



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:43 AM UTC

PDB ID : 5EAN / pdb_00005ean
Title : Crystal structure of Dna2 in complex with a 5' overhang DNA
Authors : Zhou, C.; Pourmal, S.; Pavletich, N.P.
Deposited on : 2015-10-16
Resolution : 2.36 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

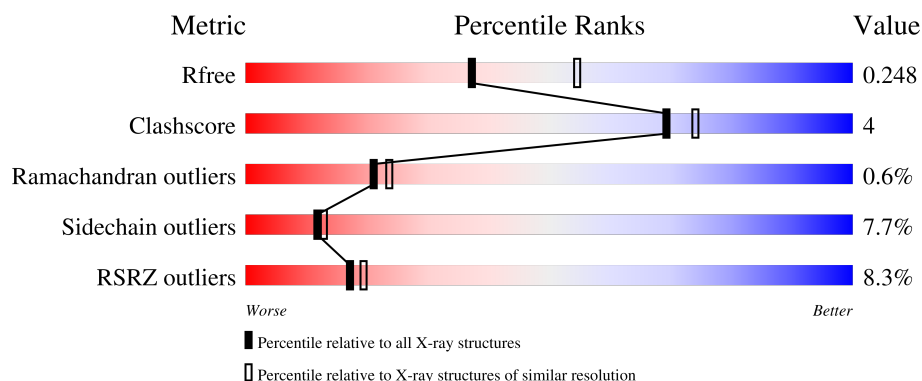
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	1059	
2	B	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8652 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 DNA replication ATP-dependent helicase/nuclease DNA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1051	Total	C	N	O	S	0	0	0
			8302	5239	1464	1554	45			

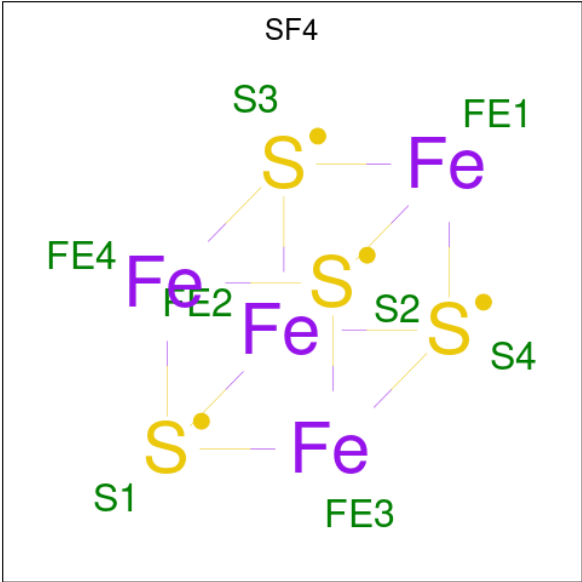
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q6ZQJ5
A	-1	GLY	-	expression tag	UNP Q6ZQJ5
A	0	HIS	-	expression tag	UNP Q6ZQJ5

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*TP*CP*TP*GP*CP*CP*AP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			309	146	61	87	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

