



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:23 PM EDT

PDB ID : 5IFW / pdb_00005ifw
Title : Quantitative interaction mapping reveals an extended ubiquitin regulatory domain in ASPL that disrupts functional p97 hexamers and induces cell death
Authors : Roske, Y.; Heinemann, U.
Deposited on : 2016-02-26
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

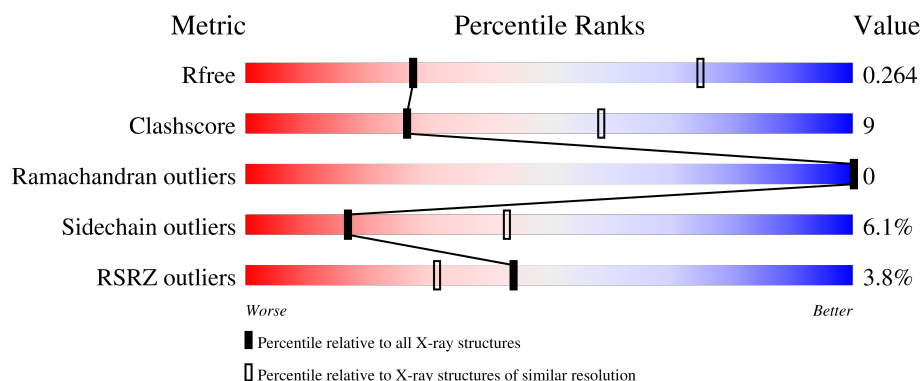
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

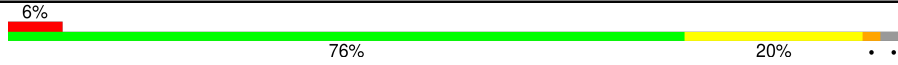
The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	188	
2	B	807	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7038 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tether containing UBX domain for GLUT4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1462	939	254	267	2			

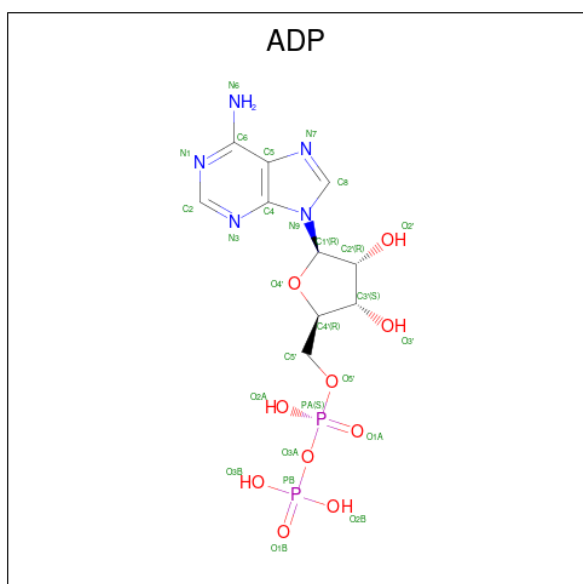
- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	702	Total	C	N	O	S	0	0	0
			5498	3451	972	1046	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P55072
B	1	SER	-	expression tag	UNP P55072

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

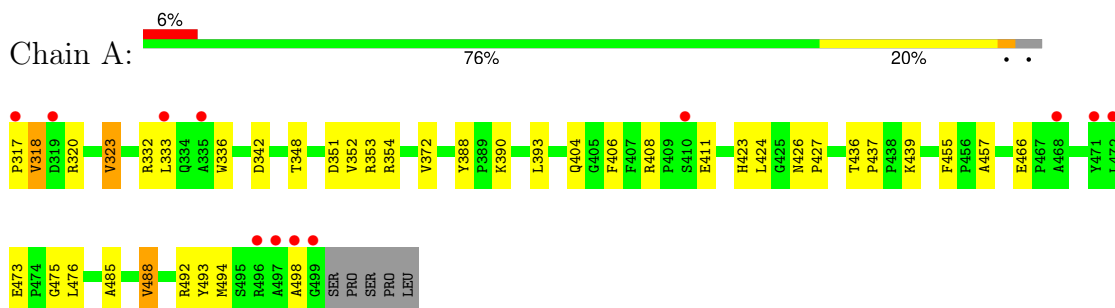
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	21	Total	O	0	0
			21	21		

