



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:25 PM UTC

PDB ID : 7R7J / pdb_00007r7j
Title : Crystal structure of RadD with ADP
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Deposited on : 2021-06-24
Resolution : 2.03 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

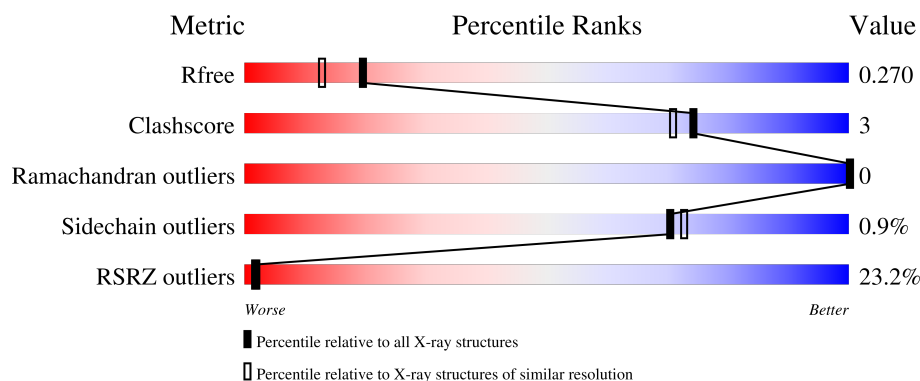
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	586	24% 89% 8%
1	B	586	21% 92% 6%

2 Entry composition [i](#)

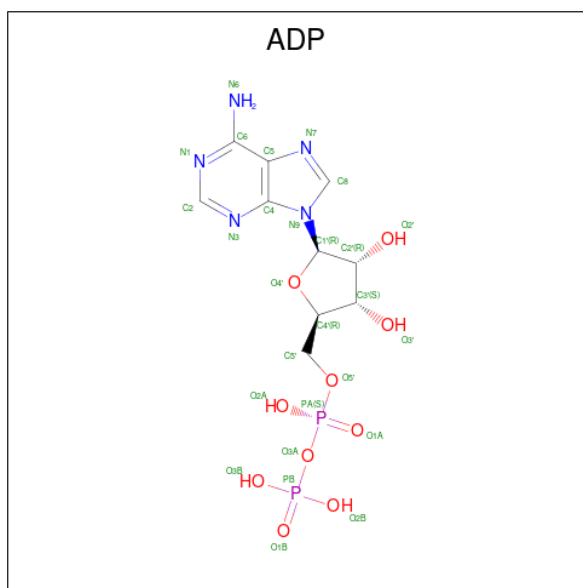
There are 5 unique types of molecules in this entry. The entry contains 17744 atoms, of which 8552 are hydrogens and 0 are deuteriums.

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 Putative DNA repair helicase RadD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	572	Total	C	H	N	O	S	0	0	0
			8576	2779	4194	786	799	18			
1	B	574	Total	C	H	N	O	S	0	0	0
			8799	2834	4335	807	805	18			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

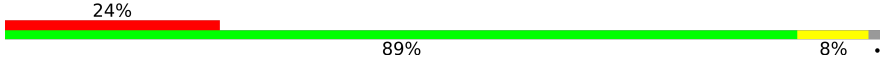
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Zn 2	0	0
4	B	2	Total 2	Zn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 131	O 131	0	0
5	B	155	Total 155	O 155	0	0

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.

- Chain A:
- 
- 24% 89% 8%

- Chain B:
-
- 21%
- 92%
- 6%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.41Å 74.45Å 109.40Å 84.66° 80.03° 82.77°	Depositor
Resolution (Å)	35.65 – 2.03 35.65 – 2.03	Depositor EDS
% Data completeness (in resolution range)	81.0 (35.65-2.03) 81.0 (35.65-2.03)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.236 , 0.269 0.238 , 0.270	Depositor DCC
R_{free} test set	1812 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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, ZN, 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	A	0.13	0/4478	0.31	0/6086
1	B	0.12	0/4565	0.29	0/6196
All	All	0.13	0/9043	0.30	0/12282

There are no bond length outliers.

There are no bond angle outliers.