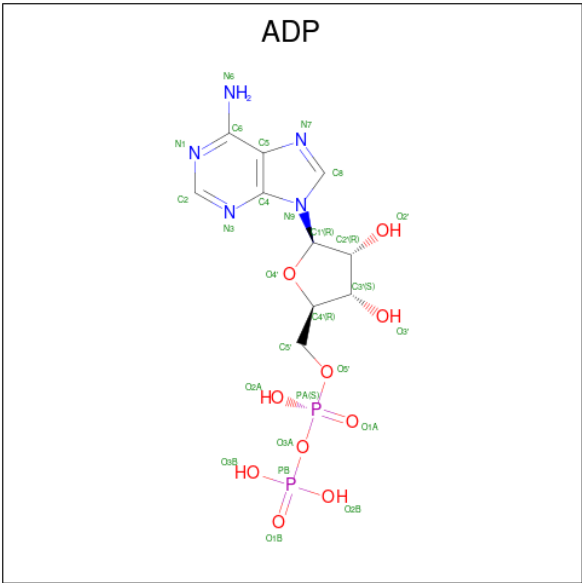


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

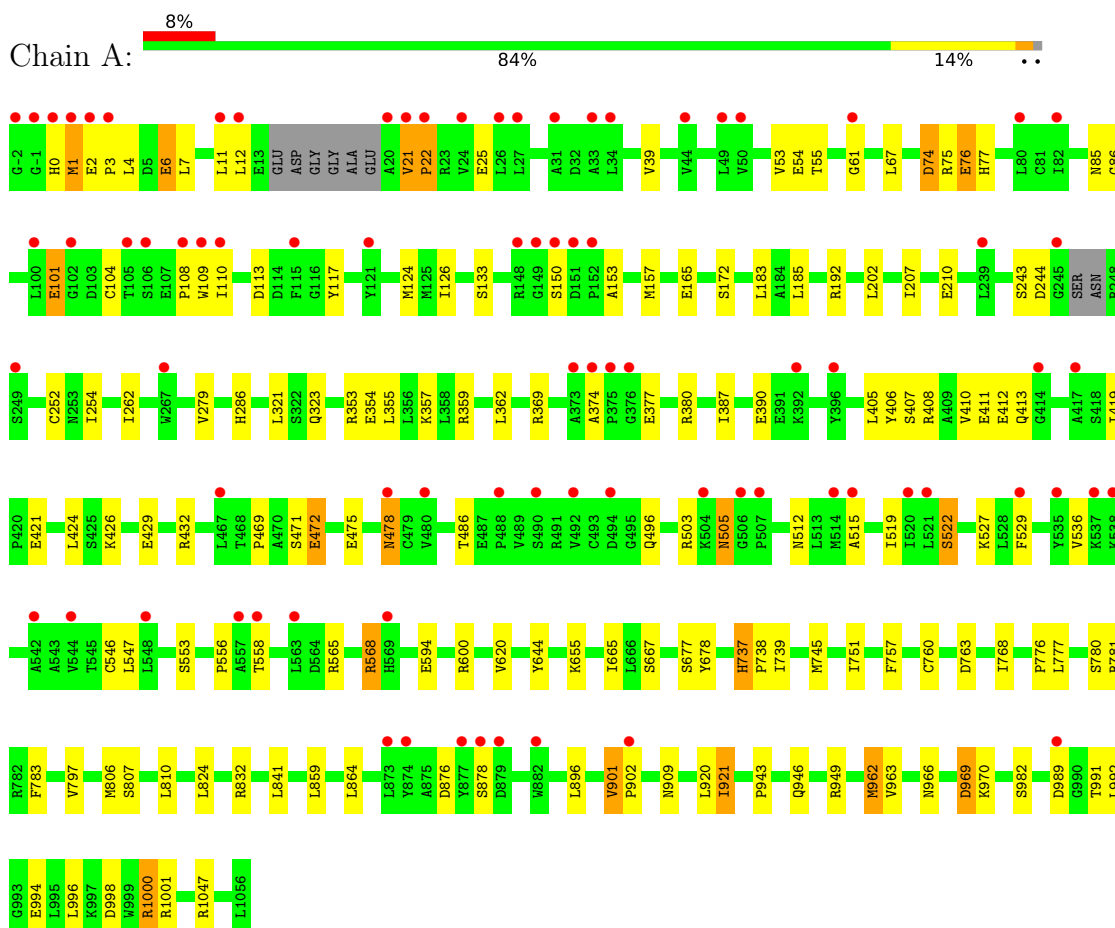
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	2	Total	O	0	0
			2	2		

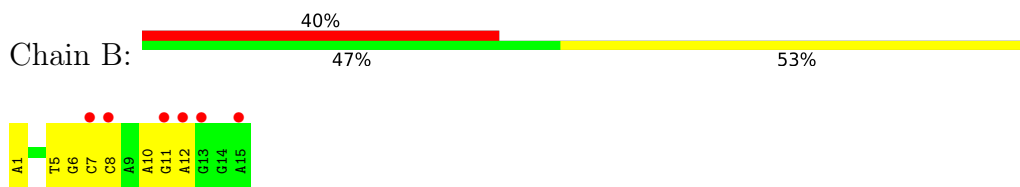
3 Residue-property plots

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: DNA replication ATP-dependent helicase/nuclease DNA2



- Molecule 2: DNA (5'-D(P*AP*CP*TP*CP*TP*GP*CP*CP*AP*AP*GP*AP*GP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	87.15Å 118.49Å 149.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.36 50.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.36) 92.6 (50.00-2.36)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.208 , 0.246 0.212 , 0.248	Depositor DCC
R_{free} test set	1918 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	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	8652	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: CA, SF4, ADP

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	0.72	0/8454	1.04	8/11432 (0.1%)
2	B	0.35	0/347	0.76	0/533
All	All	0.71	0/8801	1.03	8/11965 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	901	VAL	CA-C-N	-5.96	113.07	119.98
1	A	901	VAL	C-N-CA	-5.96	113.07	119.98
1	A	737	HIS	CA-C-N	5.73	125.41	119.56
1	A	737	HIS	C-N-CA	5.73	125.41	119.56
1	A	243	SER	N-CA-C	5.70	120.10	113.20
1	A	966	ASN	N-CA-C	5.60	117.36	108.79
1	A	909	ASN	N-CA-C	5.13	118.80	112.24
1	A	806	MET	N-CA-C	5.02	118.51	112.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLU	Peptide

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	8302	0	8436	57	0
2	B	309	0	168	8	0
3	A	8	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	27	0	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	8652	0	8616	61	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 4.

