



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 4USJ / pdb_00004usj
Title : N-acetylglutamate kinase from Arabidopsis thaliana in complex with PII from Chlamydomonas reinhardtii
Authors : Chellamuthu, V.R.; Forchhammer, K.; Hartmann, M.D.
Deposited on : 2014-07-08
Resolution : 2.85 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

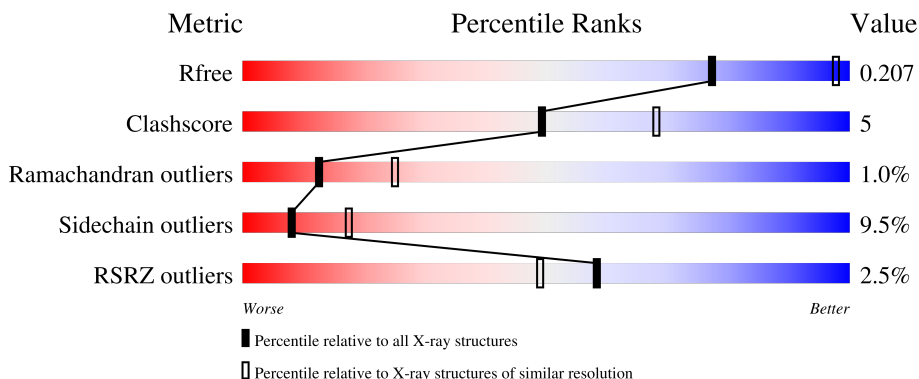
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	318	 2% 69% 16% • 12%
1	B	318	 3% 69% 16% • 12%
2	C	154	 % 85% 5% • 8%
2	D	154	 3% 82% 10% • 8%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6567 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 ACETYLGLUTAMATE KINASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2066	1304	359	393	10	0	0	0
1	B	281	2058	1298	357	393	10	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9SCL7
A	-19	GLY	-	expression tag	UNP Q9SCL7
A	-18	SER	-	expression tag	UNP Q9SCL7
A	-17	SER	-	expression tag	UNP Q9SCL7
A	-16	HIS	-	expression tag	UNP Q9SCL7
A	-15	HIS	-	expression tag	UNP Q9SCL7
A	-14	HIS	-	expression tag	UNP Q9SCL7
A	-13	HIS	-	expression tag	UNP Q9SCL7
A	-12	HIS	-	expression tag	UNP Q9SCL7
A	-11	HIS	-	expression tag	UNP Q9SCL7
A	-10	SER	-	expression tag	UNP Q9SCL7
A	-9	SER	-	expression tag	UNP Q9SCL7
A	-8	GLY	-	expression tag	UNP Q9SCL7
A	-7	LEU	-	expression tag	UNP Q9SCL7
A	-6	VAL	-	expression tag	UNP Q9SCL7
A	-5	PRO	-	expression tag	UNP Q9SCL7
A	-4	ARG	-	expression tag	UNP Q9SCL7
A	-3	GLY	-	expression tag	UNP Q9SCL7
A	-2	SER	-	expression tag	UNP Q9SCL7
A	-1	HIS	-	expression tag	UNP Q9SCL7
A	0	MET	-	expression tag	UNP Q9SCL7
B	-20	MET	-	expression tag	UNP Q9SCL7
B	-19	GLY	-	expression tag	UNP Q9SCL7
B	-18	SER	-	expression tag	UNP Q9SCL7
B	-17	SER	-	expression tag	UNP Q9SCL7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q9SCL7
B	-15	HIS	-	expression tag	UNP Q9SCL7
B	-14	HIS	-	expression tag	UNP Q9SCL7
B	-13	HIS	-	expression tag	UNP Q9SCL7
B	-12	HIS	-	expression tag	UNP Q9SCL7
B	-11	HIS	-	expression tag	UNP Q9SCL7
B	-10	SER	-	expression tag	UNP Q9SCL7
B	-9	SER	-	expression tag	UNP Q9SCL7
B	-8	GLY	-	expression tag	UNP Q9SCL7
B	-7	LEU	-	expression tag	UNP Q9SCL7
B	-6	VAL	-	expression tag	UNP Q9SCL7
B	-5	PRO	-	expression tag	UNP Q9SCL7
B	-4	ARG	-	expression tag	UNP Q9SCL7
B	-3	GLY	-	expression tag	UNP Q9SCL7
B	-2	SER	-	expression tag	UNP Q9SCL7
B	-1	HIS	-	expression tag	UNP Q9SCL7
B	0	MET	-	expression tag	UNP Q9SCL7

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN PII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	142	1087	694	188	200	5	0	1	0
2	D	142	1086	694	187	200	5	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

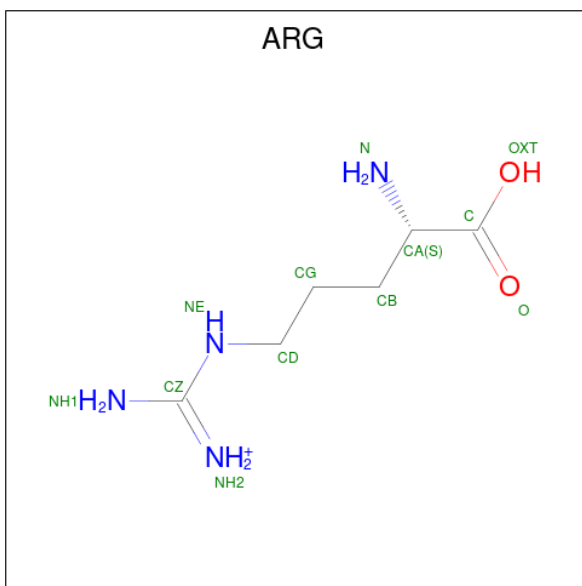
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP A8JI83
C	145	SER	-	expression tag	UNP A8JI83
C	146	ALA	-	expression tag	UNP A8JI83
C	147	TRP	-	expression tag	UNP A8JI83
C	148	SER	-	expression tag	UNP A8JI83
C	149	HIS	-	expression tag	UNP A8JI83
C	150	PRO	-	expression tag	UNP A8JI83
C	151	GLN	-	expression tag	UNP A8JI83
C	152	PHE	-	expression tag	UNP A8JI83
C	153	GLU	-	expression tag	UNP A8JI83
C	154	LYS	-	expression tag	UNP A8JI83
D	1	MET	-	expression tag	UNP A8JI83
D	145	SER	-	expression tag	UNP A8JI83