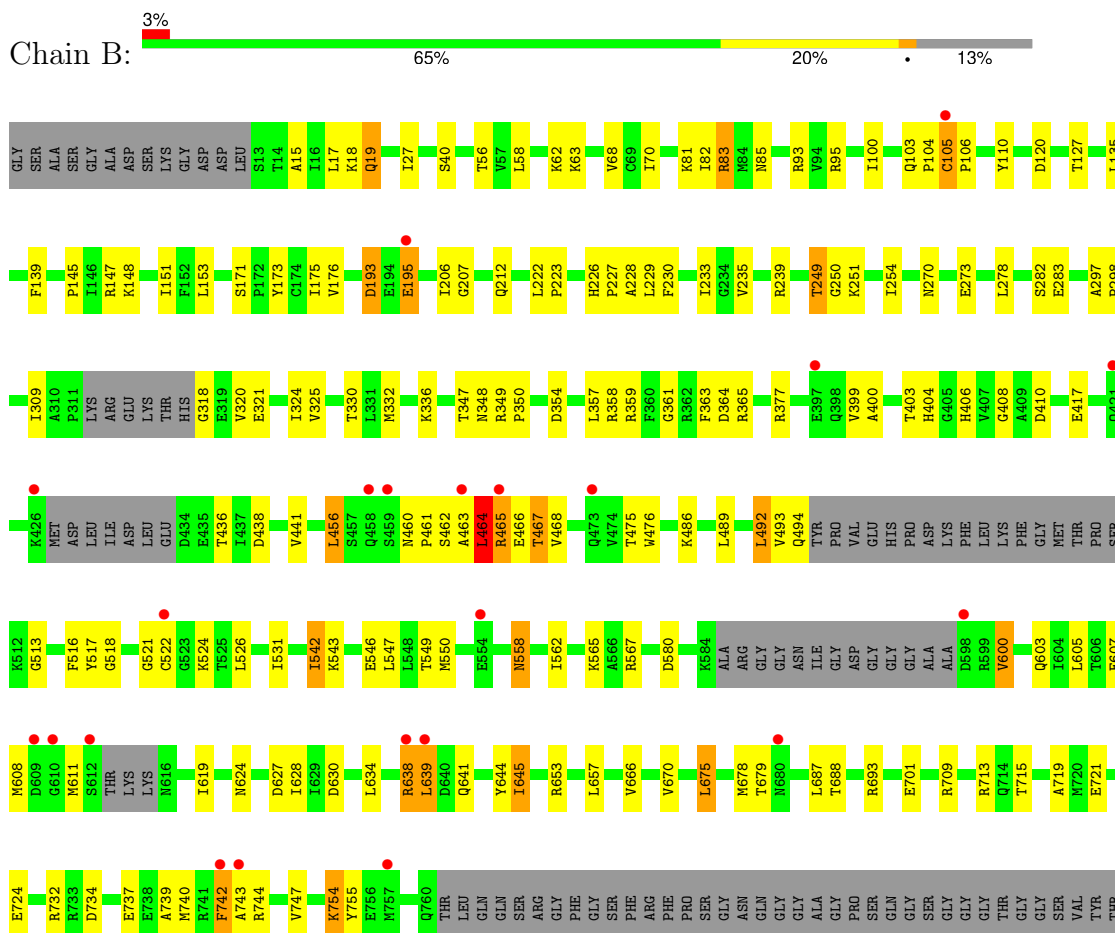
3 Residue-property plots

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: Tether containing UBX domain for GLUT4



- Molecule 2: Transitional endoplasmic reticulum ATPase



GLU
ASP
ASN
ASP
ASP
ASP
LEU
TYR
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	143.34Å 208.36Å 99.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 3.40 33.89 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.89-3.40) 99.8 (33.89-3.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.229 , 0.261 0.231 , 0.264	Depositor DCC
R_{free} test set	1040 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7038	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/1499	0.80	2/2039 (0.1%)
2	B	0.31	0/5580	0.81	7/7535 (0.1%)
All	All	0.31	0/7079	0.81	9/9574 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	105	CYS	CA-C-N	6.76	128.29	119.84
2	B	105	CYS	C-N-CA	6.76	128.29	119.84
2	B	464	LEU	CA-C-N	6.52	133.44	121.70
2	B	464	LEU	C-N-CA	6.52	133.44	121.70
1	A	466	GLU	CA-C-N	5.39	125.05	119.56
1	A	466	GLU	C-N-CA	5.39	125.05	119.56
2	B	630	ASP	CA-C-N	5.19	124.86	119.56
2	B	630	ASP	C-N-CA	5.19	124.86	119.56
2	B	120	ASP	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	464	LEU	Peptide
2	B	742	PHE	Peptide

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	A	1462	0	1455	23	0
2	B	5498	0	5547	112	1
3	B	54	0	24	5	0
4	A	3	0	0	0	0
4	B	21	0	0	1	0
All	All	7038	0	7026	130	1

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 9.

