



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 4PJ3 / pdb_00004pj3
Title : Structural insight into the function and evolution of the spliceosomal helicase Aquarius, Structure of Aquarius in complex with AMPPNP
Authors : De, I.; Bessonov, S.; Hofele, R.; dos Santos, K.F.; Will, C.L.; Urlaub, H.; Luhrmann, R.; Pena, V.
Deposited on : 2014-05-11
Resolution : 2.30 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

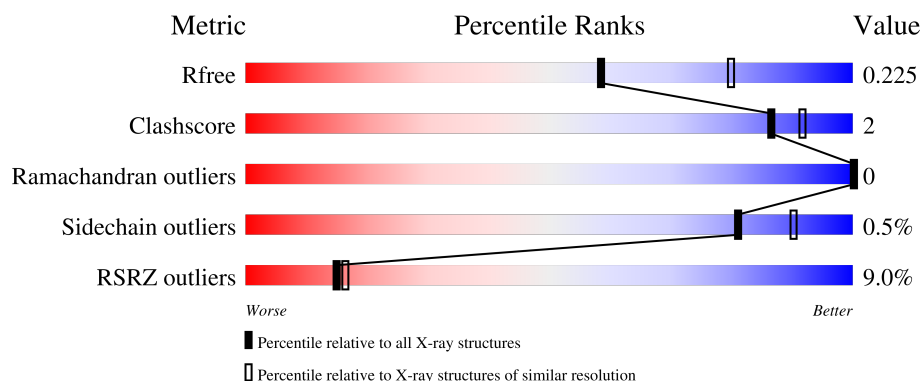
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1475	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11598 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.

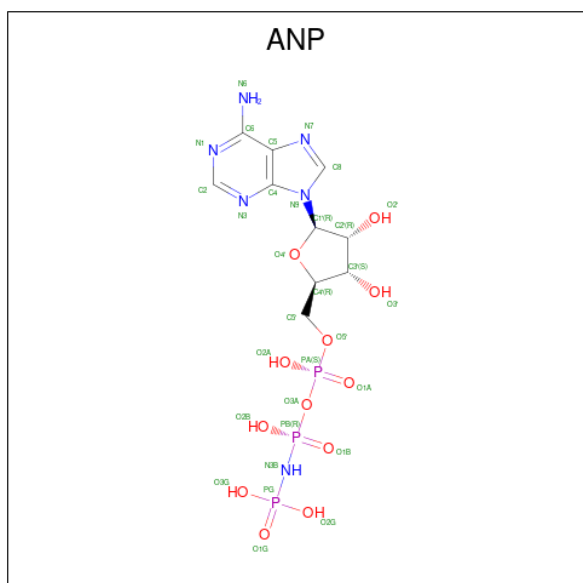
- Molecule 1 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1335	11010	7073	1895	1986	18	38	211	6	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1486	HIS	-	expression tag	UNP O60306
A	1487	HIS	-	expression tag	UNP O60306
A	1488	HIS	-	expression tag	UNP O60306
A	1489	HIS	-	expression tag	UNP O60306
A	1490	HIS	-	expression tag	UNP O60306
A	1491	HIS	-	expression tag	UNP O60306
A	1492	HIS	-	expression tag	UNP O60306
A	1493	HIS	-	expression tag	UNP O60306

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	555	Total	O	0	0
			555	555		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.99Å 140.44Å 144.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.30 47.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.49-2.30) 96.5 (47.49-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.191 , 0.226 0.193 , 0.225	Depositor DCC
R_{free} test set	7468 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11598	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MG, ANP

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	0.29	0/11256	0.69	1/15185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1379	TYR	N-CA-C	7.66	122.72	112.30

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	11010	0	10974	45	0
2	A	31	0	13	0	0
3	A	2	0	0	0	0
4	A	555	0	0	0	0
All	All	11598	0	10987	45	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 2.