All (61) 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)
2:B:10:DA:H1'	2:B:11:DG:H5''	1.67	0.76
1:A:745:MET:HG3	2:B:6:DG:H2''	1.71	0.71
1:A:3:PRO:HD2	1:A:6:GLU:OE1	1.95	0.66
1:A:678:TYR:HB2	1:A:768:ILE:HG12	1.80	0.63
1:A:620:VAL:HG13	1:A:665:ILE:HG12	1.83	0.59
1:A:989:ASP:OD1	1:A:991:THR:HG22	2.03	0.59
1:A:74:ASP:HB3	1:A:76:GLU:HG2	1.85	0.59
1:A:1:MET:SD	1:A:1:MET:N	2.75	0.54
2:B:11:DG:H4'	2:B:12:DA:OP1	2.07	0.54
1:A:85:ASN:HD22	1:A:113:ASP:H	1.55	0.53
1:A:969:ASP:OD1	1:A:969:ASP:N	2.40	0.53
1:A:998:ASP:OD1	1:A:1000:ARG:HD3	2.09	0.53
1:A:568:ARG:HD3	2:B:5:DT:O4	2.10	0.52
1:A:101:GLU:HB2	1:A:117:TYR:HB2	1.92	0.51
1:A:252:CYS:HB2	1:A:286:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:SER:HB3	1:A:763:ASP:HB3	1.93	0.50
1:A:387:ILE:HB	1:A:419:ILE:HD12	1.94	0.50
1:A:472:GLU:O	1:A:475:GLU:HG2	2.12	0.50
1:A:429:GLU:HA	1:A:432:ARG:HD3	1.95	0.48
1:A:469:PRO:HB2	1:A:471:SER:HB3	1.94	0.48
1:A:644:TYR:HA	1:A:783:PHE:O	2.14	0.47
1:A:970:LYS:HA	1:A:970:LYS:HE2	1.96	0.47
1:A:21:VAL:N	1:A:22:PRO:HD2	2.30	0.47
1:A:53:VAL:HG22	1:A:67:LEU:HD22	1.97	0.47
1:A:374:ALA:HB3	1:A:377:GLU:HG3	1.97	0.47
1:A:594:GLU:OE1	1:A:600:ARG:NH1	2.46	0.47
1:A:104:CYS:HB3	1:A:109:TRP:CG	2.50	0.46
1:A:408:ARG:HA	1:A:412:GLU:HG2	1.97	0.46
1:A:407:SER:HA	1:A:411:GLU:HG2	1.96	0.46
1:A:522:SER:HB3	1:A:529:PHE:HA	1.98	0.45
1:A:126:ILE:HG21	1:A:362:LEU:HD23	1.99	0.45
1:A:921:ILE:HD12	1:A:982:SER:HB2	1.98	0.45
1:A:153:ALA:HA	1:A:157:MET:HE2	1.97	0.45
1:A:902:PRO:HG2	1:A:1047:ARG:HH11	1.82	0.45
1:A:667:SER:HB2	1:A:739:ILE:HD11	1.97	0.45
1:A:946:GLN:HG3	1:A:949:ARG:HH12	1.81	0.45
1:A:760:CYS:SG	1:A:776:PRO:HB2	2.57	0.44
1:A:994:GLU:CG	2:B:1:DA:H5''	2.48	0.43
1:A:478:ASN:HB3	1:A:565:ARG:NH1	2.33	0.43
1:A:515:ALA:HA	1:A:536:VAL:HG13	2.00	0.43
1:A:165:GLU:CD	1:A:192:ARG:HH21	2.26	0.43
1:A:503:ARG:HE	1:A:503:ARG:HB3	1.61	0.43
1:A:353:ARG:NH1	1:A:354:GLU:OE2	2.52	0.43
1:A:202:LEU:HD13	1:A:207:ILE:HD11	2.00	0.43
1:A:556:PRO:HB2	1:A:558:THR:HG22	2.00	0.43
1:A:1:MET:HA	1:A:6:GLU:HG2	2.00	0.42
1:A:369:ARG:NH2	1:A:406:TYR:OH	2.51	0.42
1:A:478:ASN:HB3	1:A:565:ARG:HH12	1.84	0.42
1:A:757:PHE:O	1:A:780:SER:HA	2.18	0.42
1:A:876:ASP:OD1	1:A:878:SER:HB3	2.20	0.42
1:A:943:PRO:HD2	1:A:982:SER:O	2.20	0.42
2:B:11:DG:C4'	2:B:12:DA:OP1	2.67	0.42
1:A:496:GLN:HB3	1:A:547:LEU:HD22	2.00	0.41
2:B:7:DC:H3'	2:B:8:DC:H5''	2.01	0.41
1:A:85:ASN:ND2	1:A:113:ASP:H	2.18	0.41
1:A:124:MET:HE2	1:A:126:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:O	1:A:412:GLU:C	2.64	0.41
1:A:962:MET:SD	1:A:962:MET:N	2.87	0.41
1:A:86:GLY:HA3	1:A:357:LYS:NZ	2.36	0.40
1:A:737:HIS:HA	1:A:738:PRO:HD3	1.87	0.40
1:A:994:GLU:HG3	2:B:1:DA:H5''	2.02	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	1045/1059 (99%)	1004 (96%)	35 (3%)	6 (1%)	21 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	GLY
1	A	22	PRO
1	A	505	ASN
1	A	568	ARG
1	A	2	GLU
1	A	108	PRO