All (130) 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)
2:B:461:PRO:HD2	2:B:550:MET:HA	1.64	0.80
2:B:743:ALA:HB1	2:B:744:ARG:HB2	1.67	0.78
2:B:464:LEU:N	2:B:465:ARG:HB3	2.03	0.73
2:B:526:LEU:HD11	3:B:902:ADP:H2'	1.71	0.71
1:A:492:ARG:NH2	1:A:498:ALA:O	2.25	0.70
2:B:207:GLY:O	3:B:901:ADP:N6	2.24	0.69
2:B:348:ASN:OD1	2:B:349:ARG:N	2.27	0.67
2:B:461:PRO:HB2	2:B:462:SER:C	2.20	0.67
1:A:353:ARG:HB2	2:B:233:ILE:HD11	1.77	0.66
2:B:354:ASP:HB3	2:B:357:LEU:HD23	1.79	0.65
2:B:516:PHE:HB3	2:B:524:LYS:HG2	1.79	0.64
2:B:666:VAL:HG22	2:B:670:VAL:HG21	1.79	0.64
2:B:492:LEU:HD21	2:B:641:GLN:HG2	1.80	0.63
2:B:249:THR:OG1	2:B:251:LYS:NZ	2.31	0.62
1:A:423:HIS:HD2	1:A:476:LEU:HD21	1.65	0.62
2:B:40:SER:HB2	2:B:83:ARG:HG3	1.82	0.62
2:B:465:ARG:HE	2:B:467:THR:HG22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:GLU:HB3	2:B:724:GLU:HB3	1.81	0.62
2:B:151:ILE:HD12	2:B:195:GLU:HG3	1.82	0.60
2:B:567:ARG:NH1	2:B:607:GLU:OE1	2.29	0.60
2:B:63:LYS:HG3	2:B:93:ARG:HB3	1.85	0.59
2:B:549:THR:OG1	2:B:550:MET:N	2.34	0.59
2:B:357:LEU:HD12	2:B:363:PHE:HE2	1.68	0.59
2:B:282:SER:OG	2:B:283:GLU:OE1	2.20	0.59
2:B:377:ARG:NH1	2:B:400:ALA:O	2.36	0.59
2:B:542:ILE:HD13	2:B:562:ILE:HG12	1.84	0.59
2:B:701:GLU:OE2	2:B:732:ARG:NH2	2.35	0.58
2:B:226:HIS:CE1	2:B:229:LEU:HG	2.39	0.58
2:B:270:ASN:HB3	2:B:273:GLU:HB3	1.86	0.58
1:A:457:ALA:HB2	1:A:494:MET:HE3	1.86	0.57
2:B:713:ARG:NH2	2:B:719:ALA:O	2.38	0.56
2:B:464:LEU:H	2:B:465:ARG:HD3	1.70	0.55
2:B:489:LEU:HD22	2:B:531:ILE:HD11	1.90	0.54
1:A:473:GLU:OE2	1:A:475:GLY:N	2.39	0.54
2:B:139:PHE:HD1	2:B:176:VAL:HG21	1.73	0.54
2:B:82:ILE:HD13	2:B:100:ILE:HD11	1.90	0.53
1:A:436:THR:HG22	1:A:439:LYS:HA	1.90	0.53
2:B:456:LEU:O	2:B:460:ASN:ND2	2.41	0.53
2:B:226:HIS:CE1	2:B:228:ALA:HB3	2.44	0.53
2:B:657:LEU:HD13	2:B:675:LEU:HB3	1.91	0.52
1:A:323:VAL:HG23	1:A:404:GLN:HB3	1.92	0.52
2:B:147:ARG:HG3	2:B:173:TYR:HB3	1.92	0.52
2:B:318:GLY:N	2:B:321:GLU:OE1	2.43	0.51
2:B:239:ARG:NH1	2:B:361:GLY:O	2.43	0.51
1:A:408:ARG:H	1:A:411:GLU:HG3	1.74	0.51
2:B:58:LEU:HB2	2:B:105:CYS:SG	2.50	0.51
2:B:562:ILE:O	2:B:565:LYS:HG2	2.11	0.51
1:A:437:PRO:HD3	2:B:70:ILE:HG13	1.92	0.51
1:A:351:ASP:OD1	1:A:354:ARG:NH2	2.45	0.50
2:B:518:GLY:HA3	2:B:645:ILE:HD12	1.93	0.50
1:A:320:ARG:NH2	1:A:411:GLU:OE2	2.44	0.50
2:B:145:PRO:HA	2:B:175:ILE:HG22	1.92	0.50
2:B:517:TYR:CZ	2:B:644:TYR:HB2	2.47	0.50
2:B:110:TYR:CE1	2:B:175:ILE:HD11	2.47	0.50
2:B:608:MET:SD	2:B:638:ARG:NE	2.84	0.50
2:B:403:THR:OG1	2:B:406:HIS:ND1	2.44	0.50
2:B:364:ASP:HB2	2:B:365:ARG:HD2	1.94	0.49
2:B:104:PRO:O	2:B:106:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TYR:HB2	1:A:455:PHE:CZ	2.48	0.48
2:B:580:ASP:HB2	2:B:628:ILE:HD11	1.95	0.48
2:B:461:PRO:HB2	2:B:463:ALA:N	2.29	0.48
2:B:361:GLY:N	2:B:364:ASP:OD1	2.43	0.47
2:B:399:VAL:O	2:B:403:THR:HG22	2.14	0.47
2:B:350:PRO:HB2	2:B:358:ARG:HH11	1.79	0.47
2:B:634:LEU:HA	2:B:639:LEU:CD1	2.44	0.47
2:B:230:PHE:O	2:B:233:ILE:HG22	2.15	0.47
2:B:56:THR:OG1	2:B:105:CYS:O	2.32	0.47
2:B:324:ILE:HD12	2:B:325:VAL:N	2.30	0.47