All (45) 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:1059:ILE:HG13	1:A:1088:LEU:HD11	1.72	0.71
1:A:323:GLU:HA	1:A:326[A]:MSE:HE3	1.75	0.67
1:A:362:ARG:NH2	1:A:405:GLU:OE1	2.35	0.58
1:A:867:MSE:HE1	1:A:889:GLU:HB3	1.86	0.58
1:A:204:ASP:HA	1:A:207:MSE:HE2	1.87	0.56
1:A:571:LYS:HD2	1:A:586:GLN:O	2.07	0.55
1:A:913:LYS:HD2	1:A:917:LYS:HE2	1.90	0.54
1:A:673:ILE:HG22	1:A:677:MSE:HE2	1.90	0.53
1:A:1027:LEU:HA	1:A:1031:GLU:HB3	1.90	0.53
1:A:814:MSE:SE	1:A:839:ASN:HD22	2.43	0.52
1:A:225:LEU:HG	1:A:253:PHE:HE1	1.74	0.51
1:A:19:ASN:HB3	1:A:22:PHE:HB3	1.94	0.50
1:A:204:ASP:O	1:A:212:ARG:NH1	2.45	0.50
1:A:748:ARG:NH1	1:A:780:GLU:OE1	2.43	0.48
1:A:830:THR:HG22	1:A:865:LYS:HD2	1.94	0.48
1:A:1355:ILE:HG21	1:A:1361:MSE:HB2	1.96	0.48
1:A:1237:ILE:O	1:A:1241:ILE:HG12	2.14	0.47
1:A:790:TYR:OH	1:A:976:ASN:ND2	2.47	0.47
1:A:790:TYR:HB3	1:A:792:TYR:CE2	2.51	0.46
1:A:509:ARG:HG3	1:A:549:ILE:HD12	1.97	0.46
1:A:444:TYR:CZ	1:A:446:GLY:HA2	2.51	0.45
1:A:987:TYR:CZ	1:A:991:MSE:HE3	2.51	0.45
1:A:1220:PRO:HD3	1:A:1338:PHE:CE2	2.52	0.45
1:A:1284:LEU:HD23	1:A:1310:PHE:CE1	2.51	0.45
1:A:362:ARG:HH22	1:A:405:GLU:CD	2.24	0.45
1:A:1208:VAL:HG13	1:A:1241:ILE:HD13	2.00	0.44
1:A:1021:LEU:HD22	1:A:1021:LEU:HA	1.85	0.43
1:A:987:TYR:CE1	1:A:991:MSE:HE3	2.53	0.43
1:A:61:ILE:O	1:A:65:MSE:HG3	2.19	0.43
1:A:941:MSE:SE	1:A:998:PHE:HZ	2.52	0.43
1:A:163:ARG:O	1:A:167:GLN:HG2	2.19	0.42
1:A:1358:MSE:HB3	1:A:1359:PRO:HD3	2.01	0.42
1:A:173:PRO:HG3	1:A:200:ILE:HD13	2.01	0.42
1:A:961:VAL:HG12	1:A:987:TYR:N	2.34	0.42
1:A:565:ILE:HB	1:A:655:ILE:HB	2.02	0.42
1:A:21:GLU:H	1:A:21:GLU:CD	2.28	0.41
1:A:1248:ASN:HA	1:A:1249:PRO:HD3	1.90	0.41
1:A:676:LEU:HD23	1:A:676:LEU:HA	1.96	0.41
1:A:902:LEU:O	1:A:906:ILE:HG12	2.21	0.41
1:A:109:TRP:CD2	1:A:162:ILE:HD11	2.56	0.41
1:A:735:VAL:HG11	1:A:743:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD12	1:A:140:LEU:HA	1.87	0.40
1:A:1138:ARG:NE	1:A:1267:GLN:OE1	2.48	0.40
1:A:748:ARG:HG3	1:A:782:HIS:CD2	2.57	0.40

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	1333/1475 (90%)	1308 (98%)	25 (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	1217/1292 (94%)	1211 (100%)	6 (0%)	81	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	84	GLU
1	A	881	HIS

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Mol	Chain	Res	Type
1	A	960	ASP
1	A	986	SER
1	A	1021	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	125	HIS
1	A	165	GLN
1	A	542	ASN
1	A	1007	GLN
1	A	1082	GLN
1	A	1255	ASN
1	A	1311	GLN
1	A	1380	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	ANP	A	1501	-	33,33,33	1.85	11 (33%)	45,52,52	2.08	15 (33%)

