Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:56 PM EDT

PDB ID	:	7R7J
Title	:	Crystal structure of RadD with ADP
Authors	:	Osorio Garcia, M.A.; Satyshur, K.A.; Keck, J.L.; Cox, M.M.
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:

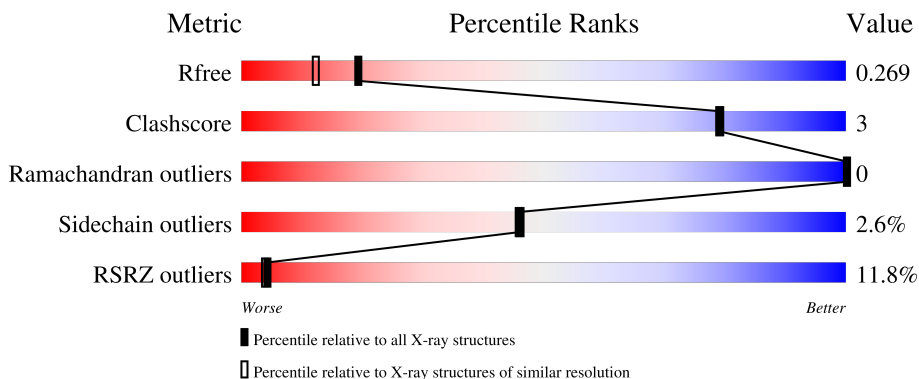|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.269
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.6%
RSRZ outliers		11.8%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (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 <=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	10% / 88% / 9% ·
1	B	586	13% / 91% / 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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

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: Putative DNA repair helicase RadD
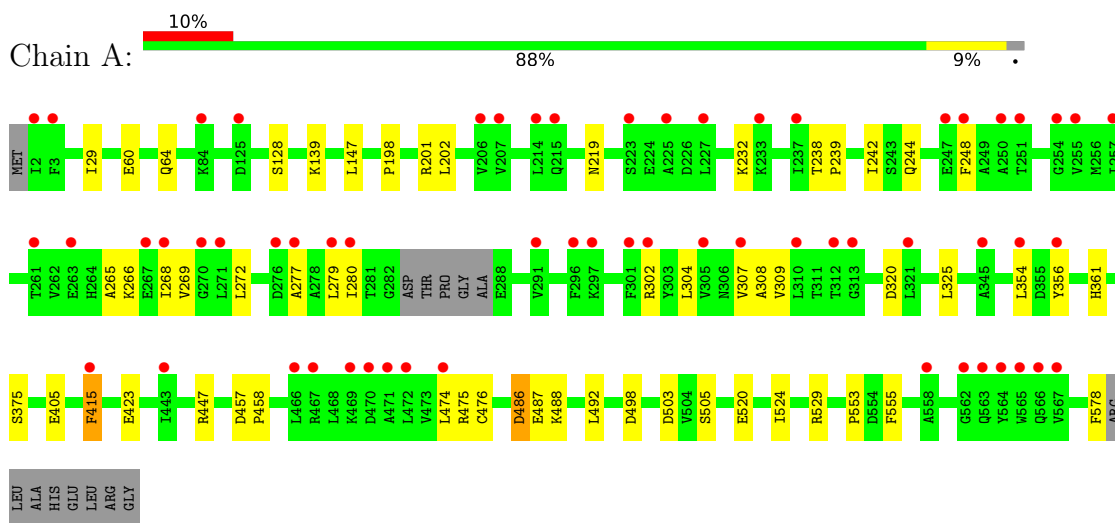
• Molecule 1: Putative DNA repair helicase RadD
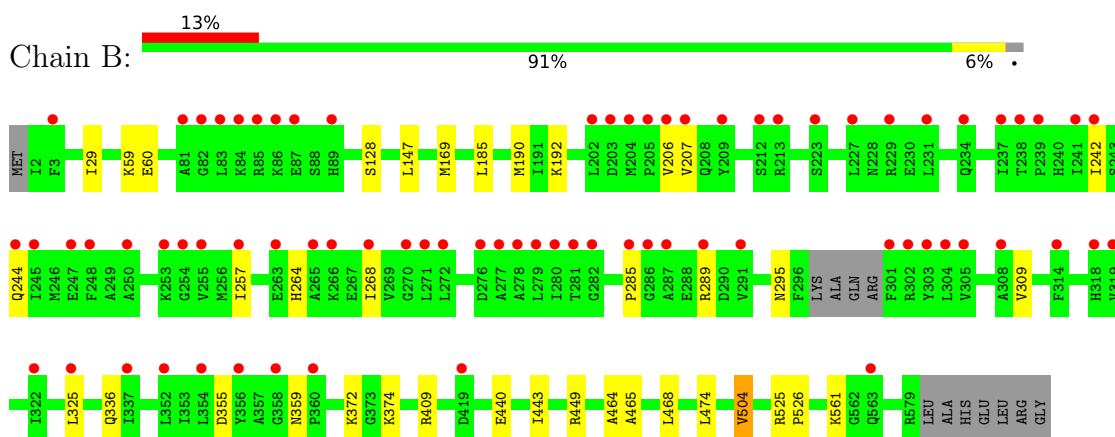
4 Data and refinement statistics ⓘ