2:B:543:LYS:NZ	4:B:1001:HOH:O	2.33	0.47
2:B:493:VAL:HG22	2:B:494:GLN:H	1.80	0.47
2:B:135:LEU:HD22	2:B:139:PHE:HE2	1.80	0.46
1:A:348:THR:OG1	2:B:18:LYS:NZ	2.47	0.46
2:B:408:GLY:HA3	3:B:901:ADP:C8	2.51	0.46
2:B:250:GLY:N	3:B:901:ADP:O2B	2.35	0.46
2:B:565:LYS:HE2	2:B:565:LYS:HB3	1.69	0.46
2:B:558:ASN:OD1	2:B:558:ASN:N	2.47	0.46
1:A:342:ASP:HB3	2:B:62:LYS:HE3	1.97	0.46
2:B:212:GLN:OE1	2:B:212:GLN:N	2.41	0.46
2:B:634:LEU:HA	2:B:639:LEU:HD11	1.97	0.46
2:B:580:ASP:OD1	2:B:580:ASP:N	2.43	0.46
2:B:521:GLY:N	3:B:902:ADP:O3B	2.45	0.46
2:B:644:TYR:CE1	2:B:755:TYR:HB3	2.50	0.46
2:B:653:ARG:NE	2:B:679:THR:O	2.49	0.45
2:B:406:HIS:NE2	2:B:550:MET:SD	2.88	0.45
2:B:734:ASP:HA	2:B:737:GLU:HB3	1.98	0.45
1:A:352:VAL:HG13	2:B:222:LEU:HD22	1.98	0.45
2:B:522:CYS:SG	2:B:645:ILE:HD13	2.56	0.45
1:A:485:ALA:O	1:A:488:VAL:HG12	2.17	0.45
2:B:82:ILE:HG21	2:B:100:ILE:HD11	1.99	0.45
1:A:390:LYS:HD2	1:A:493:TYR:CE1	2.52	0.44
2:B:27:ILE:HG13	2:B:81:LYS:HG2	1.98	0.44
2:B:239:ARG:HD3	2:B:332:MET:O	2.17	0.44
2:B:465:ARG:HD2	2:B:546:GLU:HB3	1.99	0.44
1:A:423:HIS:CD2	1:A:476:LEU:HD21	2.49	0.44
2:B:465:ARG:HE	2:B:467:THR:CG2	2.29	0.44
2:B:139:PHE:CD1	2:B:176:VAL:HG21	2.50	0.44
2:B:359:ARG:HD2	2:B:359:ARG:HA	1.77	0.44
1:A:390:LYS:HD3	1:A:406:PHE:HB3	1.99	0.44
1:A:426:ASN:N	1:A:426:ASN:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:ASP:OD2	2:B:754:LYS:HE3	2.18	0.43
2:B:233:ILE:CG2	2:B:235:VAL:HG12	2.48	0.43
2:B:476:TRP:O	2:B:486:LYS:NZ	2.45	0.43
1:A:318:VAL:HG13	1:A:408:ARG:HH11	1.84	0.43
2:B:693:ARG:HB2	2:B:739:ALA:HB1	2.00	0.43
2:B:85:ASN:OD1	2:B:85:ASN:N	2.43	0.42
2:B:297:ALA:HA	2:B:298:PRO:C	2.44	0.42
2:B:336:LYS:HA	2:B:336:LYS:HD2	1.78	0.42
2:B:93:ARG:HH12	2:B:195:GLU:HG2	1.84	0.42
2:B:193:ASP:OD1	2:B:193:ASP:N	2.52	0.42
2:B:223:PRO:HG3	2:B:230:PHE:CE2	2.54	0.42
2:B:406:HIS:HD2	2:B:410:ASP:HB3	1.85	0.42
2:B:465:ARG:HH21	2:B:467:THR:HG21	1.84	0.42
2:B:678:MET:HE2	2:B:740:MET:HE1	2.00	0.42
2:B:347:THR:OG1	2:B:348:ASN:N	2.53	0.41
2:B:600:VAL:O	2:B:603:GLN:HG2	2.20	0.41
2:B:404:HIS:O	2:B:406:HIS:ND1	2.53	0.41
2:B:103:GLN:HA	2:B:104:PRO:HD3	1.75	0.41
2:B:309:ILE:HG23	2:B:324:ILE:HD13	2.02	0.41
2:B:653:ARG:HG2	2:B:687:LEU:HD11	2.02	0.41
2:B:17:LEU:HD12	2:B:17:LEU:H	1.85	0.41
2:B:513:GLY:HA3	2:B:639:LEU:HB3	2.02	0.41
2:B:226:HIS:HA	2:B:227:PRO:HD2	1.92	0.41
1:A:317:PRO:HB2	1:A:318:VAL:H	1.71	0.41
1:A:426:ASN:HA	1:A:427:PRO:HD3	1.89	0.41
2:B:466:GLU:O	2:B:468:VAL:HG23	2.20	0.41
2:B:206:ILE:HD13	2:B:254:ILE:HG12	2.03	0.40
2:B:438:ASP:HB3	2:B:441:VAL:HG22	2.03	0.40
2:B:475:THR:OG1	2:B:476:TRP:N	2.54	0.40
2:B:15:ALA:O	2:B:19:GLN:HB2	2.22	0.40
2:B:709:ARG:O	2:B:713:ARG:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:THR:OG1	2:B:330:THR:OG1[2_565]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	B	690/807 (86%)	661 (96%)	29 (4%)	0	100	100
All	All	871/995 (88%)	835 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/163 (96%)	147 (94%)	9 (6%)	18	45
2	B	598/678 (88%)	561 (94%)	37 (6%)	16	43
All	All	754/841 (90%)	708 (94%)	46 (6%)	17	43