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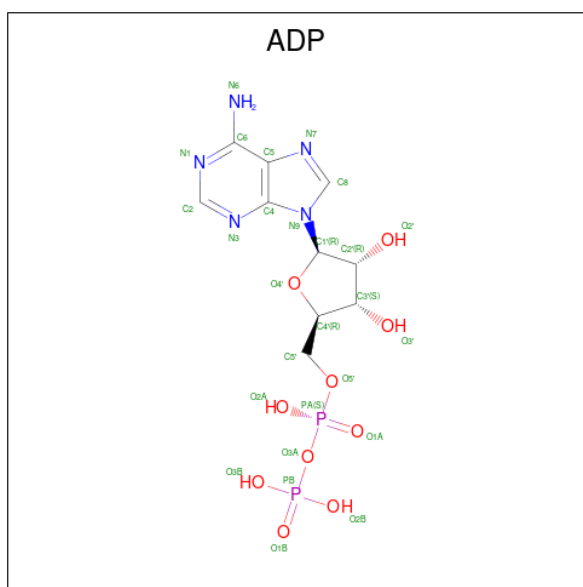
Chain	Residue	Modelled	Actual	Comment	Reference
D	146	ALA	-	expression tag	UNP A8JI83
D	147	TRP	-	expression tag	UNP A8JI83
D	148	SER	-	expression tag	UNP A8JI83
D	149	HIS	-	expression tag	UNP A8JI83
D	150	PRO	-	expression tag	UNP A8JI83
D	151	GLN	-	expression tag	UNP A8JI83
D	152	PHE	-	expression tag	UNP A8JI83
D	153	GLU	-	expression tag	UNP A8JI83
D	154	LYS	-	expression tag	UNP A8JI83

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



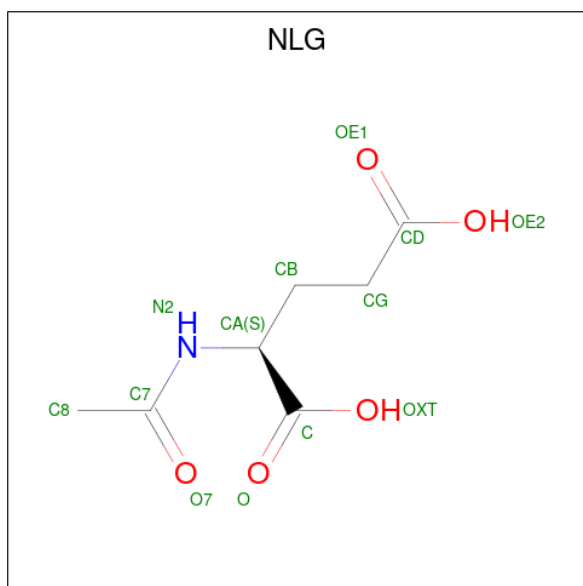
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is N-ACETYL-L-GLUTAMATE (CCD ID: NLG) (formula: $C_7H_{11}NO_5$).

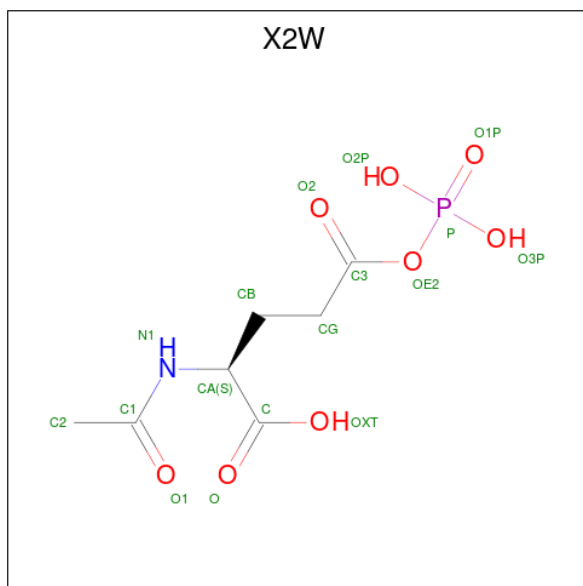


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	13	7	1	5	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

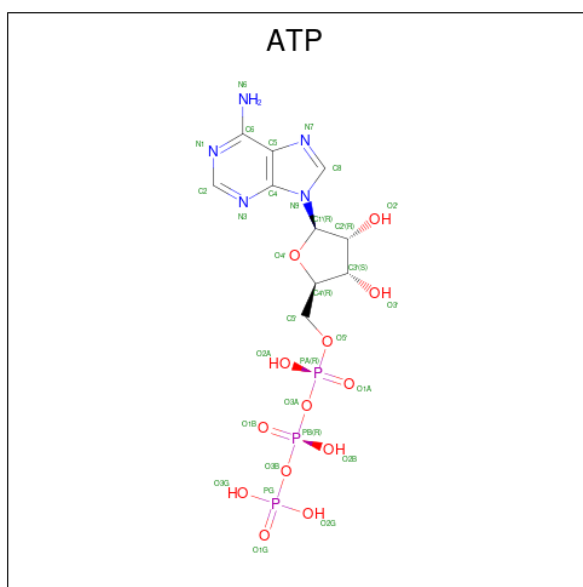
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is N-ACETYL-L-GLUTAMYL 5-PHOSPHATE (CCD ID: X2W) (formula: C₇H₁₂NO₈P).



