



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 12:50 AM EDT

PDB ID : 2H39
Title : Crystal Structure of an ADP-Glucose Phosphorylase from Arabidopsis thaliana with bound ADP-Glucose
Authors : McCoy, J.G.; Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2006-05-22
Resolution : 2.23 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
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

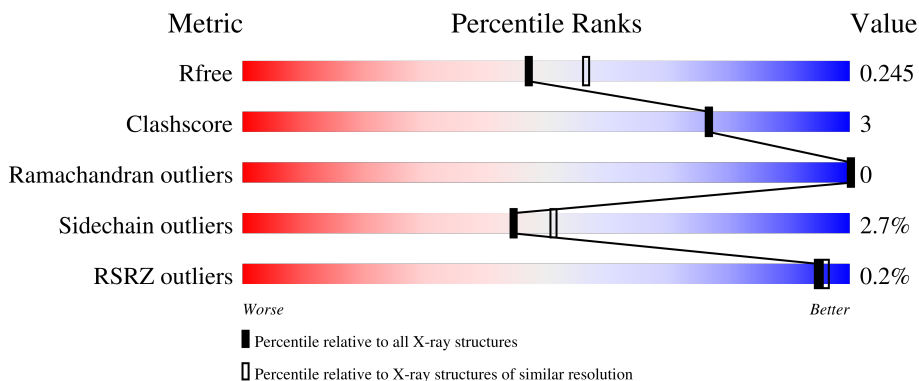
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	351	 77% 11% • 12%
1	B	351	 82% 6% 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5357 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 Probable galactose-1-phosphate uridyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2434	1561	414	446	13	0	0	0
1	B	313	2470	1582	420	455	13	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	HIS	engineered mutation	UNP Q9FK51
B	186	GLY	HIS	engineered mutation	UNP Q9FK51

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: C₁₆H₂₅N₅O₁₅P₂).

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.32Å 95.45Å 110.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.73 – 2.23 47.73 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.73-2.23) 99.9 (47.73-2.23)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.243 0.176 , 0.245	Depositor DCC
R_{free} test set	1639 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: ADQ, ZN, CL

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	0.78	0/2501	0.80	3/3399 (0.1%)
1	B	0.80	0/2538	0.78	3/3450 (0.1%)
All	All	0.79	0/5039	0.79	6/6849 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	41	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	33	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	41	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	147	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	346	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2434	0	2396	20	0
1	B	2470	0	2429	11	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	38	0	23	0	0
4	B	38	0	23	0	0
5	A	184	0	0	2	0
5	B	187	0	0	4	0
All	All	5357	0	4871	30	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 (30) 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:106:GLN:O	1:A:107:SER:HB2	1.99	0.62
1:B:81:PRO:HD3	1:B:88:LYS:HE2	1.82	0.62
1:A:67:ILE:O	5:A:549:HOH:O	2.16	0.60
1:B:182:MET:O	5:B:585:HOH:O	2.17	0.58
1:B:33:ARG:HD2	5:B:514:HOH:O	2.03	0.58
1:A:80:VAL:HB	1:A:89:LEU:HG	1.89	0.55
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.49	0.53
1:A:149:LEU:HD13	1:A:270:LEU:HD23	1.92	0.52
1:A:197:PRO:HD3	5:B:627:HOH:O	2.09	0.52
1:B:153:LYS:HE3	1:B:260:HIS:O	2.10	0.51
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.51	0.50
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.48	0.49
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.95	0.49
1:A:154:LYS:HE2	5:A:634:HOH:O	2.13	0.48
1:A:71:GLN:NE2	1:A:71:GLN:HA	2.29	0.48
1:A:89:LEU:C	1:A:89:LEU:HD12	2.34	0.48
1:B:88:LYS:HB2	1:B:88:LYS:HE3	1.58	0.47
1:A:88:LYS:HE2	1:A:147:ASP:OD1	2.15	0.46
1:A:170:VAL:HG22	1:A:189:MET:HG2	1.98	0.46
1:B:41:ARG:HD3	5:B:544:HOH:O	2.15	0.45
1:B:207:LYS:HE2	1:B:211:GLU:OE1	2.16	0.44
1:B:234:PHE:CE1	1:B:270:LEU:HB2	2.52	0.44
1:A:101:ARG:NH2	1:A:125:ASP:OD1	2.35	0.44
1:A:175:GLY:HA3	1:A:289:PRO:HB3	1.99	0.44
1:A:297:SER:HB2	1:A:309:THR:HG21	1.98	0.44
1:A:153:LYS:HE3	1:A:260:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:O	1:A:93:GLU:HG3	2.19	0.43
1:A:25:LEU:HD12	1:B:120:GLY:HA2	2.01	0.42
1:B:248:ILE:HD12	1:B:281:ILE:HD11	2.02	0.41
1:A:229:ASP:OD2	1:A:277:MET:HE1	2.21	0.41