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
1	A	323	VAL
1	A	332	ARG
1	A	333	LEU
1	A	336	TRP
1	A	372	VAL
1	A	393	LEU
1	A	424	LEU

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Mol	Chain	Res	Type
1	A	488	VAL
2	B	19	GLN
2	B	68	VAL
2	B	83	ARG
2	B	95	ARG
2	B	127	THR
2	B	148	LYS
2	B	153	LEU
2	B	171	SER
2	B	193	ASP
2	B	195	GLU
2	B	249	THR
2	B	278	LEU
2	B	320	VAL
2	B	417	GLU
2	B	436	THR
2	B	456	LEU
2	B	464	LEU
2	B	465	ARG
2	B	467	THR
2	B	492	LEU
2	B	542	ILE
2	B	547	LEU
2	B	558	ASN
2	B	600	VAL
2	B	605	LEU
2	B	611	MET
2	B	619	ILE
2	B	624	ASN
2	B	638	ARG
2	B	639	LEU
2	B	645	ILE
2	B	675	LEU
2	B	688	THR
2	B	715	THR
2	B	742	PHE
2	B	747	VAL
2	B	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
2	B	24	ASN
2	B	296	ASN
2	B	340	HIS
2	B	660	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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$
3	ADP	B	902	-	28,29,29	1.46	5 (17%)	43,45,45	1.88	8 (18%)
3	ADP	B	901	-	28,29,29	1.43	5 (17%)	43,45,45	1.87	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
3	ADP	B	902	-	-	3/16/32/32	0/3/3/3
3	ADP	B	901	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ADP	C5-C4	4.83	1.47	1.39
3	B	901	ADP	C5-C4	4.75	1.47	1.39
3	B	902	ADP	C5-C6	2.74	1.48	1.41
3	B	901	ADP	C5-C6	2.69	1.48	1.41
3	B	902	ADP	C5-N7	-2.45	1.34	1.39
3	B	901	ADP	C5-N7	-2.40	1.34	1.39
3	B	902	ADP	PA-O3A	2.28	1.62	1.59
3	B	901	ADP	C8-N7	2.26	1.36	1.31
3	B	902	ADP	C8-N7	2.25	1.36	1.31
3	B	901	ADP	PA-O3A	2.04	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ADP	C5-C4-N3	-6.14	118.26	126.72
3	B	902	ADP	C5-C4-N3	-6.13	118.27	126.72
3	B	901	ADP	N3-C4-N9	4.95	135.59	127.17
3	B	902	ADP	N3-C4-N9	4.85	135.41	127.17
3	B	901	ADP	C2-N3-C4	3.72	120.92	111.83
3	B	902	ADP	C2-N3-C4	3.70	120.86	111.83
3	B	902	ADP	C4-C5-N7	-3.57	106.50	110.58
3	B	901	ADP	C4-C5-N7	-3.47	106.61	110.58
3	B	901	ADP	N3-C2-N1	-3.11	123.87	128.58
3	B	902	ADP	N3-C2-N1	-3.09	123.91	128.58
3	B	902	ADP	C5-N7-C8	2.68	107.67	103.45
3	B	901	ADP	C5-N7-C8	2.67	107.64	103.45
3	B	902	ADP	C3'-C2'-C1'	2.64	106.46	101.46
3	B	901	ADP	C4-N9-C8	2.63	108.50	105.74
3	B	901	ADP	C3'-C2'-C1'	2.55	106.28	101.46
3	B	902	ADP	C4-N9-C8	2.42	108.28	105.74
3	B	901	ADP	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