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	A	4382	4194	4194	31	0
1	B	4464	4335	4335	23	0
2	A	27	12	12	0	0
2	B	27	11	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	131	0	0	0	0
5	B	155	0	0	1	0
All	All	9192	8552	8553	54	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 (54) 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:B:257:ILE:HG23	1:B:325:LEU:HD23	1.67	0.75
1:B:206:VAL:HG13	1:B:207:VAL:H	1.59	0.68
1:B:242:ILE:CD1	1:B:268:ILE:HG23	2.24	0.67
1:A:307:VAL:O	1:A:309:VAL:N	2.30	0.65
1:B:440:GLU:O	1:B:449:ARG:NH1	2.29	0.64
1:A:268:ILE:HD11	1:A:325:LEU:HD12	1.81	0.62
1:B:242:ILE:HD11	1:B:268:ILE:HG23	1.81	0.62
1:A:280:ILE:HG12	1:A:304:LEU:HD21	1.84	0.58
1:A:307:VAL:HG12	1:A:308:ALA:H	1.70	0.57
1:B:465:ALA:HA	1:B:468:LEU:HD12	1.88	0.56
1:A:405:GLU:HG3	1:A:529:ARG:HB3	1.88	0.56
1:A:280:ILE:HG13	1:A:304:LEU:HD11	1.89	0.55
1:A:29:ILE:HG12	1:A:147:LEU:HD11	1.89	0.53
1:B:185:LEU:HD21	1:B:190:MET:SD	2.48	0.53
1:B:409:ARG:CZ	1:B:443:ILE:HD11	2.40	0.52
1:B:206:VAL:HG13	1:B:207:VAL:N	2.26	0.51
1:B:29:ILE:HG13	1:B:147:LEU:HD11	1.93	0.51
1:B:474:LEU:HD22	1:B:504:VAL:HG22	1.91	0.51
1:A:265:ALA:O	1:A:269:VAL:HG23	2.12	0.49
1:B:525:ARG:HB3	1:B:526:PRO:HD3	1.95	0.49
1:A:201:ARG:HD2	1:A:361:HIS:CE1	2.49	0.48
1:A:476:CYS:HB3	1:A:553:PRO:O	2.14	0.48
1:A:520:GLU:HG2	1:A:524:ILE:HD12	1.95	0.48
1:B:59:LYS:HG2	1:B:60:GLU:OE1	2.14	0.48
1:B:264:HIS:O	1:B:268:ILE:HG13	2.13	0.47
1:A:266:LYS:HZ2	1:A:279:LEU:HD11	1.79	0.47
1:B:35:ALA:HA	1:B:190:MET:HE1	1.96	0.47
1:A:256:MET:HE3	1:A:304:LEU:HD12	1.96	0.46
1:A:487:GLU:H	1:A:487:GLU:CD	2.23	0.46
1:A:475:ARG:O	1:A:498:ASP:HB3	2.16	0.46
1:B:242:ILE:HD12	1:B:268:ILE:HG23	1.95	0.46
1:A:475:ARG:HD2	1:A:555:PHE:CZ	2.51	0.45
1:A:457:ASP:CG	1:A:458:PRO:HD2	2.42	0.45
1:A:415:PHE:CE1	1:A:423:GLU:HG3	2.52	0.45
1:A:242:ILE:HD11	1:A:268:ILE:HG12	1.99	0.44
1:A:486:ASP:OD1	1:A:486:ASP:C	2.61	0.44
1:B:372:LYS:HB3	1:B:372:LYS:HE2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:O	1:A:64:GLN:HG3	2.18	0.43
1:A:29:ILE:CG1	1:A:147:LEU:HD11	2.49	0.43
1:A:486:ASP:OD1	1:A:487:GLU:N	2.52	0.43
1:A:324:ILE:C	1:A:325:LEU:HD23	2.45	0.42
1:B:174:GLU:H	1:B:174:GLU:CD	2.27	0.42
1:B:355:ASP:OD1	1:B:359:ASN:ND2	2.52	0.42
1:B:309:VAL:HG21	1:B:336:GLN:HG2	2.00	0.41
1:A:238:THR:HB	1:A:239:PRO:HD3	2.02	0.41
1:A:475:ARG:NH1	1:A:578:PHE:CB	2.84	0.41
1:A:244:GLN:NE2	1:A:248:PHE:CE2	2.89	0.41
1:B:464:ALA:O	5:B:701:HOH:O	2.21	0.41
1:A:325:LEU:HD22	1:A:356:TYR:HB2	2.04	0.40
1:A:486:ASP:OD1	1:A:488:LYS:N	2.48	0.40
1:B:285:PRO:O	1:B:289:ARG:N	2.54	0.40
1:A:272:LEU:HD23	1:A:277:ALA:HB2	2.04	0.40
1:A:202:LEU:HB2	1:A:354:LEU:HD23	2.04	0.40
1:B:560:MET:HE2	1:B:560:MET:HB2	1.94	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	
1	A	568/586 (97%)	546 (96%)	22 (4%)	0	100	100
1	B	570/586 (97%)	550 (96%)	20 (4%)	0	100	100
All	All	1138/1172 (97%)	1096 (96%)	42 (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	436/491 (89%)	432 (99%)	4 (1%)	70	73
1	B	452/491 (92%)	448 (99%)	4 (1%)	70	73
All	All	888/982 (90%)	880 (99%)	8 (1%)	70	73