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	ANP	A	1501	-	-	5/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	ANP	C6-N6	4.61	1.46	1.34
2	A	1501	ANP	C4-N3	3.25	1.40	1.34
2	A	1501	ANP	PG-O1G	3.09	1.50	1.46
2	A	1501	ANP	C2'-C3'	-2.82	1.45	1.53
2	A	1501	ANP	PB-O1B	2.81	1.50	1.46
2	A	1501	ANP	PG-O2G	-2.60	1.49	1.56
2	A	1501	ANP	PB-O2B	-2.49	1.50	1.56
2	A	1501	ANP	C3'-C4'	-2.19	1.47	1.53
2	A	1501	ANP	C8-N7	2.16	1.35	1.31
2	A	1501	ANP	O2'-C2'	-2.13	1.37	1.43
2	A	1501	ANP	O3'-C3'	-2.03	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	ANP	C5-C4-N3	-4.97	119.87	126.72
2	A	1501	ANP	O2G-PG-O1G	-4.85	101.28	113.45
2	A	1501	ANP	N3-C2-N1	-4.31	122.05	128.58
2	A	1501	ANP	N3-C4-N9	3.72	133.50	127.17
2	A	1501	ANP	O2B-PB-O1B	-3.68	101.98	109.87
2	A	1501	ANP	N9-C8-N7	-3.40	109.12	113.94
2	A	1501	ANP	C2-N3-C4	3.29	119.86	111.83
2	A	1501	ANP	C5-N7-C8	2.95	108.09	103.45
2	A	1501	ANP	C4-N9-C8	2.86	108.74	105.74
2	A	1501	ANP	C4-C5-N7	-2.76	107.42	110.58
2	A	1501	ANP	O2A-PA-O1A	-2.55	100.60	112.44
2	A	1501	ANP	O3A-PB-N3B	2.51	113.56	106.59
2	A	1501	ANP	O2A-PA-O3A	2.26	113.38	107.27
2	A	1501	ANP	O5'-C5'-C4'	2.15	116.30	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	ANP	O4'-C1'-N9	2.01	111.96	108.09

There are no chirality outliers.

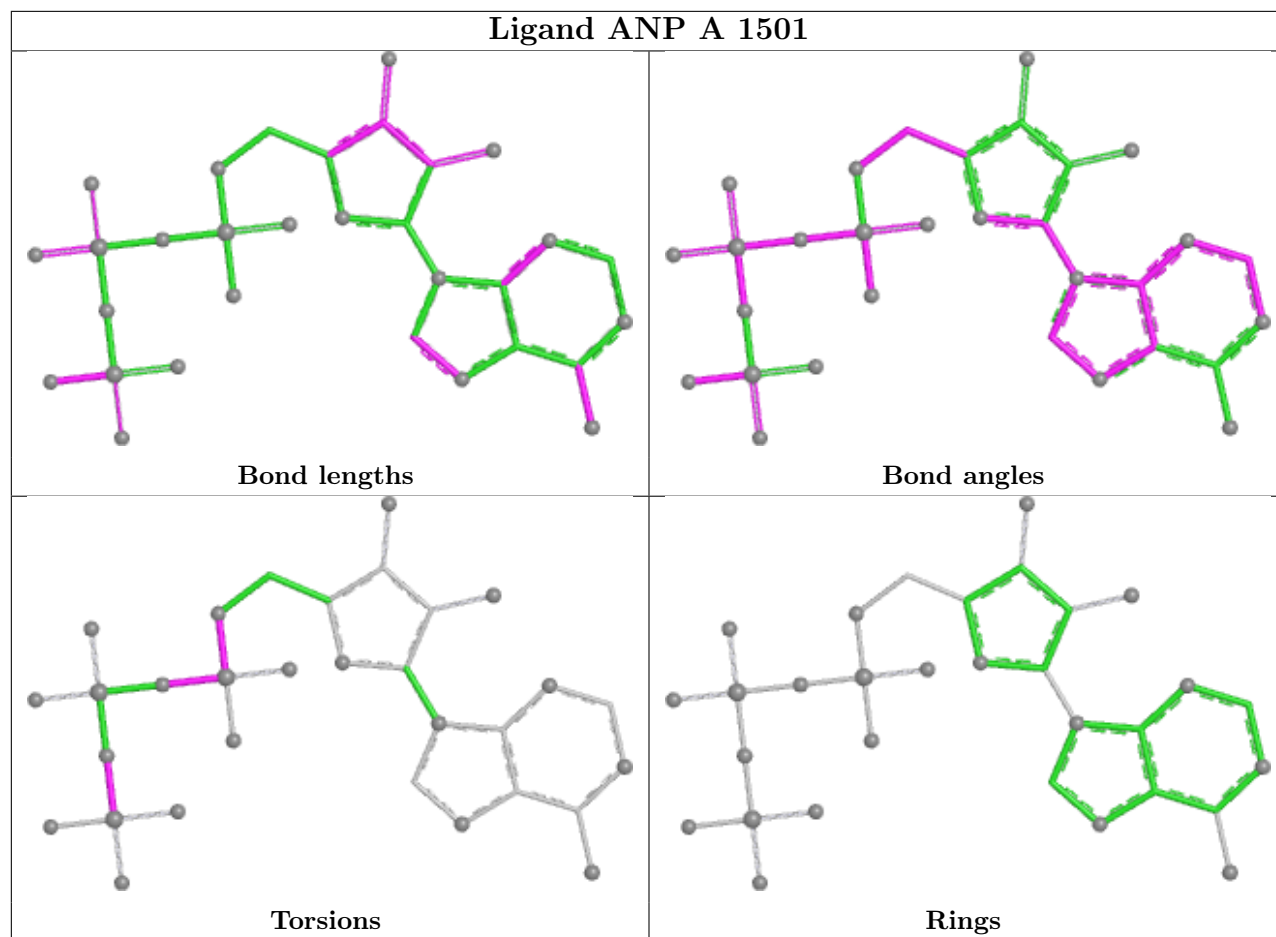
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	ANP	PB-N3B-PG-O1G
2	A	1501	ANP	C5'-O5'-PA-O1A
2	A	1501	ANP	C5'-O5'-PA-O2A
2	A	1501	ANP	C5'-O5'-PA-O3A
2	A	1501	ANP	PB-O3A-PA-O2A