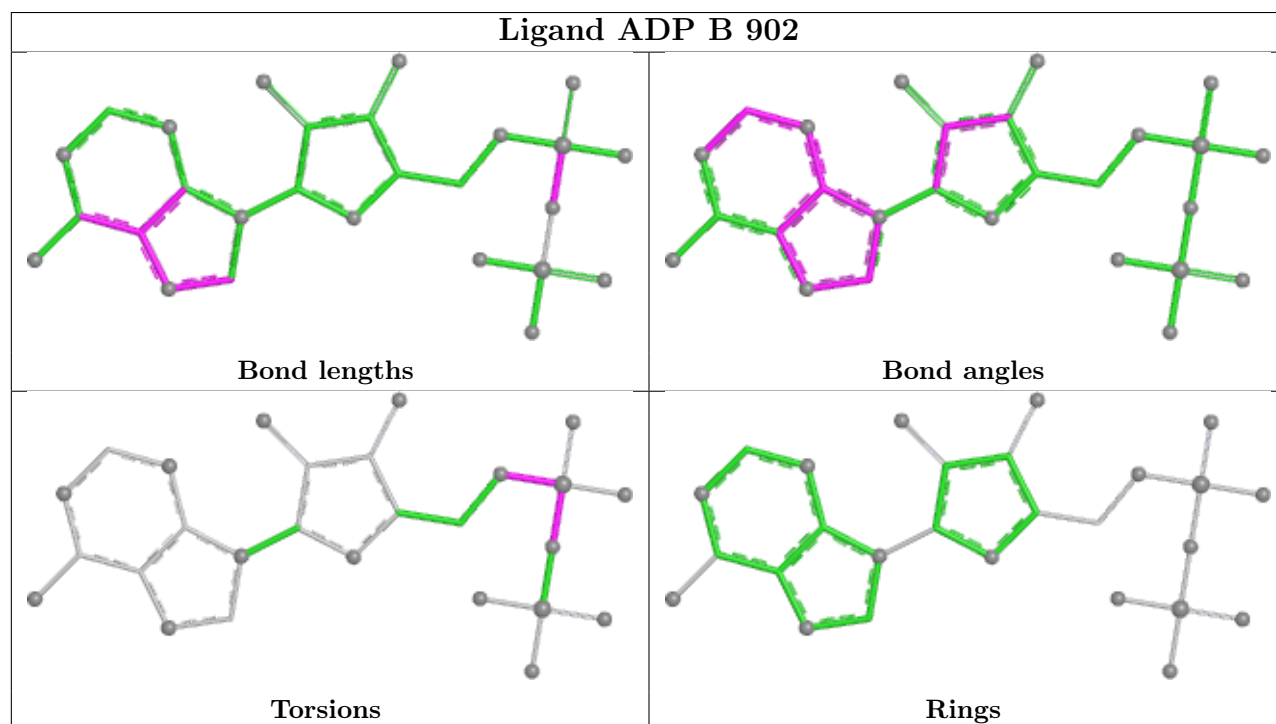
Mol	Chain	Res	Type	Atoms
3	B	901	ADP	PB-O3A-PA-O1A
3	B	902	ADP	PB-O3A-PA-O2A
3	B	902	ADP	C5'-O5'-PA-O1A
3	B	901	ADP	PB-O3A-PA-O2A
3	B	902	ADP	PB-O3A-PA-O1A