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	302/351 (86%)	295 (98%)	7 (2%)	0	100	100
1	B	307/351 (88%)	300 (98%)	7 (2%)	0	100	100
All	All	609/702 (87%)	595 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	274/311 (88%)	268 (98%)	6 (2%)	52	59
1	B	279/311 (90%)	270 (97%)	9 (3%)	39	44
All	All	553/622 (89%)	538 (97%)	15 (3%)	44	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	116	ARG
1	A	117	THR
1	A	292	TYR
1	A	297	SER
1	A	318	GLN
1	B	22	SER
1	B	33	ARG
1	B	41	ARG
1	B	69	ARG
1	B	108	THR
1	B	117	THR
1	B	161	GLN
1	B	190	MET
1	B	292	TYR

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	71	GLN
1	A	136	GLN
1	A	157	ASN
1	A	260	HIS
1	B	260	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 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
4	ADQ	A	506	-	35,41,41	0.86	2 (5%)	45,63,63	1.27	4 (8%)
4	ADQ	B	507	-	35,41,41	0.85	1 (2%)	45,63,63	1.23	5 (11%)

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
4	ADQ	A	506	-	-	9/19/59/59	0/4/4/4
4	ADQ	B	507	-	-	7/19/59/59	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	ADQ	O4D-C1D	3.20	1.45	1.41
4	B	507	ADQ	O4D-C1D	2.10	1.44	1.41
4	A	506	ADQ	C2-N3	2.10	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	ADQ	N3-C2-N1	-4.69	121.34	128.68
4	B	507	ADQ	N3-C2-N1	-3.72	122.86	128.68
4	A	506	ADQ	O5'-C5'-C4'	2.61	114.44	109.69
4	A	506	ADQ	C2D-C3D-C4D	2.59	107.68	102.64
4	B	507	ADQ	C1D-N9-C4	-2.43	122.37	126.64
4	B	507	ADQ	C4'-C3'-C2'	-2.34	106.74	110.82
4	B	507	ADQ	O4D-C1D-C2D	-2.23	103.67	106.93
4	B	507	ADQ	PA-O3A-PB	-2.12	125.55	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	ADQ	C4'-C3'-C2'	-2.07	107.21	110.82

There are no chirality outliers.