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 45.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	81.0 (35.65-2.03) 81.0 (45.00-2.03)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.236 , 0.269 0.236 , 0.269	Depositor DCC
R_{free} test set	1812 reflections (2.28%)	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 , 46.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.26	0/4478	0.52	0/6086
1	B	0.25	0/4565	0.51	0/6196
All	All	0.26	0/9043	0.52	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	28	0
1	B	4464	4335	4335	20	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	48	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 (48) 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: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:266:LYS:HZ2	1:A:279:LEU:HD11	1.81	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:B:372:LYS:HB3	1:B:372:LYS:HE2	1.81	0.43
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:B:355:ASP:OD1	1:B:359:ASN:ND2	2.52	0.42
1:A:487:GLU:H	1:A:487:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:457:ASP:CG	1:A:458:PRO:HD2	2.42	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%)	421 (97%)	15 (3%)	37	35
1	B	452/491 (92%)	444 (98%)	8 (2%)	59	61
All	All	888/982 (90%)	865 (97%)	23 (3%)	46	46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER
1	A	139	LYS
1	A	198	PRO
1	A	219	ASN
1	A	232	LYS
1	A	302	ARG
1	A	320	ASP
1	A	375	SER
1	A	415	PHE
1	A	447	ARG
1	A	474	LEU
1	A	486	ASP
1	A	492	LEU
1	A	503	ASP
1	A	505	SER
1	B	128	SER
1	B	169	MET
1	B	192	LYS
1	B	244	GLN
1	B	295	ASN
1	B	374	LYS
1	B	504	VAL
1	B	561	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	B	132	GLN

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 monosaccharides 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	B	601	3	24,29,29	1.05	2 (8%)	29,45,45	1.26	3 (10%)
2	ADP	A	601	3	24,29,29	0.98	2 (8%)	29,45,45	1.33	3 (10%)

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	B	601	3	-	2/12/32/32	0/3/3/3
2	ADP	A	601	3	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	O4'-C1'	2.93	1.45	1.41
2	A	601	ADP	O4'-C1'	2.65	1.44	1.41
2	B	601	ADP	C5-C4	2.33	1.47	1.40
2	A	601	ADP	C5-C4	2.18	1.46	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ADP	N3-C2-N1	-3.79	122.76	128.68
2	B	601	ADP	N3-C2-N1	-3.66	122.95	128.68
2	A	601	ADP	PA-O3A-PB	-3.38	121.23	132.83
2	B	601	ADP	PA-O3A-PB	-2.63	123.81	132.83
2	B	601	ADP	C4-C5-N7	-2.47	106.83	109.40
2	A	601	ADP	C4-C5-N7	-2.20	107.11	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ADP	PA-O3A-PB-O3B
2	A	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	C4'-C5'-O5'-PA
2	A	601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ADP B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 601