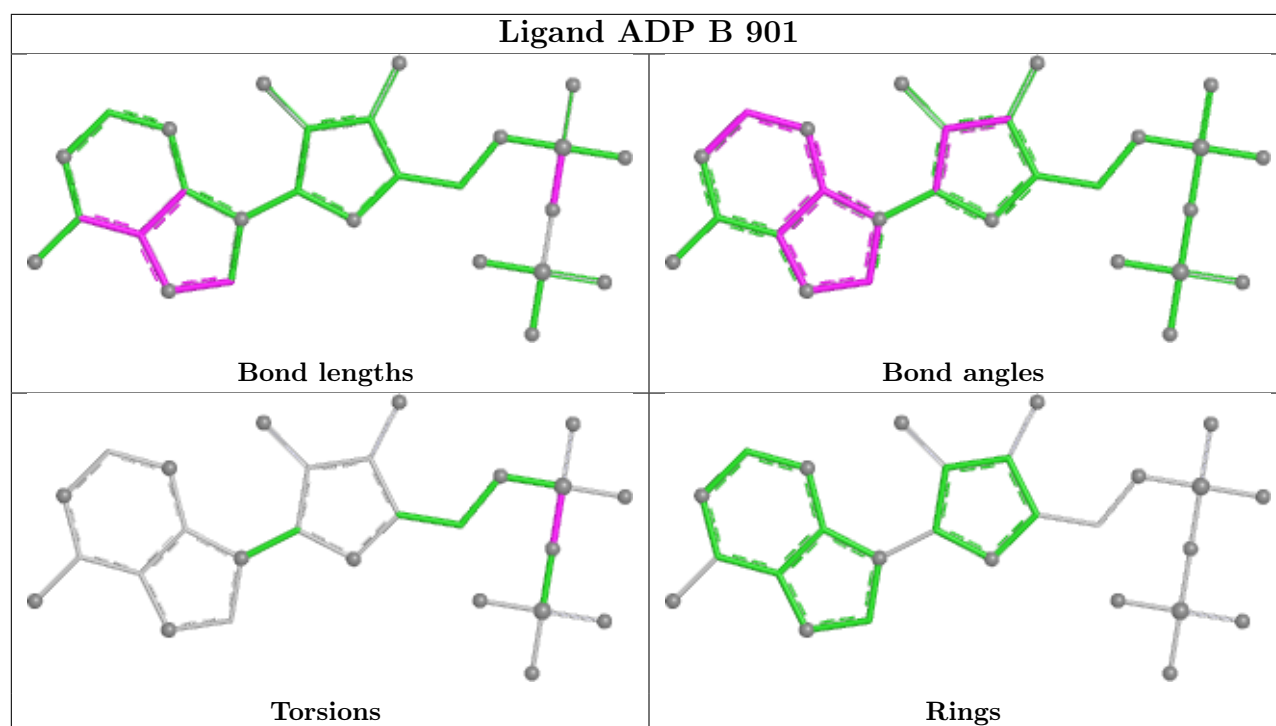
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	ADP	2	0
3	B	901	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	183/188 (97%)	0.49	12 (6%)	24 19	71, 97, 132, 138	0
2	B	702/807 (86%)	0.37	22 (3%)	51 38	65, 91, 124, 138	0
All	All	885/995 (88%)	0.39	34 (3%)	44 31	65, 92, 126, 138	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ALA	4.9
2	B	554	GLU	4.2
2	B	638	ARG	3.9
1	A	497	ALA	3.6
1	A	499	GLY	3.4
2	B	459	SER	3.2
2	B	612	SER	3.2
1	A	471	TYR	3.1
1	A	317	PRO	3.1
2	B	680	ASN	3.0
2	B	458	GLN	2.8
1	A	496	ARG	2.8
2	B	522	CYS	2.7
2	B	397	GLU	2.6
1	A	319	ASP	2.4
2	B	639	LEU	2.4
2	B	757	MET	2.4
2	B	742	PHE	2.4
2	B	610	GLY	2.3
2	B	426	LYS	2.3
2	B	473	GLN	2.3
2	B	195	GLU	2.3
1	A	335	ALA	2.2
2	B	598	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	421	GLN	2.2
2	B	743	ALA	2.2
2	B	609	ASP	2.2
1	A	333	LEU	2.1
2	B	463	ALA	2.1
2	B	105	CYS	2.1
1	A	468	ALA	2.1
1	A	472	LEU	2.0
2	B	465	ARG	2.0
1	A	410	SER	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](#)