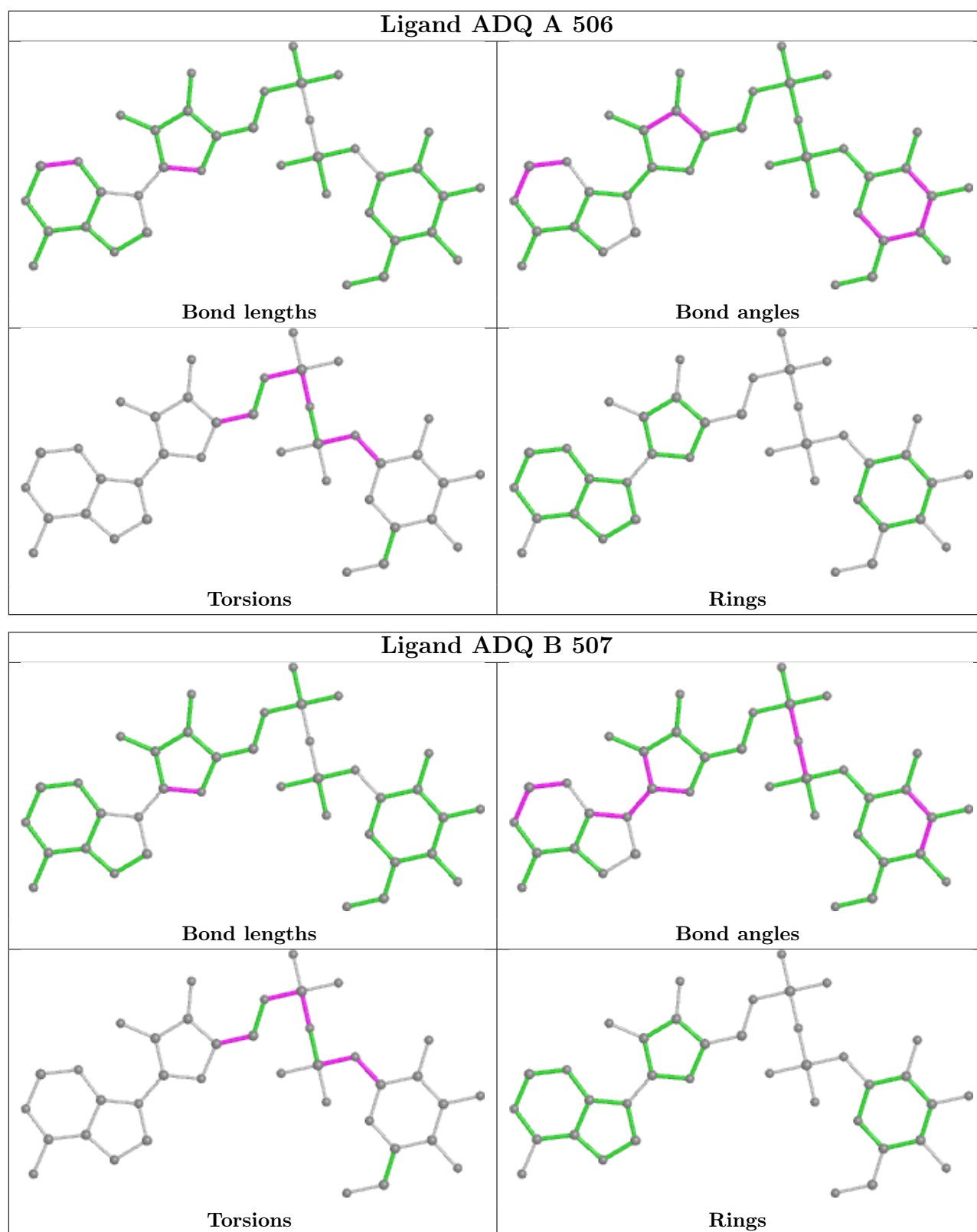
All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	ADQ	PB-O3A-PA-O5D
4	A	506	ADQ	C5D-O5D-PA-O1A
4	B	507	ADQ	C5D-O5D-PA-O1A
4	B	507	ADQ	C5D-O5D-PA-O2A
4	A	506	ADQ	C1'-O3B-PB-O3A
4	A	506	ADQ	C2'-C1'-O3B-PB
4	B	507	ADQ	C2'-C1'-O3B-PB
4	B	507	ADQ	C1'-O3B-PB-O3A
4	A	506	ADQ	O4D-C4D-C5D-O5D
4	B	507	ADQ	PB-O3A-PA-O5D
4	A	506	ADQ	C5D-O5D-PA-O3A
4	A	506	ADQ	C5D-O5D-PA-O2A
4	A	506	ADQ	C3D-C4D-C5D-O5D
4	B	507	ADQ	C5D-O5D-PA-O3A
4	A	506	ADQ	PB-O3A-PA-O2A
4	B	507	ADQ	O4D-C4D-C5D-O5D

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

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	308/351 (87%)	-0.62	0 100 100	6, 17, 34, 52	1 (0%)
1	B	313/351 (89%)	-0.66	1 (0%) 94 94	7, 16, 33, 55	1 (0%)
All	All	621/702 (88%)	-0.64	1 (0%) 95 96	6, 17, 34, 55	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	HIS	2.7

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 monosaccharides 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.