Bond lengths

Bond angles

Torsions

Rings
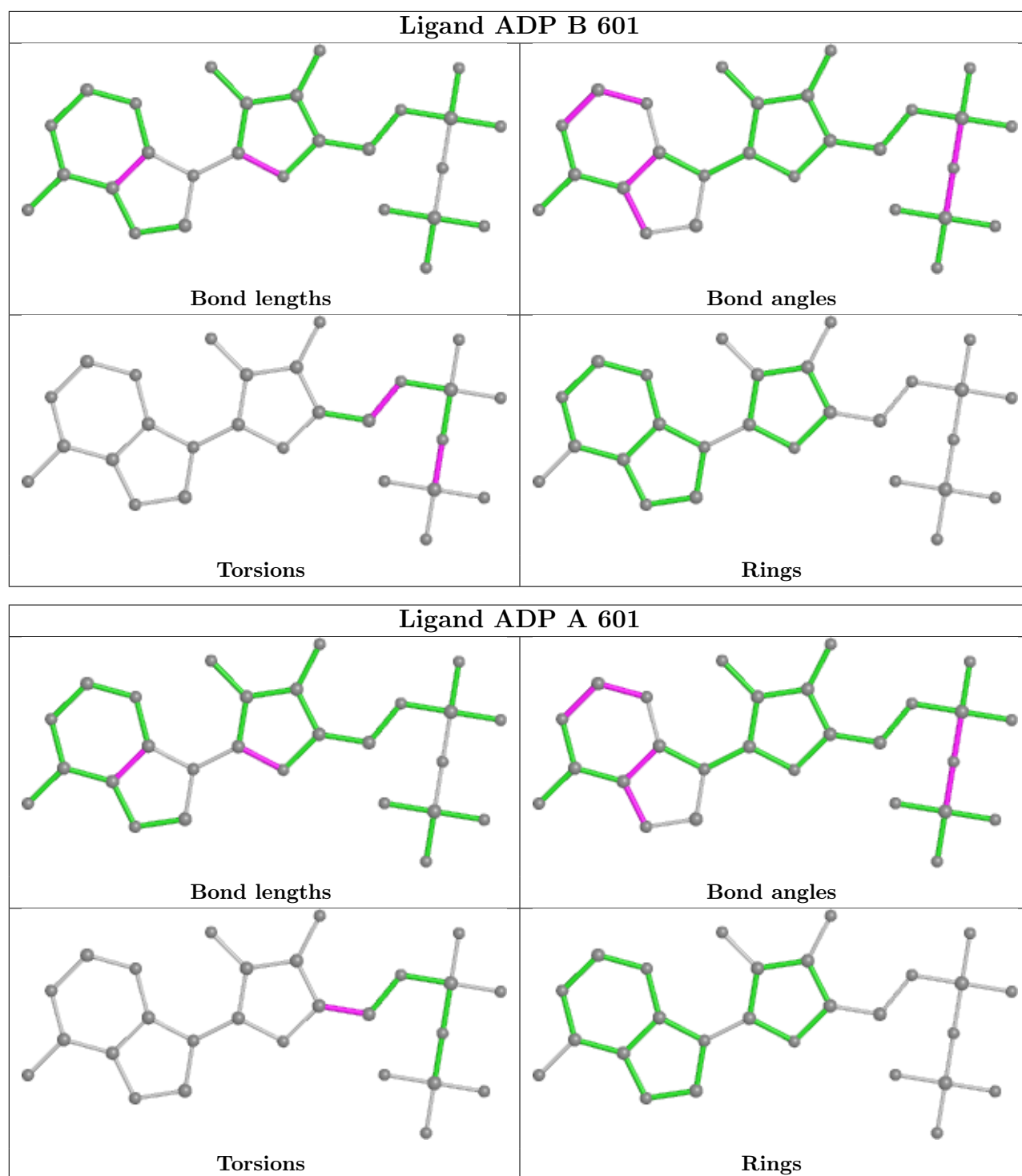
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	572/586 (97%)	0.75	60 (10%)	6	5	22, 53, 94, 118	0
1	B	574/586 (97%)	0.73	75 (13%)	3	3	21, 47, 103, 115	0
All	All	1146/1172 (97%)	0.74	135 (11%)	4	4	21, 50, 100, 118	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254	GLY	9.9
1	B	206	VAL	9.7
1	B	241	ILE	8.4
1	B	248	PHE	7.1
1	A	279	LEU	7.0
1	B	205	PRO	6.9
1	B	278	ALA	6.8
1	B	279	LEU	6.7
1	B	319	VAL	6.7
1	A	471	ALA	6.7
1	A	237	ILE	6.6
1	B	356	TYR	6.5
1	A	305	VAL	5.7
1	B	250	ALA	5.6
1	B	272	LEU	5.5
1	B	245	ILE	5.3
1	B	268	ILE	5.0
1	A	474	LEU	4.9
1	B	352	LEU	4.8
1	A	280	ILE	4.8
1	B	239	PRO	4.7
1	B	305	VAL	4.6
1	B	285	PRO	4.6
1	A	125	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	268	ILE	4.5
1	B	83	LEU	4.4
1	B	281	THR	4.4
1	B	255	VAL	4.4
1	B	277	ALA	4.2
1	A	563	GLN	4.2
1	B	82	GLY	4.2
1	A	227	LEU	4.1
1	B	354	LEU	4.1
1	A	257	ILE	4.1
1	A	277	ALA	4.0
1	B	314	PHE	3.9
1	B	322	ILE	3.8
1	A	214	LEU	3.8
1	A	267	GLU	3.7
1	B	360	PRO	3.7
1	A	301	PHE	3.7
1	B	3	PHE	3.7
1	A	248	PHE	3.6
1	B	203	ASP	3.6
1	B	204	MET	3.6
1	B	207	VAL	3.6
1	A	562	GLY	3.6
1	A	296	PHE	3.6
1	B	303	TYR	3.6
1	A	567	VAL	3.6
1	A	250	ALA	3.5
1	B	289	ARG	3.5
1	B	308	ALA	3.4
1	A	223	SER	3.4
1	A	312	THR	3.4
1	A	466	LEU	3.4
1	A	215	GLN	3.4
1	A	207	VAL	3.3
1	B	213	ARG	3.3