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	ASP
1	A	375	SER
1	A	415	PHE
1	A	505	SER
1	B	128	SER
1	B	268	ILE
1	B	295	ASN
1	B	504	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	64	GLN
1	A	235	GLN
1	A	299	GLN
1	A	335	GLN
1	A	336	GLN
1	A	361	HIS
1	B	98	GLN
1	B	131	GLN
1	B	132	GLN
1	B	244	GLN
1	B	381	GLN
1	B	412	GLN
1	B	421	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	601	3	28,29,29	1.35	4 (14%)	43,45,45	1.88	9 (20%)
2	ADP	B	601	3	28,29,29	1.41	5 (17%)	43,45,45	1.90	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
2	ADP	A	601	3	-	1/16/32/32	0/3/3/3
2	ADP	B	601	3	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	4.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C5-C4	4.26	1.46	1.39
2	B	601	ADP	C5-C6	2.65	1.48	1.41
2	A	601	ADP	C5-C6	2.46	1.47	1.41
2	A	601	ADP	C8-N7	2.31	1.36	1.31
2	B	601	ADP	C5-N7	-2.31	1.34	1.39
2	B	601	ADP	C8-N7	2.29	1.36	1.31
2	A	601	ADP	C5-N7	-2.26	1.35	1.39
2	B	601	ADP	PA-O3A	2.03	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-6.04	118.40	126.72
2	A	601	ADP	C5-C4-N3	-5.68	118.90	126.72
2	B	601	ADP	N3-C4-N9	5.15	135.92	127.17
2	A	601	ADP	N3-C4-N9	4.95	135.59	127.17
2	B	601	ADP	C2-N3-C4	3.95	121.49	111.83
2	A	601	ADP	C2-N3-C4	3.90	121.36	111.83
2	A	601	ADP	N3-C2-N1	-3.85	122.75	128.58
2	A	601	ADP	C4-N9-C8	3.75	109.67	105.74
2	B	601	ADP	N3-C2-N1	-3.72	122.95	128.58
2	B	601	ADP	C4-N9-C8	3.41	109.32	105.74
2	B	601	ADP	C4-C5-N7	-3.28	106.83	110.58
2	A	601	ADP	C4-C5-N7	-3.03	107.11	110.58
2	B	601	ADP	C5-N7-C8	2.75	107.77	103.45
2	A	601	ADP	N9-C8-N7	-2.64	110.19	113.94
2	A	601	ADP	C5-N7-C8	2.58	107.50	103.45
2	B	601	ADP	N9-C8-N7	-2.50	110.39	113.94
2	A	601	ADP	C6-C5-N7	2.16	136.25	132.09
2	B	601	ADP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