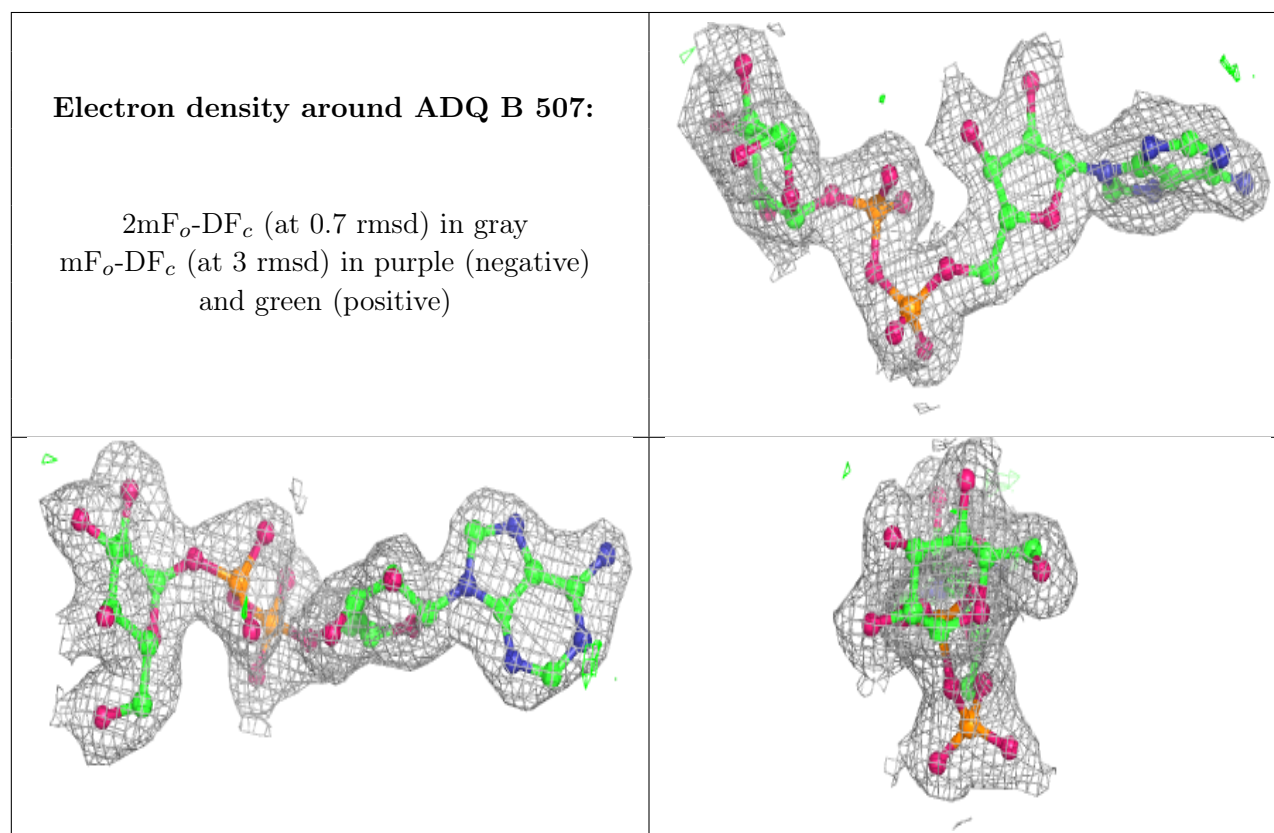
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	352	1/1	0.96	0.06	37,37,37,37	0
4	ADQ	B	507	38/38	0.96	0.10	6,16,22,24	0
4	ADQ	A	506	38/38	0.98	0.08	7,16,19,19	0
2	ZN	B	352	1/1	0.99	0.06	26,26,26,26	0