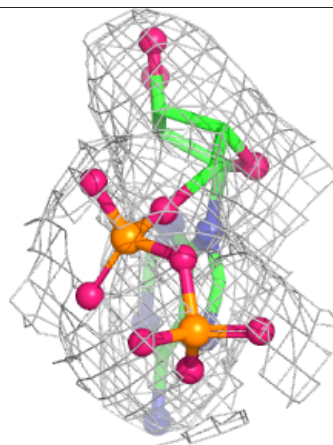
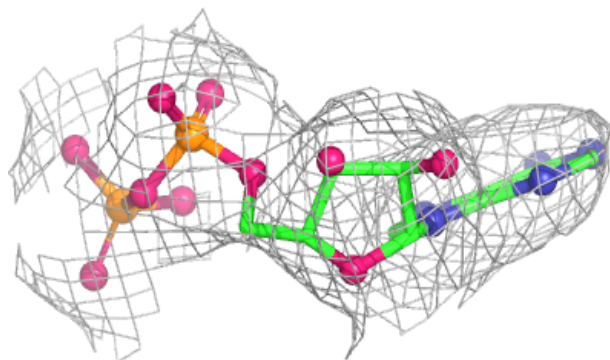
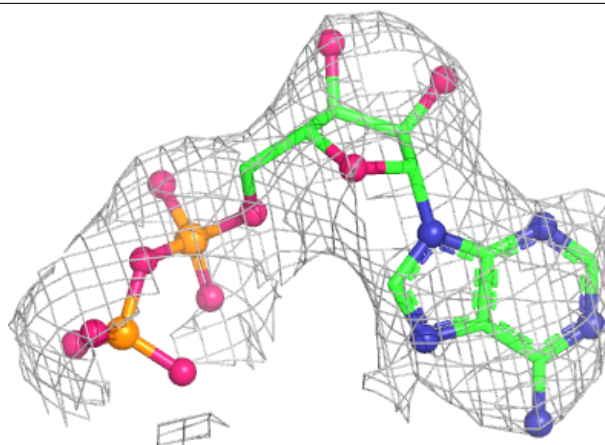
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	902	27/27	0.94	0.10	73,82,90,92	0
3	ADP	B	901	27/27	0.95	0.08	66,77,88,91	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.

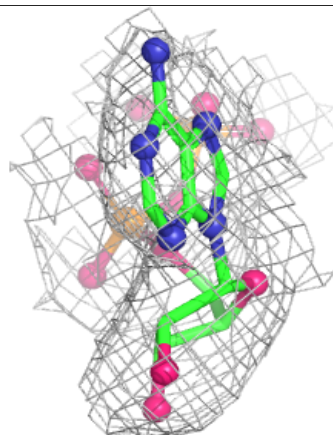
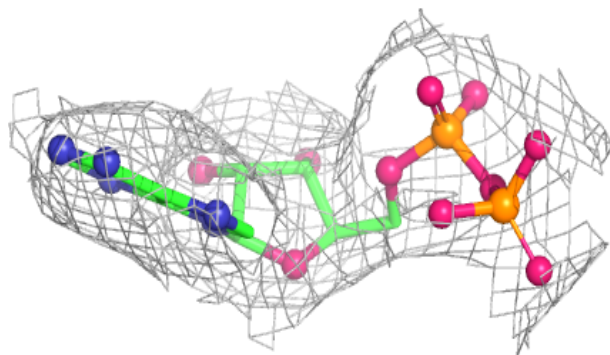
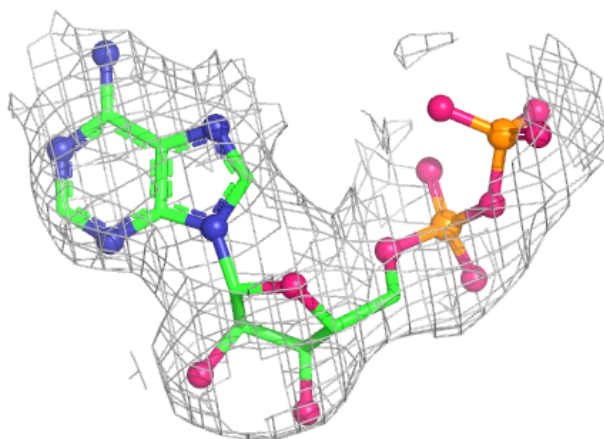
Electron density around ADP B 902:

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



Electron density around ADP B 901:

$2mF_o-DF_c$ (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.