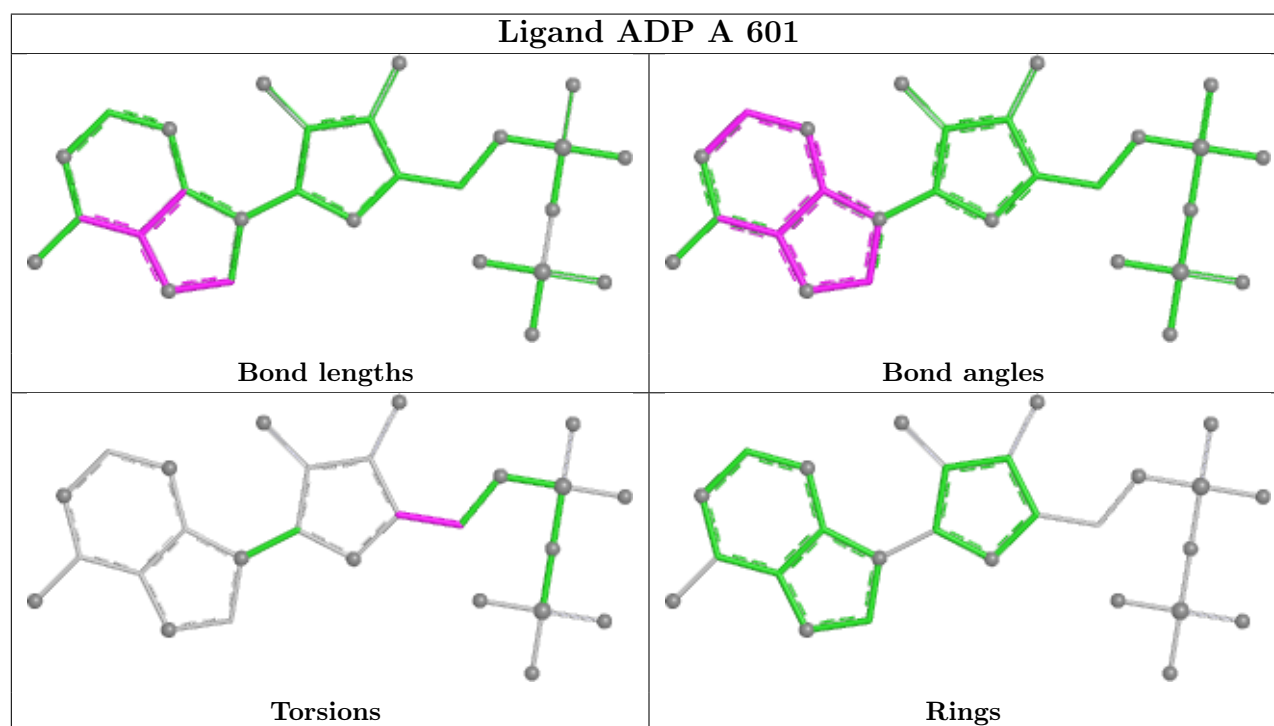
All (3) torsion outliers are listed below:

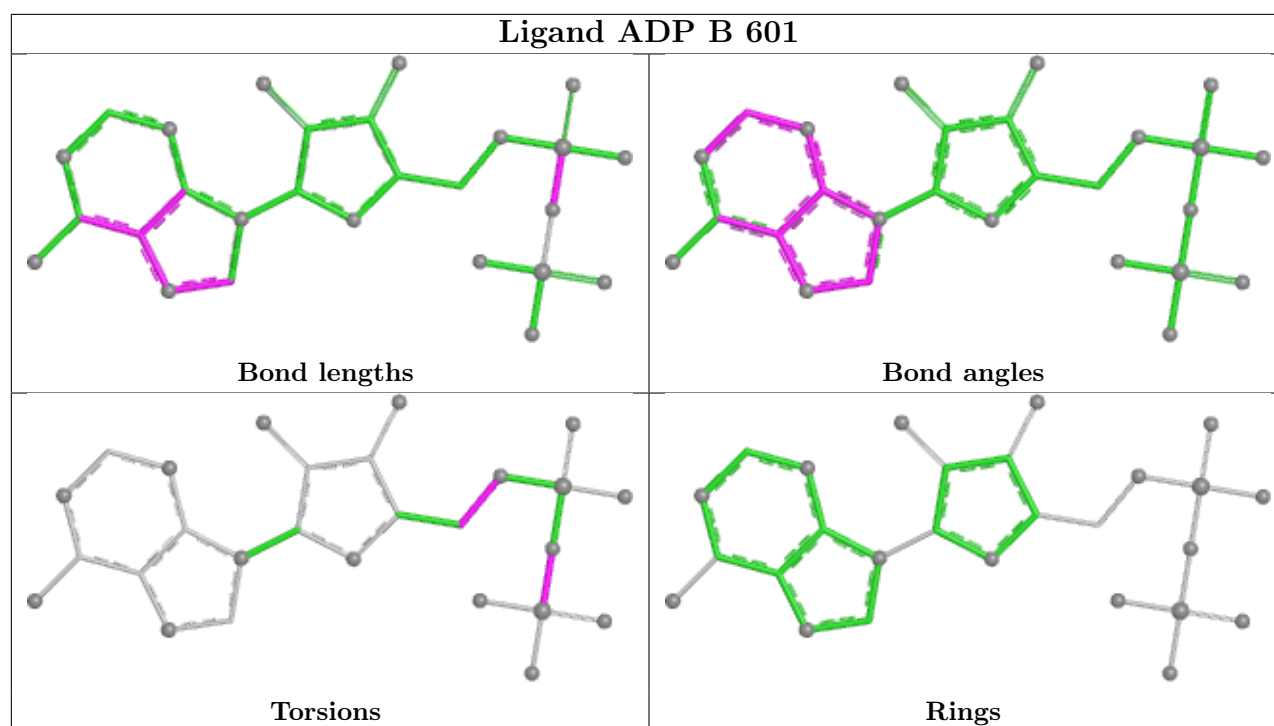
Mol	Chain	Res	Type	Atoms
2	B	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	C4'-C5'-O5'-PA
2	A	601	ADP	O4'-C4'-C5'-O5'