1	B	302	ARG	3.2
1	B	202	LEU	3.2
1	A	84	LYS	3.2
1	A	469	LYS	3.2
1	B	87	GLU	3.2
1	B	287	ALA	3.1
1	A	251	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	THR	3.1
1	B	231	LEU	3.1
1	B	257	ILE	3.1
1	B	337	ILE	3.1
1	B	84	LYS	3.1
1	A	470	ASP	3.1
1	B	265	ALA	3.0
1	B	237	ILE	2.9
1	B	227	LEU	2.8
1	B	276	ASP	2.8
1	B	286	GLY	2.7
1	A	270	GLY	2.7
1	B	358	GLY	2.7
1	B	301	PHE	2.7
1	A	310	LEU	2.6
1	B	223	SER	2.6
1	B	253	LYS	2.6
1	B	85	ARG	2.6
1	A	271	LEU	2.6
1	B	89	HIS	2.6
1	B	318	HIS	2.6
1	B	419	ASP	2.6
1	B	325	LEU	2.5
1	A	307	VAL	2.5
1	B	271	LEU	2.5
1	A	225	ALA	2.5
1	A	255	VAL	2.4
1	A	354	LEU	2.4
1	A	313	GLY	2.4
1	B	86	LYS	2.4
1	B	229	ARG	2.4
1	A	356	TYR	2.3
1	B	266	LYS	2.3
1	A	321	LEU	2.3
1	A	472	LEU	2.3
1	A	564	TYR	2.3
1	A	558	ALA	2.3
1	A	297	LYS	2.3
1	A	206	VAL	2.3
1	A	276	ASP	2.3
1	B	563	GLN	2.2
1	B	238	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLN	2.2
1	A	263	GLU	2.2
1	A	443	ILE	2.2
1	B	212	SER	2.2
1	B	244	GLN	2.2
1	B	81	ALA	2.2
1	B	209	TYR	2.2
1	A	302	ARG	2.2
1	A	2	ILE	2.1
1	A	565	TRP	2.1
1	B	304	LEU	2.1
1	A	415	PHE	2.1
1	A	467	ARG	2.1
1	A	254	GLY	2.1
1	A	566	GLN	2.1
1	B	270	GLY	2.1
1	A	233	LYS	2.1
1	A	345	ALA	2.1
1	B	263	GLU	2.1
1	B	291	VAL	2.1
1	A	3	PHE	2.1
1	A	247	GLU	2.1
1	B	282	GLY	2.1
1	B	247	GLU	2.0
1	B	242	ILE	2.0
1	B	280	ILE	2.0
1	A	291	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