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	1295/1475 (87%)	0.28	117 (9%)	15 16	9, 31, 66, 107	34 (2%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	HIS	8.0
1	A	738	GLU	6.9
1	A	1239	ASP	6.8
1	A	1380	HIS	6.5
1	A	614	PRO	6.3
1	A	293	GLU	5.9
1	A	546	ARG	5.6
1	A	959	PRO	5.5
1	A	1381	GLN	5.5
1	A	500	GLY	4.9
1	A	753	VAL	4.9
1	A	1246	GLY	4.9
1	A	507	TRP	4.8
1	A	1376	THR	4.7
1	A	210	GLU	4.5
1	A	547	ASP	4.5
1	A	34	HIS	4.5
1	A	1378	HIS	4.4
1	A	960	ASP	4.4
1	A	1231	ASN	4.4
1	A	1105	LYS	4.3
1	A	1373	ILE	4.3
1	A	292	GLU	4.2
1	A	1374	GLN	4.1
1	A	792	TYR	4.0
1	A	1379	TYR	4.0
1	A	1152	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1195	PRO	3.9
1	A	527	ILE	3.8
1	A	531	TRP	3.8
1	A	1247	ASN	3.8
1	A	20	ALA	3.7
1	A	619	ARG	3.7
1	A	36	LYS	3.7
1	A	618	LEU	3.7
1	A	1188	VAL	3.6
1	A	774	ALA	3.6
1	A	1377	HIS	3.5
1	A	1196	TYR	3.5
1	A	528	GLY	3.5
1	A	498	GLU	3.5
1	A	133	GLU	3.5
1	A	443	TYR	3.4
1	A	1243	ARG	3.4
1	A	609	GLU	3.2
1	A	19	ASN	3.2
1	A	1369	TYR	3.2
1	A	392	LYS	3.2
1	A	35	ILE	3.2
1	A	1262	ARG	3.1
1	A	22	PHE	3.1
1	A	1245	CYS	3.1
1	A	1018	ARG	3.1
1	A	734	LYS	3.1
1	A	1356	LYS	3.0
1	A	1189	GLY	3.0
1	A	773	GLU	2.9
1	A	1187	GLY	2.8
1	A	1366	TYR	2.8
1	A	1055	LYS	2.8
1	A	549	ILE	2.8
1	A	1240	ILE	2.7
1	A	1253	ARG	2.7
1	A	682	VAL	2.7
1	A	1375	THR	2.7
1	A	576	LYS	2.7
1	A	544	ASN	2.7
1	A	884	GLU	2.7
1	A	1372	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1171	ALA	2.6
1	A	1185	PHE	2.6
1	A	739	ASP	2.6
1	A	414	ARG	2.6
1	A	953	ASN	2.6
1	A	1236	LEU	2.6
1	A	976	ASN	2.6
1	A	1197	PHE	2.6
1	A	524	LYS	2.5
1	A	33	PRO	2.5
1	A	791	PRO	2.5
1	A	1345	GLY	2.5
1	A	1251	ILE	2.5
1	A	1359	PRO	2.5
1	A	530	ASN	2.4
1	A	615	ARG	2.4
1	A	1249	PRO	2.4
1	A	616	PRO	2.4
1	A	1248	ASN	2.3
1	A	1250	LEU	2.3
1	A	211	ALA	2.3
1	A	1201	LEU	2.3
1	A	617	ASN	2.3
1	A	895	TYR	2.3
1	A	1280	ALA	2.3
1	A	1085	PHE	2.3
1	A	192	LYS	2.3
1	A	680	ASP	2.2
1	A	209	PRO	2.2
1	A	1312	ASN	2.2
1	A	1348	PRO	2.2
1	A	1354	ILE	2.2
1	A	1344	ASN	2.2
1	A	525	PRO	2.2
1	A	620	GLY	2.2
1	A	1349	SER	2.2
1	A	880	GLY	2.1
1	A	23	VAL	2.1
1	A	1186	GLN	2.1
1	A	1019	SER	2.1
1	A	501	GLY	2.1
1	A	962	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	2.0
1	A	1355	ILE	2.0
1	A	1193	PRO	2.0
1	A	725	LYS	2.0
1	A	621	GLU	2.0
1	A	393	ASN	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](#)