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	A	572/586 (97%)	1.18	142 (24%) 2 1	24, 58, 103, 135	0
1	B	574/586 (97%)	1.07	124 (21%) 2 2	24, 52, 112, 125	0
All	All	1146/1172 (97%)	1.12	266 (23%) 2 2	24, 55, 108, 135	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	VAL	9.7
1	B	301	PHE	7.2
1	B	254	GLY	6.3
1	A	578	PHE	5.9
1	B	321	LEU	5.8
1	B	352	LEU	5.8
1	B	320	ASP	5.8
1	B	245	ILE	5.8
1	B	248	PHE	5.7
1	B	354	LEU	5.7
1	B	317	PRO	5.5
1	B	252	ARG	5.5
1	B	322	ILE	5.4
1	B	278	ALA	5.4
1	B	279	LEU	5.3
1	B	250	ALA	5.0
1	B	296	PHE	5.0
1	B	292	LEU	5.0
1	A	257	ILE	5.0
1	A	293	ILE	4.9
1	B	356	TYR	4.9
1	A	567	VAL	4.9
1	A	280	ILE	4.8
1	A	291	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	305	VAL	4.8
1	B	207	VAL	4.8
1	B	255	VAL	4.7
1	A	288	GLU	4.6
1	B	337	ILE	4.6
1	A	255	VAL	4.5
1	A	290	ASP	4.4
1	B	290	ASP	4.4
1	A	3	PHE	4.4
1	A	279	LEU	4.4
1	A	2	ILE	4.4
1	A	470	ASP	4.4
1	B	257	ILE	4.4
1	B	293	ILE	4.4
1	B	304	LEU	4.3
1	A	89	HIS	4.3
1	B	323	ALA	4.3
1	A	305	VAL	4.3
1	A	254	GLY	4.2
1	A	281	THR	4.2
1	A	565	TRP	4.2
1	A	311	THR	4.2
1	B	241	ILE	4.1
1	A	560	MET	4.1
1	B	281	THR	4.1
1	B	308	ALA	4.0
1	A	310	LEU	4.0
1	A	125	ASP	4.0
1	A	214	LEU	3.9
1	B	318	HIS	3.9
1	B	246	MET	3.9
1	B	253	LYS	3.9
1	A	471	ALA	3.9
1	A	467	ARG	3.9
1	B	302	ARG	3.9
1	B	360	PRO	3.9
1	B	206	VAL	3.8
1	A	561	LYS	3.8
1	A	260	ALA	3.8
1	A	237	ILE	3.8
1	B	280	ILE	3.8
1	B	324	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	312	THR	3.8
1	B	272	LEU	3.8
1	A	485	HIS	3.8
1	A	227	LEU	3.8
1	A	248	PHE	3.8
1	B	314	PHE	3.8
1	A	564	TYR	3.7
1	A	474	LEU	3.7
1	B	214	LEU	3.7
1	B	231	LEU	3.7
1	B	242	ILE	3.7
1	B	284	THR	3.6
1	B	303	TYR	3.6
1	A	292	LEU	3.6
1	B	268	ILE	3.5
1	B	325	LEU	3.5
1	A	559	ARG	3.5
1	B	204	MET	3.5
1	A	319	VAL	3.5
1	B	249	ALA	3.5
1	A	277	ALA	3.4
1	A	204	MET	3.4
1	A	566	GLN	3.4
1	A	558	ALA	3.4
1	A	275	GLU	3.4
1	A	289	ARG	3.4
1	A	468	LEU	3.4
1	B	271	LEU	3.4
1	A	207	VAL	3.4
1	A	354	LEU	3.4
1	A	472	LEU	3.4
1	B	351	CYS	3.3
1	B	312	THR	3.3
1	A	221	LEU	3.3
1	B	283	ASP	3.3
1	A	356	TYR	3.2
1	B	251	THR	3.2
1	A	309	VAL	3.2
1	A	296	PHE	3.2
1	B	258	PHE	3.2
1	B	259	ALA	3.2
1	B	87	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	3.1
1	A	321	LEU	3.1
1	B	202	LEU	3.1
1	A	361	HIS	3.1
1	A	314	PHE	3.1
1	A	466	LEU	3.1
1	B	353	ILE	3.1
1	A	462	LEU	3.0
1	A	504	VAL	3.0
1	B	256	MET	3.0
1	B	285	PRO	3.0
1	B	262	VAL	3.0
1	A	562	GLY	3.0
1	B	316	ALA	3.0
1	B	357	ALA	3.0
1	A	344	LEU	3.0
1	A	231	LEU	2.9
1	A	278	ALA	2.9