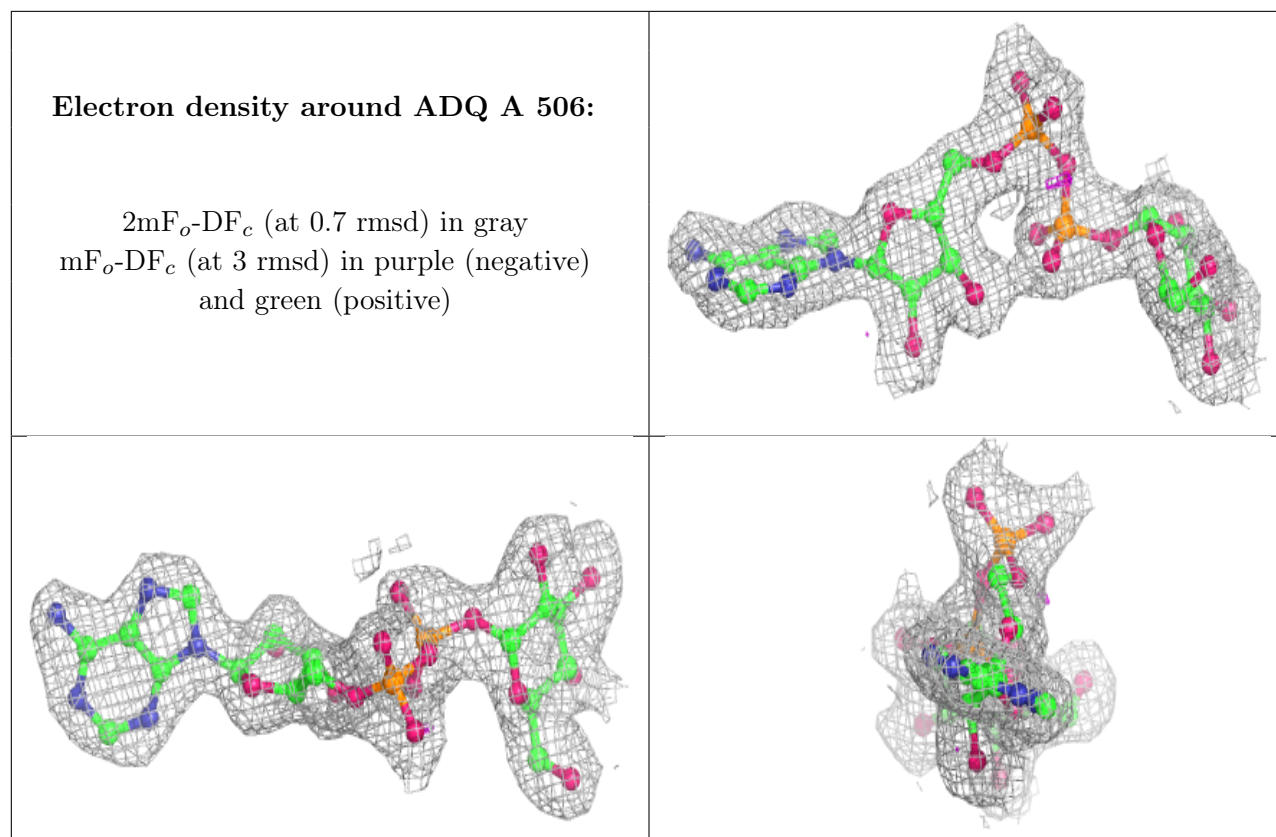
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	402	1/1	0.99	0.04	15,15,15,15	0
3	CL	B	401	1/1	1.00	0.06	13,13,13,13	0
2	ZN	B	353	1/1	1.00	0.05	16,16,16,16	0
2	ZN	A	353	1/1	1.00	0.04	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.