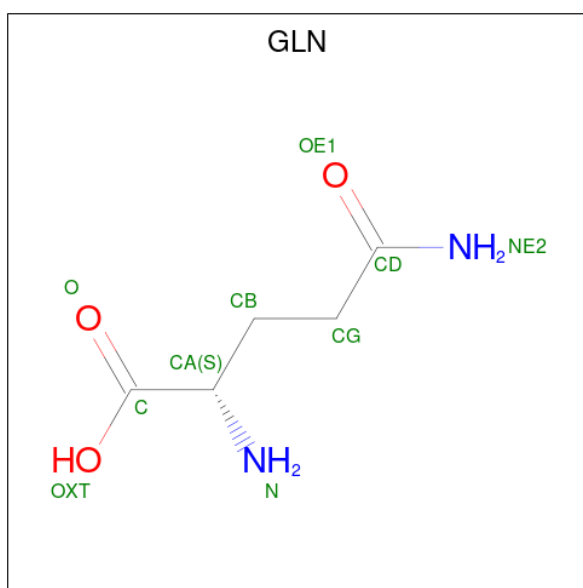
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 17 7 1 8 1	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
8	C	1	Total	31	10	5	13	3	0	0
8	D	1	Total	31	10	5	13	3	0	0

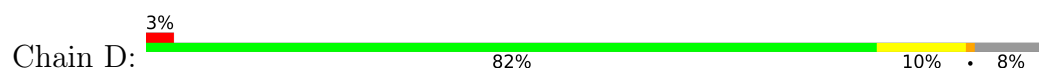
- Molecule 9 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
9	C	1	Total	10	5	2	3	0	0
9	D	1	Total	10	5	2	3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	37	Total 37	O 37	0	0
10	B	30	Total 30	O 30	0	0
10	C	20	Total 20	O 20	0	0
10	D	17	Total 17	O 17	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	171.43Å 171.43Å 171.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.85 39.36 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.36-2.85) 99.1 (39.36-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.189 , 0.220 0.173 , 0.207	Depositor DCC
R_{free} test set	2027 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG, NLG, X2W

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	1.19	3/2091 (0.1%)	1.23	6/2832 (0.2%)
1	B	1.13	2/2083 (0.1%)	1.18	2/2824 (0.1%)
2	C	1.03	1/1109 (0.1%)	1.11	2/1496 (0.1%)
2	D	1.04	0/1108	1.13	3/1495 (0.2%)
All	All	1.12	6/6391 (0.1%)	1.18	13/8647 (0.2%)

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
1	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	VAL	N-CA	-6.31	1.38	1.46
1	A	70	PRO	C-O	-6.09	1.17	1.23
2	C	74	VAL	C-O	-5.47	1.18	1.24
1	B	115	LYS	CA-C	5.30	1.57	1.52
1	B	273	ILE	CA-C	-5.17	1.47	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	107	GLY	N-CA-C	6.79	119.05	111.85
1	B	285	ILE	N-CA-C	6.24	117.80	111.00
1	A	152	GLN	CB-CA-C	-6.22	99.70	109.34
1	A	147	VAL	N-CA-CB	-6.20	102.53	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	25	PHE	N-CA-C	5.74	115.68	108.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	SER	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	2066	0	2153	28	0
1	B	2058	0	2131	29	0
2	C	1087	0	1096	7	0
2	D	1086	0	1091	8	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
4	A	27	0	12	0	0
5	A	13	0	9	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	17	0	9	0	0
8	C	31	0	12	2	0
8	D	31	0	12	2	0
9	C	10	0	7	0	0
9	D	10	0	7	0	0
10	A	37	0	0	0	0
10	B	30	0	0	1	0
10	C	20	0	0	0	0
10	D	17	0	0	0	0
All	All	6567	0	6563	70	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 5.

The worst 5 of 70 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)
1:A:269:THR:HB	1:A:294:MET:HE2	1.63	0.81
1:B:161:ARG:HA	2:C:66:THR:HB	1.68	0.76
2:C:69:GLY:H	2:C:72:ASN:HD22	1.31	0.76
1:A:161:ARG:HA	2:D:66:THR:HB	1.68	0.74
2:D:69:GLY:H	2:D:72:ASN:HD22	1.37	0.73

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	
1	A	279/318 (88%)	261 (94%)	13 (5%)	5 (2%)	6	15
1	B	279/318 (88%)	262 (94%)	14 (5%)	3 (1%)	11	24
2	C	141/154 (92%)	135 (96%)	6 (4%)	0	100	100
2	D	141/154 (92%)	134 (95%)	7 (5%)	0	100	100
All	All	840/944 (89%)	792 (94%)	40 (5%)	8 (1%)	12	25

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA
1	B	46	ALA
1	A	245	ASP
1	B	19	ARG
1	A	76	GLY

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
1	A	223/256 (87%)	195 (87%)	28 (13%)	4 8
1	B	221/256 (86%)	196 (89%)	25 (11%)	5 11
2	C	113/127 (89%)	109 (96%)	4 (4%)	32 57
2	D	112/127 (88%)	107 (96%)	5 (4%)	24 48
All	All	669/766 (87%)	607 (91%)	62 (9%)	8 18

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	TYR
2	C	66	THR
1	B	48	THR
2	C	51	LYS
2	D	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	47	ASN
2	C	72	ASN
2	D	72	ASN
2	C	112	HIS
1	A	283	HIS