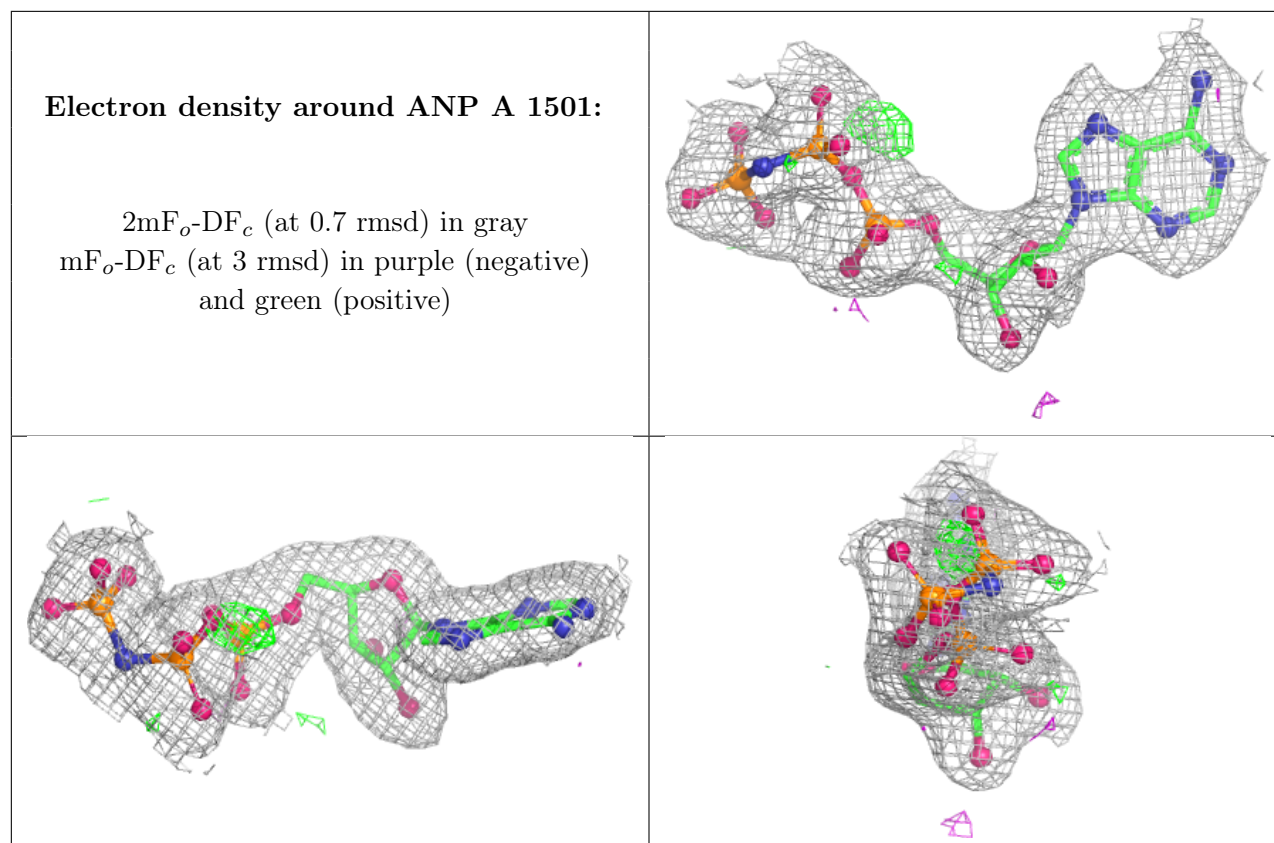
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	MG	A	1503	1/1	0.91	0.46	66,66,66,66	0
3	MG	A	1502	1/1	0.93	0.09	47,47,47,47	0
2	ANP	A	1501	31/31	0.96	0.07	22,29,39,42	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.