1	B	82	GLY	2.9
1	B	3	PHE	2.9
1	B	86	LYS	2.9
1	B	240	HIS	2.9
1	A	205	PRO	2.8
1	B	224	GLU	2.8
1	B	564	TYR	2.8
1	A	259	ALA	2.8
1	A	316	ALA	2.8
1	B	265	ALA	2.8
1	A	55	LEU	2.8
1	B	310	LEU	2.8
1	A	239	PRO	2.8
1	A	241	ILE	2.8
1	A	225	ALA	2.8
1	B	83	LEU	2.8
1	A	349	THR	2.8
1	B	89	HIS	2.8
1	A	226	ASP	2.8
1	B	277	ALA	2.8
1	B	361	HIS	2.7
1	A	84	LYS	2.7
1	B	209	TYR	2.7
1	A	206	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	LYS	2.7
1	A	577	ARG	2.7
1	A	268	ILE	2.7
1	A	443	ILE	2.7
1	A	223	SER	2.7
1	B	347	GLY	2.7
1	A	301	PHE	2.7
1	B	345	ALA	2.7
1	A	83	LEU	2.7
1	B	313	GLY	2.7
1	A	211	PHE	2.6
1	A	415	PHE	2.6
1	A	346	PRO	2.6
1	A	122	ILE	2.6
1	B	2	ILE	2.6
1	A	87	GLU	2.6
1	B	306	ASN	2.6
1	A	85	ARG	2.6
1	A	262	VAL	2.6
1	B	270	GLY	2.6
1	A	249	ALA	2.6
1	A	444	ALA	2.6
1	A	271	LEU	2.6
1	B	227	LEU	2.6
1	B	88	SER	2.6
1	A	215	GLN	2.6
1	B	200	GLU	2.6
1	B	421	HIS	2.6
1	B	201	ARG	2.6
1	B	239	PRO	2.6
1	B	346	PRO	2.6
1	B	125	ASP	2.5
1	A	267	GLU	2.5
1	B	211	PHE	2.5
1	B	269	VAL	2.5
1	B	349	THR	2.5
1	B	578	PHE	2.5
1	B	291	VAL	2.5
1	A	272	LEU	2.5
1	B	295	ASN	2.5
1	A	78	ILE	2.5
1	A	282	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	358	GLY	2.4
1	B	307	VAL	2.4
1	B	199	PRO	2.4
1	A	244	GLN	2.4
1	A	469	LYS	2.4
1	A	352	LEU	2.4
1	A	127	GLU	2.4
1	B	286	GLY	2.4
1	B	229	ARG	2.4
1	B	233	LYS	2.4
1	A	246	MET	2.3
1	A	456	VAL	2.3
1	A	473	VAL	2.3
1	A	209	TYR	2.3
1	A	303	TYR	2.3
1	A	213	ARG	2.3
1	B	223	SER	2.3
1	A	100	VAL	2.3
1	B	273	PRO	2.3
1	A	265	ALA	2.3
1	A	298	ALA	2.3
1	B	334	TYR	2.3
1	B	266	LYS	2.3
1	A	258	PHE	2.3
1	B	404	ILE	2.3
1	B	205	PRO	2.3
1	A	491	TRP	2.3
1	B	264	HIS	2.2
1	A	99	SER	2.2
1	A	222	PHE	2.2
1	A	269	VAL	2.2
1	B	309	VAL	2.2
1	A	233	LYS	2.2
1	A	320	ASP	2.2
1	A	274	ALA	2.2
1	B	288	GLU	2.2
1	A	318	HIS	2.2
1	A	219	ASN	2.2
1	A	307	VAL	2.2
1	B	84	LYS	2.2
1	A	576	GLY	2.2
1	A	325	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	2.2
1	B	85	ARG	2.2
1	A	251	THR	2.2
1	B	287	ALA	2.2
1	A	403	LEU	2.2
1	B	213	ARG	2.2
1	A	400	ASP	2.2
1	B	327	PRO	2.1
1	A	97	VAL	2.1
1	A	81	ALA	2.1
1	A	102	ARG	2.1
1	A	128	SER	2.1
1	A	80	ALA	2.1
1	A	464	ALA	2.1
1	B	260	ALA	2.1
1	A	59	LYS	2.1
1	A	105	ASP	2.1
1	A	337	ILE	2.1
1	B	220	GLY	2.1
1	B	282	GLY	2.1
1	A	304	LEU	2.1
1	B	294	GLU	2.1
1	A	362	ASP	2.1
1	A	323	ALA	2.1
1	A	461	MET	2.0
1	B	219	ASN	2.0
1	A	555	PHE	2.0
1	A	465	ALA	2.0
1	B	474	LEU	2.0
1	A	240	HIS	2.0
1	A	138	THR	2.0
1	B	311	THR	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](#)