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](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
9	GLN	D	303	-	8,9,9	0.92	1 (12%)	8,11,11	1.32	1 (12%)
3	ARG	B	301	-	10,11,11	0.67	0	9,13,13	1.43	1 (11%)
4	ADP	A	302	6	28,29,29	1.61	5 (17%)	43,45,45	1.86	10 (23%)
7	X2W	B	303	-	15,16,16	2.23	2 (13%)	20,22,22	1.84	6 (30%)
9	GLN	C	303	-	8,9,9	0.90	1 (12%)	8,11,11	0.97	1 (12%)
8	ATP	D	301	6	32,33,33	1.56	6 (18%)	48,52,52	2.19	14 (29%)
3	ARG	A	301	-	10,11,11	0.87	1 (10%)	9,13,13	1.72	2 (22%)
5	NLG	A	303	-	12,12,12	0.99	0	15,15,15	1.06	1 (6%)
8	ATP	C	301	6	32,33,33	1.43	6 (18%)	48,52,52	1.88	13 (27%)

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
9	GLN	D	303	-	-	1/9/9/9	-
3	ARG	B	301	-	-	4/11/11/11	-
4	ADP	A	302	6	-	8/16/32/32	0/3/3/3
7	X2W	B	303	-	-	0/16/18/18	-
9	GLN	C	303	-	-	2/9/9/9	-
8	ATP	D	301	6	-	5/22/38/38	0/3/3/3
3	ARG	A	301	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NLG	A	303	-	-	0/13/13/13	-
8	ATP	C	301	6	-	4/22/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	303	X2W	P-OE2	7.62	1.73	1.59
4	A	302	ADP	C5-C4	5.51	1.48	1.39
8	D	301	ATP	C5-C4	4.52	1.47	1.39
8	C	301	ATP	C5-C4	4.06	1.46	1.39
8	C	301	ATP	C5-N7	-3.58	1.32	1.39

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	301	ATP	O2B-PB-O3A	6.72	125.43	107.27
8	D	301	ATP	C5-C4-N3	-6.35	117.97	126.72
8	C	301	ATP	C5-C4-N3	-4.90	119.97	126.72
8	D	301	ATP	C4-C5-N7	-4.83	105.06	110.58
4	A	302	ADP	O5'-PA-O1A	4.83	128.08	108.94

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	ARG	N-CA-CB-CG
3	B	301	ARG	C-CA-CB-CG
4	A	302	ADP	PA-O3A-PB-O3B
8	C	301	ATP	C5'-O5'-PA-O2A
8	C	301	ATP	C5'-O5'-PA-O3A

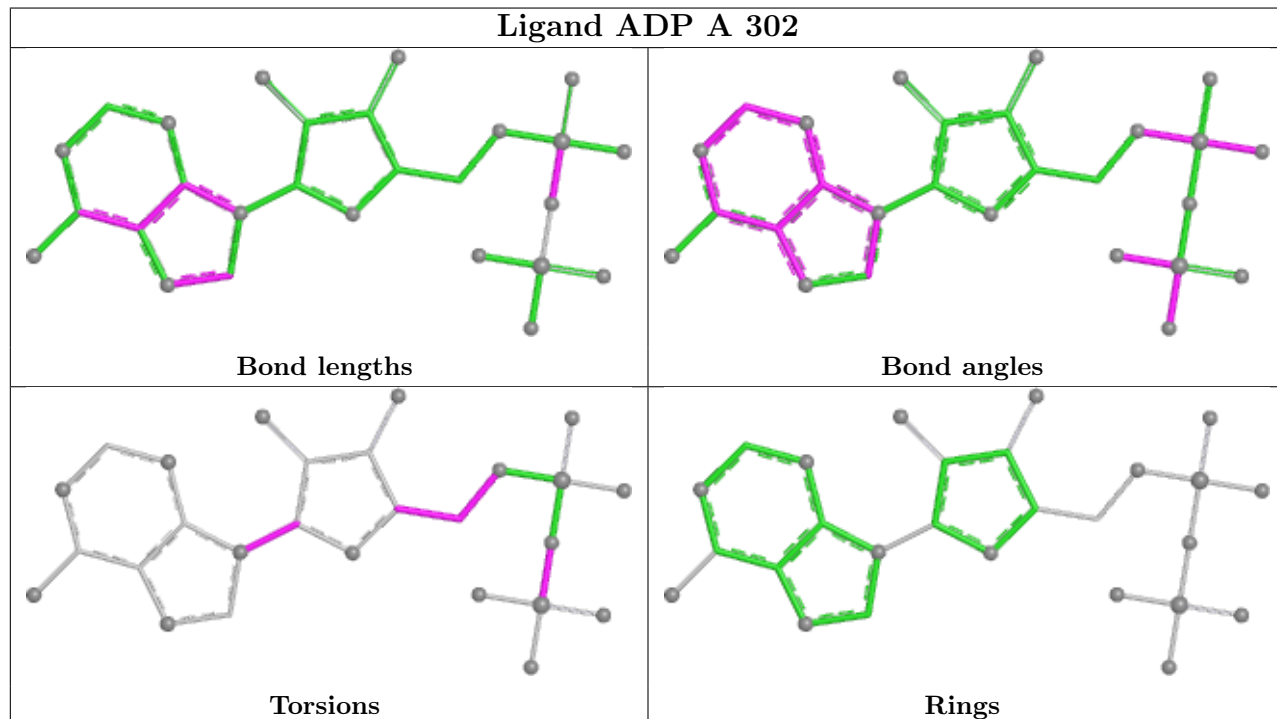
There are no ring outliers.