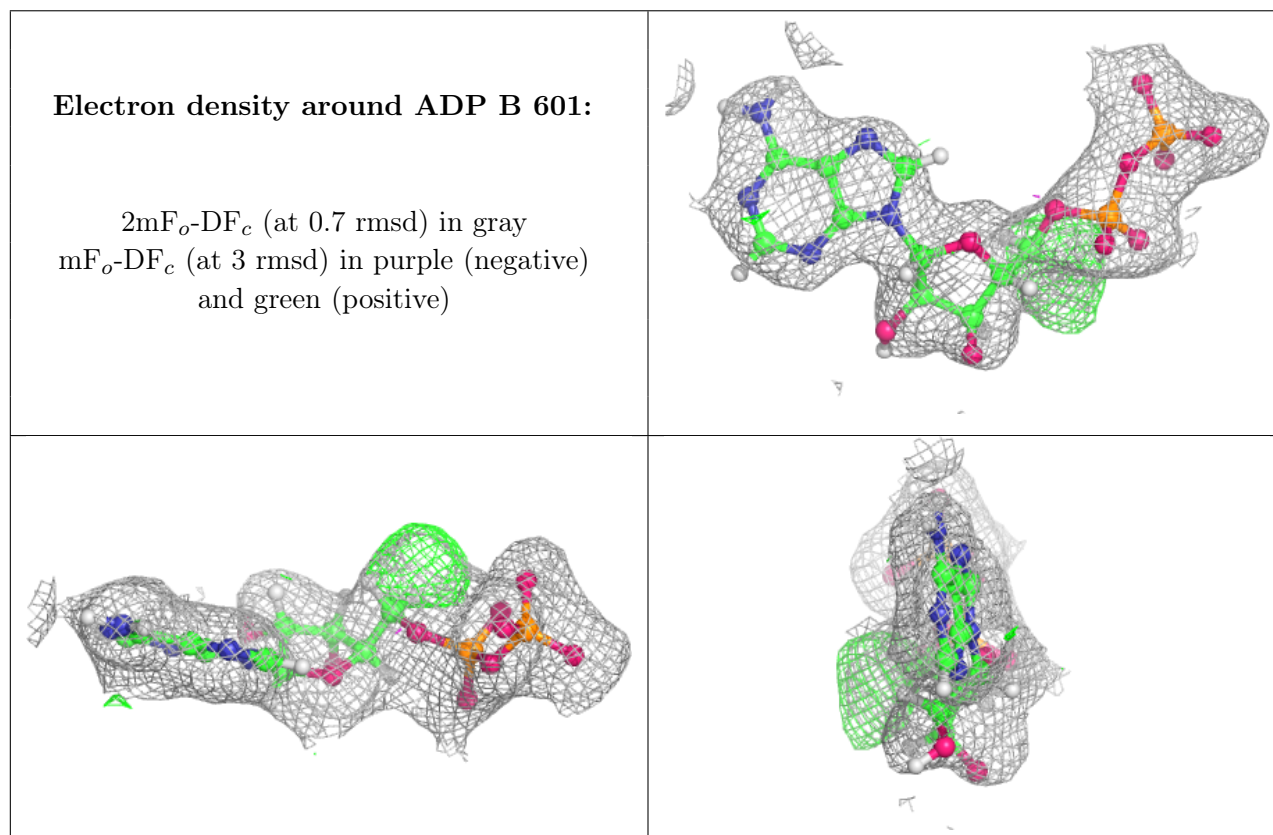## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
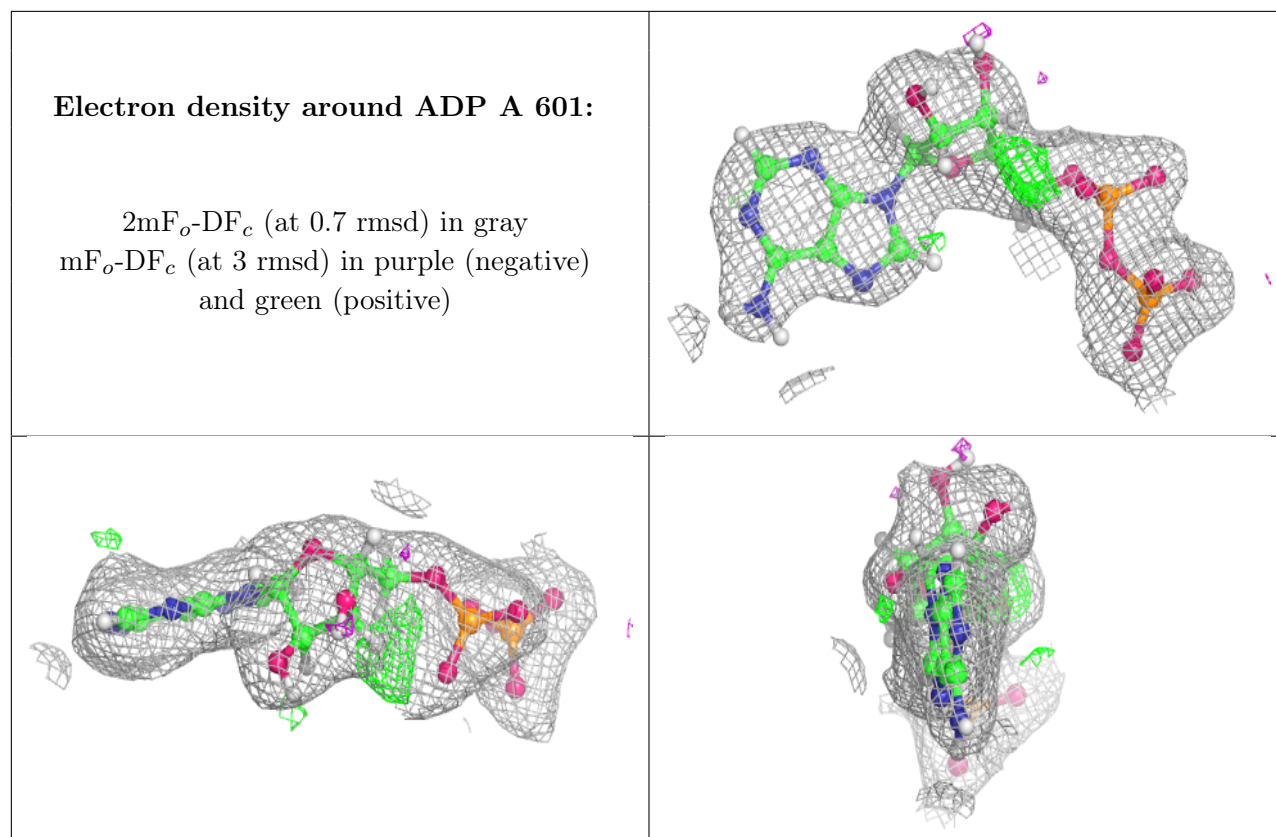
6.4 Ligands ⓘ

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	0.19	46,46,46,46	0
2	ADP	B	601	27/27	0.93	0.15	35,57,73,79	0
4	ZN	B	604	1/1	0.94	0.15	57,57,57,57	0
3	MG	A	602	1/1	0.95	0.12	41,41,41,41	0
2	ADP	A	601	27/27	0.96	0.14	32,51,66,74	0
4	ZN	A	604	1/1	0.97	0.19	44,44,44,44	0
4	ZN	B	603	1/1	0.99	0.17	29,29,29,29	0
4	ZN	A	603	1/1	1.00	0.18	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.

Electron density around ADP B 601:

$2mF_o$-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 A 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.