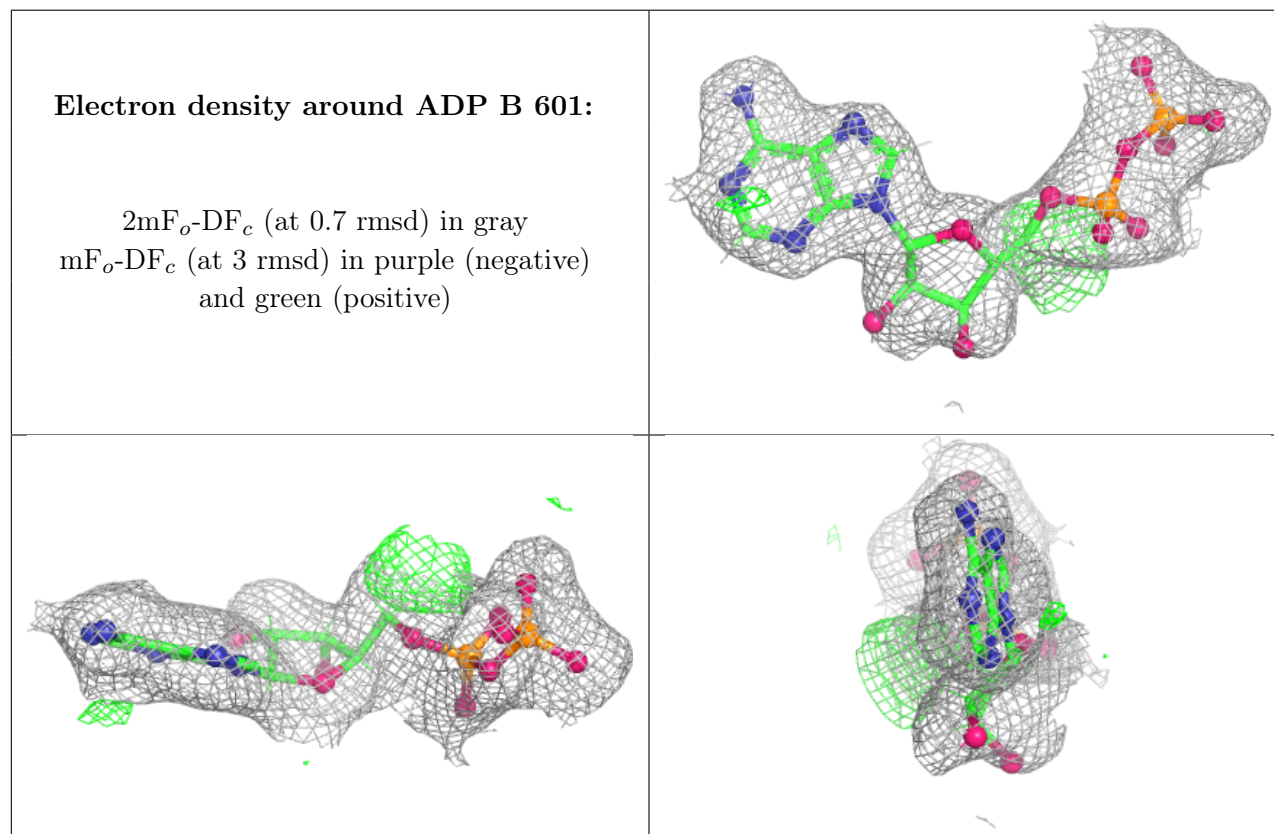
There are no oligosaccharides in this entry.