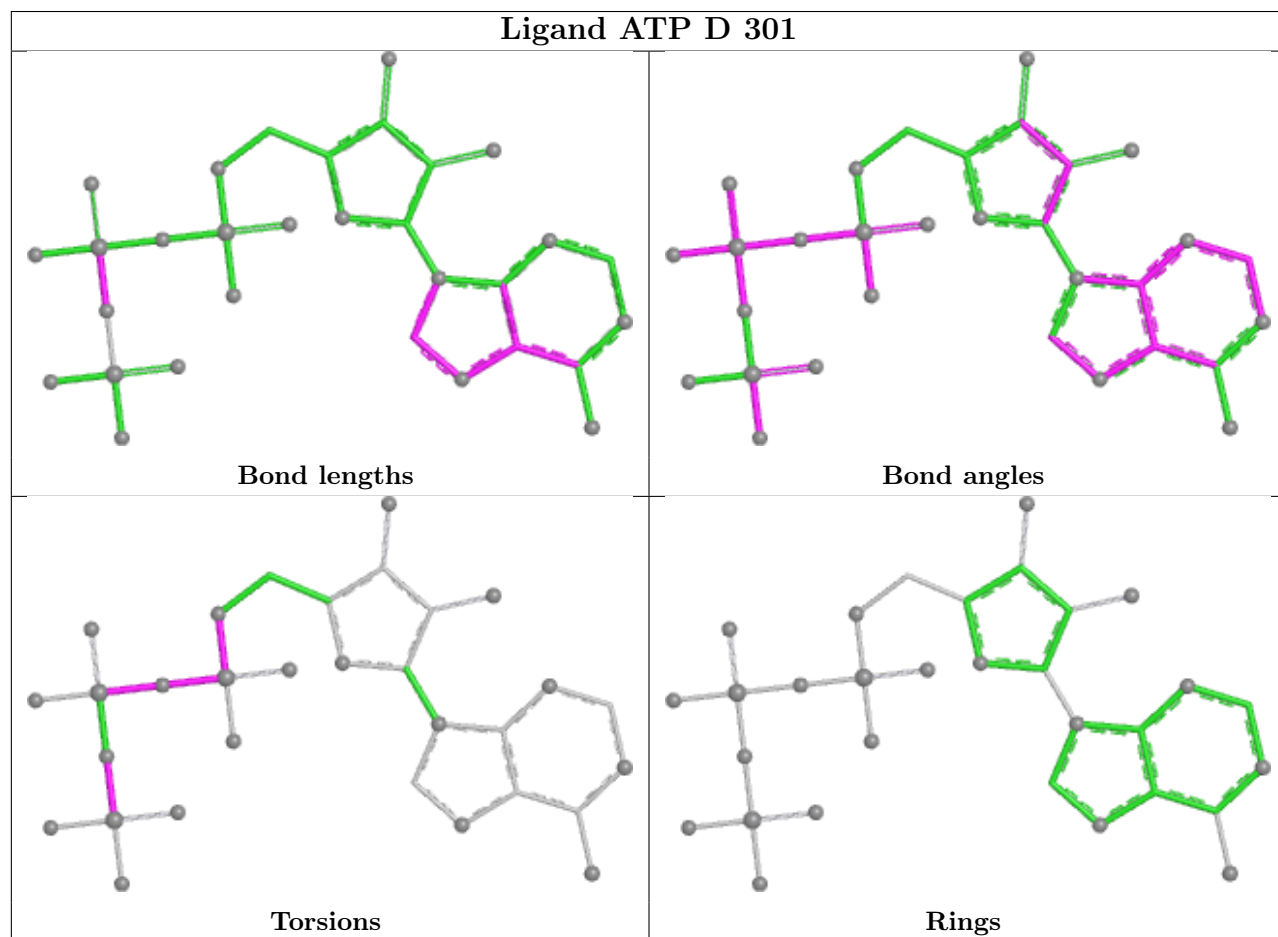
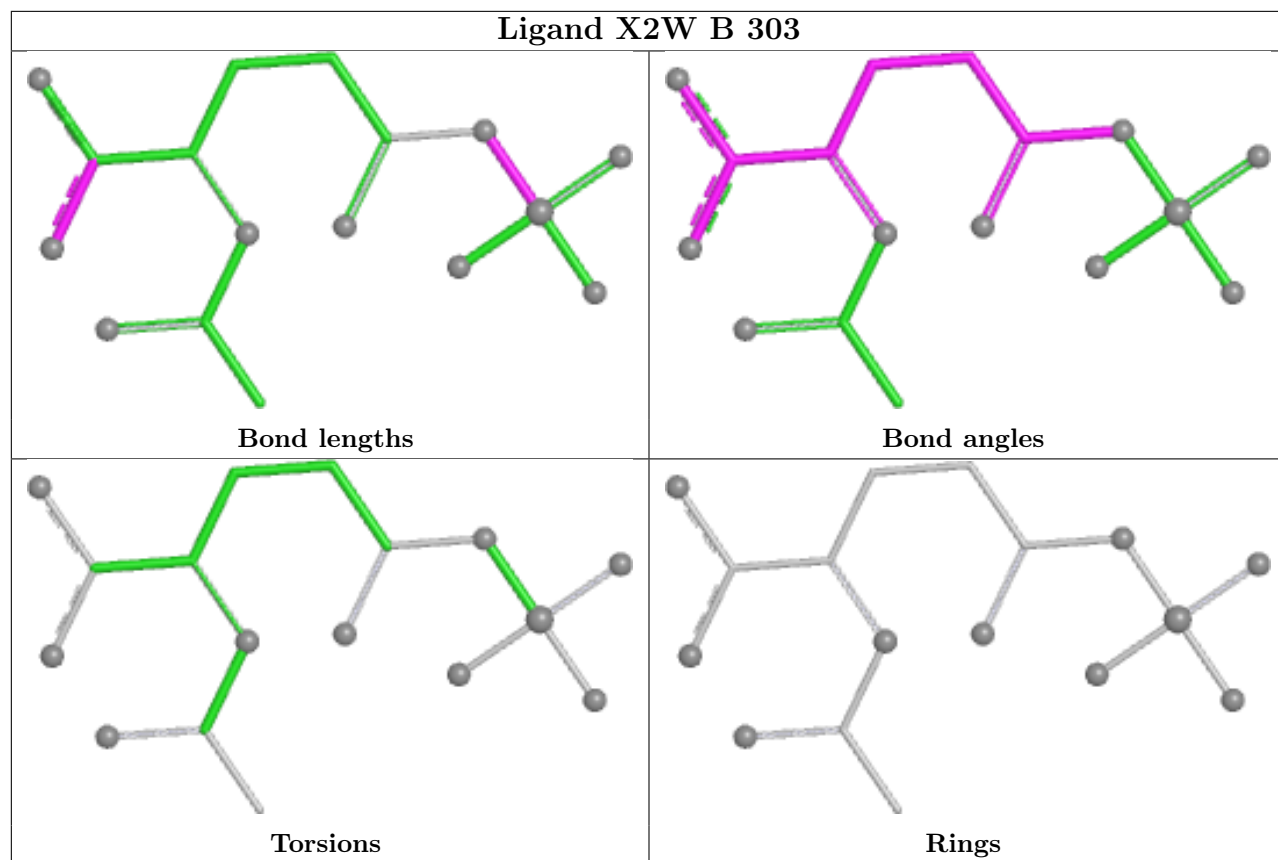
3 monomers are involved in 6 short contacts:

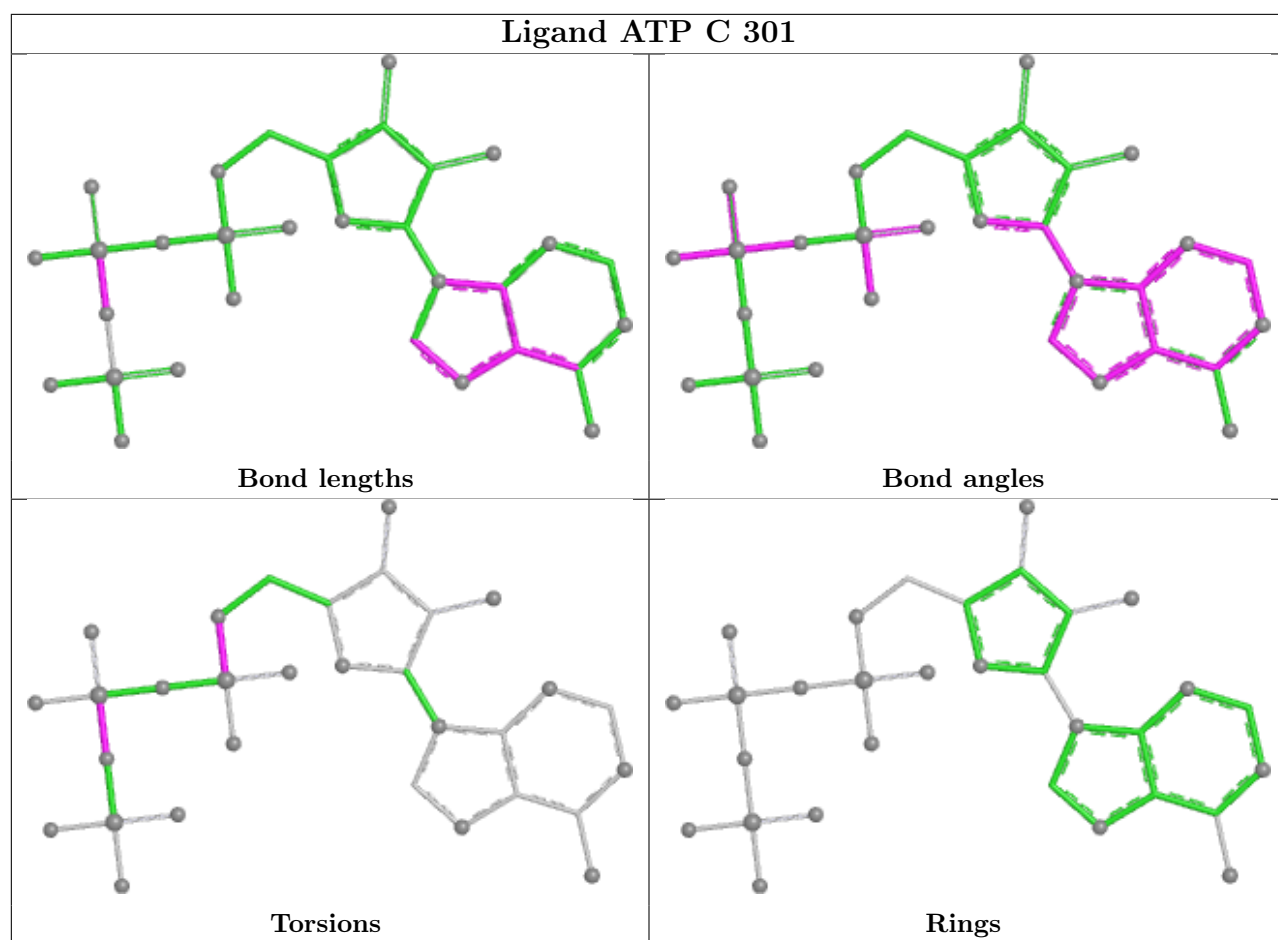
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	ARG	2	0
8	D	301	ATP	2	0
8	C	301	ATP	2	0

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 [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	A	281/318 (88%)	-0.38	5 (1%) 67 61	36, 53, 89, 132	0
1	B	281/318 (88%)	-0.25	10 (3%) 46 36	38, 56, 110, 143	0
2	C	142/154 (92%)	-0.48	2 (1%) 73 67	29, 58, 80, 102	1 (0%)
2	D	142/154 (92%)	-0.51	4 (2%) 55 46	30, 56, 76, 115	1 (0%)
All	All	846/944 (89%)	-0.37	21 (2%) 58 49	29, 56, 98, 143	2 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	VAL	5.1
2	D	3	LEU	4.9
1	B	227	PRO	3.9
1	A	297	GLY	3.6
2	C	3	LEU	3.3

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](#)

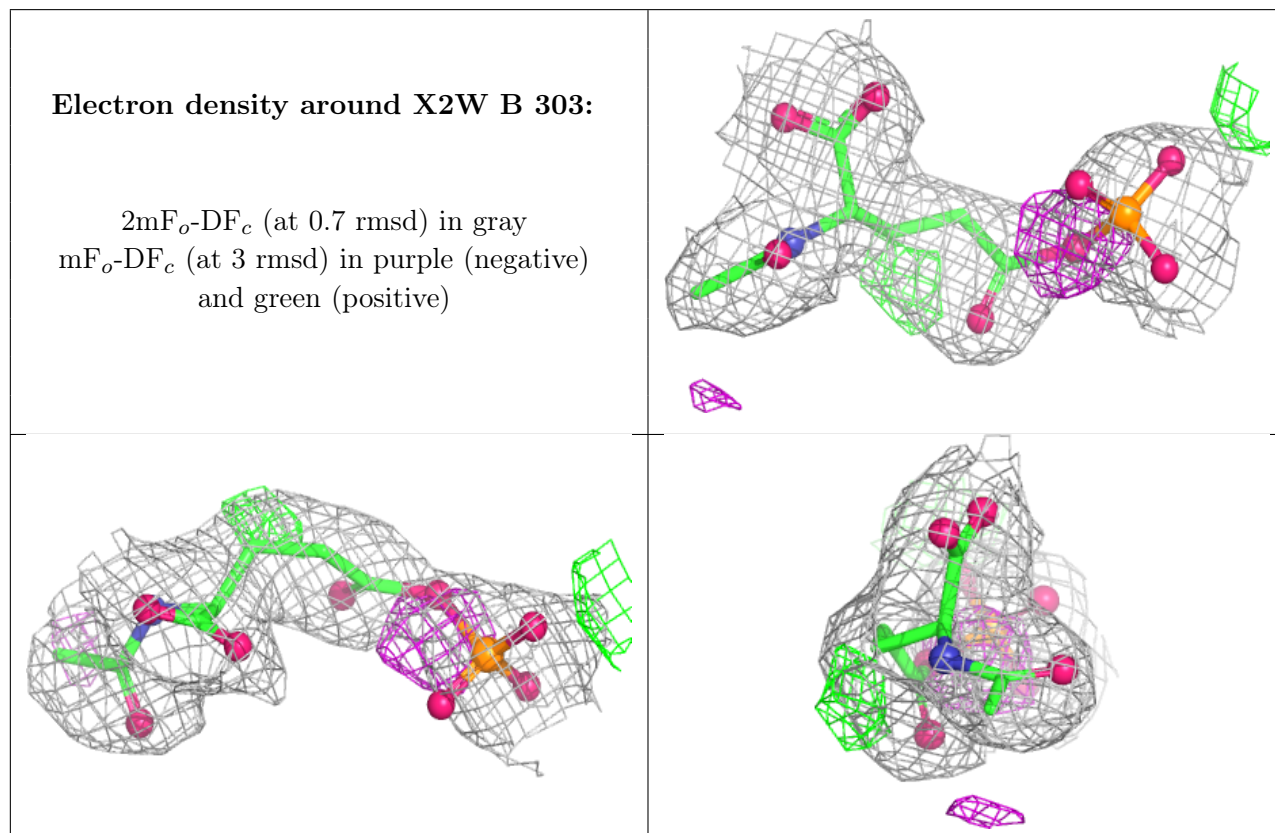
There are no oligosaccharides in this entry.

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.

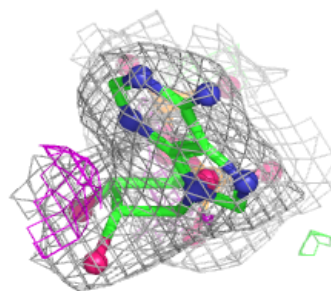
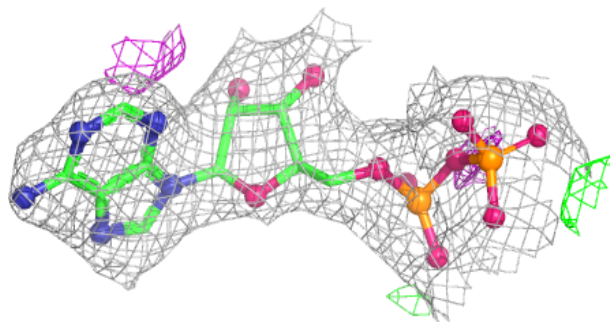
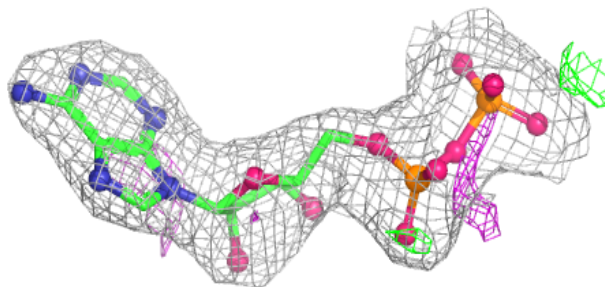
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	GLN	C	303	10/10	0.92	0.12	54,62,76,82	0
7	X2W	B	303	17/17	0.93	0.10	47,51,102,105	0
3	ARG	B	301	12/12	0.94	0.10	69,75,86,86	0
9	GLN	D	303	10/10	0.95	0.10	44,59,71,80	0
3	ARG	A	301	12/12	0.96	0.09	66,68,71,77	0
5	NLG	A	303	13/13	0.97	0.08	40,45,49,50	0
4	ADP	A	302	27/27	0.98	0.06	45,59,63,64	0
8	ATP	D	301	31/31	0.99	0.04	41,48,52,54	0
6	MG	A	304	1/1	0.99	0.04	41,41,41,41	0
8	ATP	C	301	31/31	0.99	0.04	42,48,52,56	0
6	MG	D	302	1/1	1.00	0.02	53,53,53,53	0
6	MG	C	302	1/1	1.00	0.01	58,58,58,58	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.