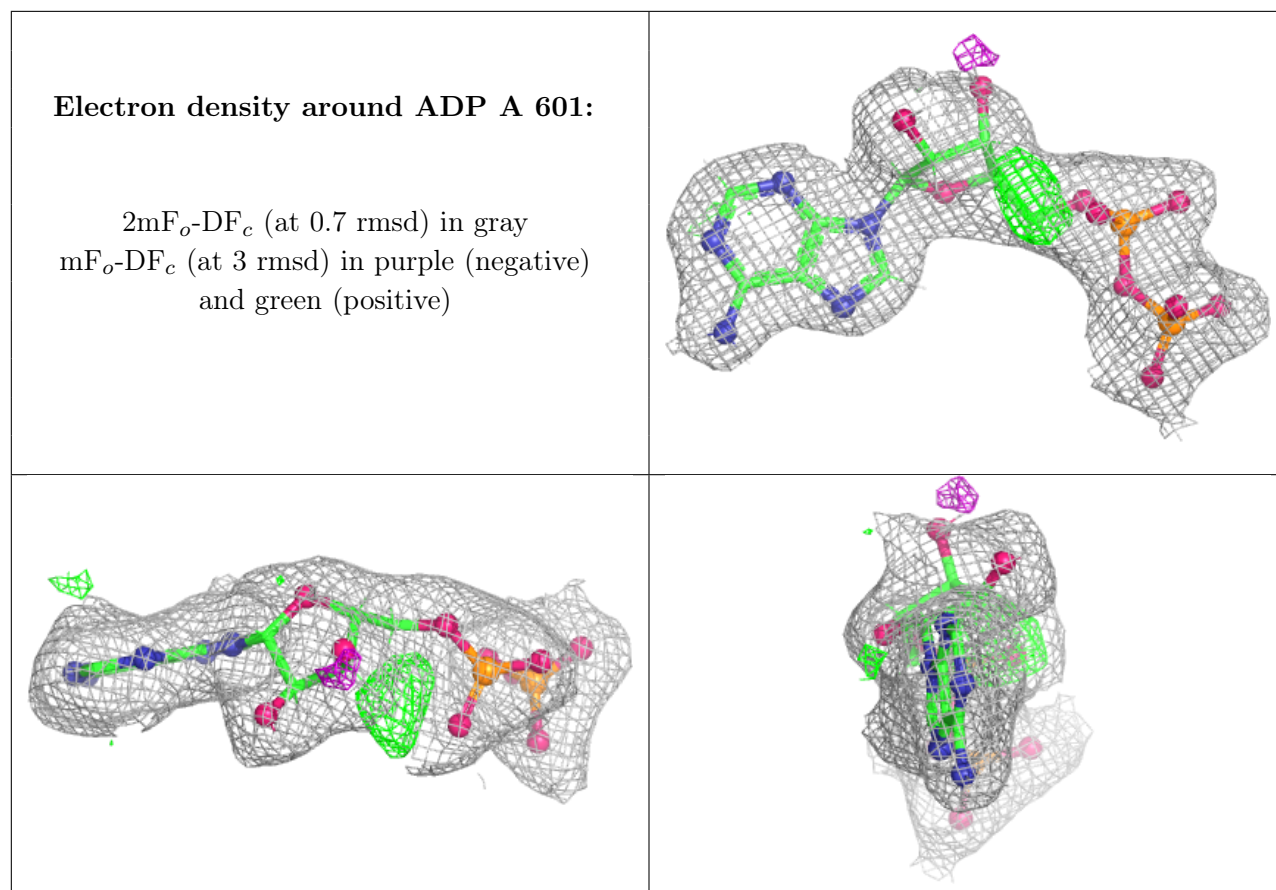
6.4 Ligands ⓘ

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	MG	B	602	1/1	0.84	0.13	46,46,46,46	0
2	ADP	B	601	27/27	0.89	0.11	35,57,73,79	0
3	MG	A	602	1/1	0.92	0.15	41,41,41,41	0
2	ADP	A	601	27/27	0.94	0.09	32,51,66,74	0
4	ZN	B	604	1/1	0.98	0.05	57,57,57,57	0
4	ZN	A	604	1/1	0.99	0.03	44,44,44,44	0
4	ZN	B	603	1/1	0.99	0.02	29,29,29,29	0
4	ZN	A	603	1/1	0.99	0.03	24,24,24,24	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 ⓘ

There are no such residues in this entry.