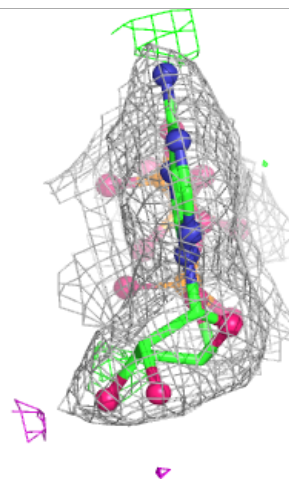
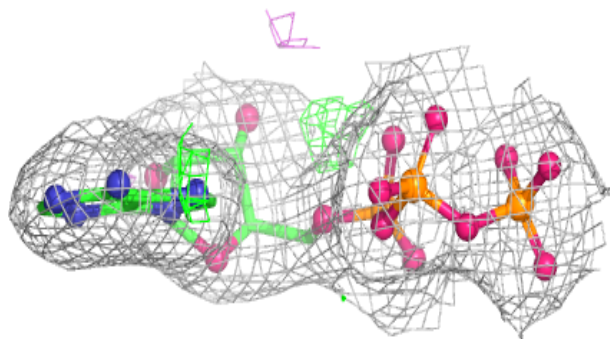
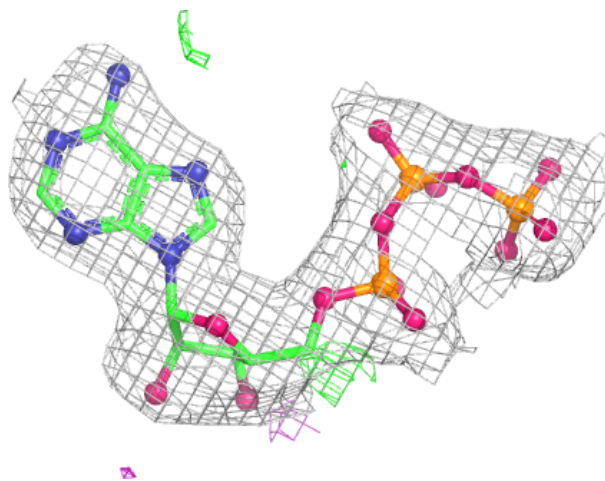
Electron density around ADP A 302:

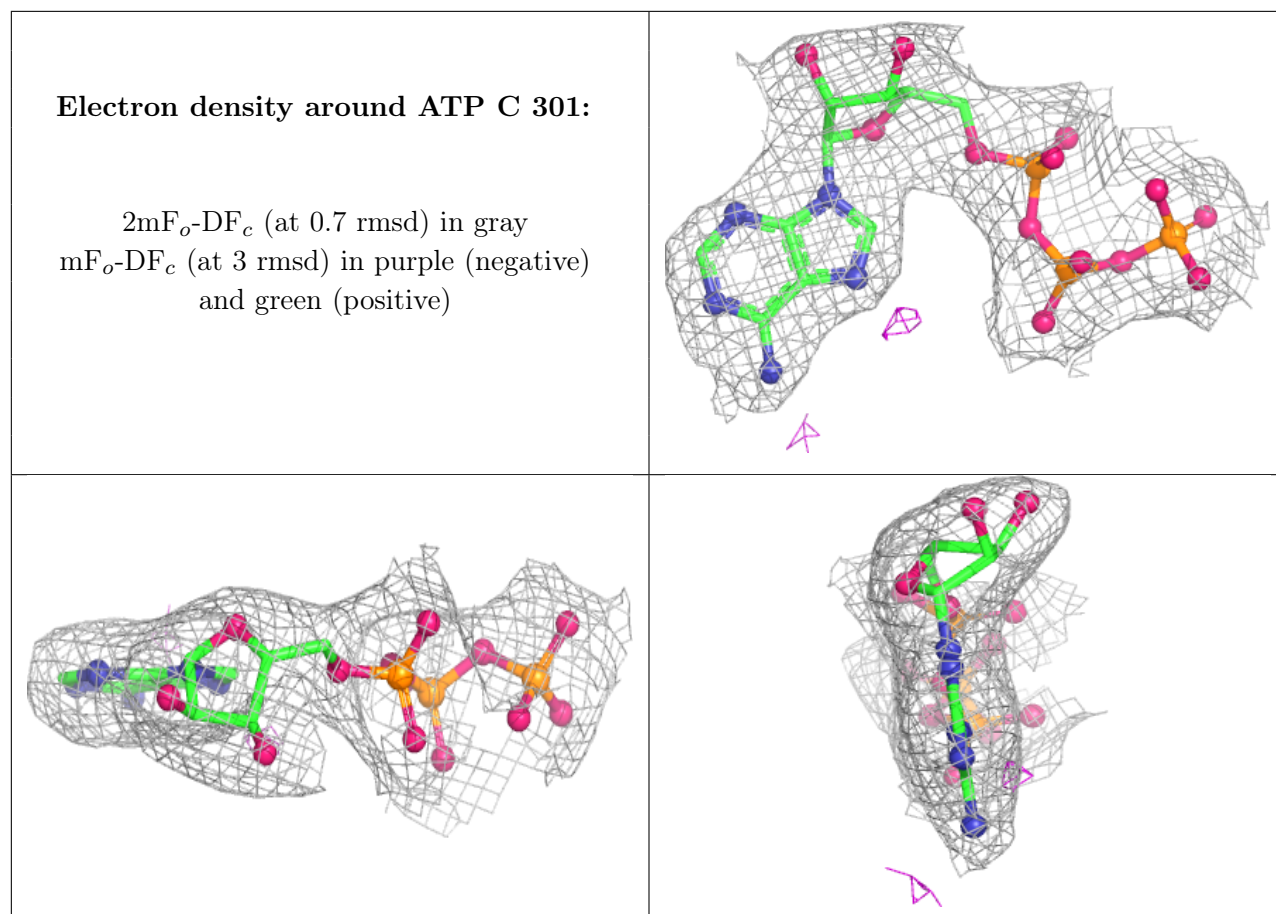
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP D 301:

$2mF_o-DF_c$ (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.