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	933/938 (100%)	861 (92%)	72 (8%)	12	13

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	A	4	LEU
1	A	6	GLU
1	A	7	LEU
1	A	11	LEU
1	A	12	LEU
1	A	21	VAL
1	A	25	GLU
1	A	39	VAL
1	A	54	GLU
1	A	55	THR
1	A	74	ASP
1	A	75	ARG
1	A	76	GLU
1	A	77	HIS
1	A	110	ILE
1	A	133	SER
1	A	150	SER
1	A	172	SER
1	A	183	LEU
1	A	185	LEU
1	A	210	GLU
1	A	244	ASP
1	A	254	ILE
1	A	262	ILE
1	A	279	VAL
1	A	321	LEU
1	A	323	GLN
1	A	355	LEU
1	A	359	ARG
1	A	380	ARG
1	A	390	GLU
1	A	405	LEU
1	A	410	VAL
1	A	413	GLN
1	A	421	GLU
1	A	424	LEU

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Mol	Chain	Res	Type
1	A	426	LYS
1	A	472	GLU
1	A	478	ASN
1	A	486	THR
1	A	505	ASN
1	A	512	ASN
1	A	519	ILE
1	A	522	SER
1	A	527	LYS
1	A	546	CYS
1	A	553	SER
1	A	655	LYS
1	A	751	ILE
1	A	777	LEU
1	A	781	ARG
1	A	797	VAL
1	A	807	SER
1	A	810	LEU
1	A	824	LEU
1	A	832	ARG
1	A	841	LEU
1	A	859	LEU
1	A	864	LEU
1	A	896	LEU
1	A	901	VAL
1	A	920	LEU
1	A	921	ILE
1	A	962	MET
1	A	963	VAL
1	A	969	ASP
1	A	992	LEU
1	A	996	LEU
1	A	1000	ARG
1	A	1001	ARG

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	57	GLN
1	A	58	ASN
1	A	85	ASN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	413	GLN
1	A	482	ASN
1	A	500	ASN
1	A	505	ASN
1	A	633	GLN
1	A	729	HIS
1	A	770	GLN
1	A	817	ASN
1	A	823	GLN
1	A	946	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
3	SF4	A	1101	1	0,12,12	-	-	-		
5	ADP	A	1103	-	28,29,29	1.56	5 (17%)	43,45,45	1.79	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
3	SF4	A	1101	1	-	-	0/6/5/5
5	ADP	A	1103	-	-	4/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	ADP	C5-C4	5.35	1.48	1.39
5	A	1103	ADP	C5-C6	3.06	1.49	1.41
5	A	1103	ADP	C8-N7	2.57	1.36	1.31
5	A	1103	ADP	PA-O3A	2.17	1.61	1.59
5	A	1103	ADP	C5-N7	-2.09	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	ADP	C5-C4-N3	-5.42	119.26	126.72
5	A	1103	ADP	N3-C4-N9	4.25	134.40	127.17
5	A	1103	ADP	C2-N3-C4	3.91	121.38	111.83
5	A	1103	ADP	N3-C2-N1	-3.67	123.03	128.58
5	A	1103	ADP	C4-C5-N7	-3.05	107.10	110.58
5	A	1103	ADP	C6-C5-N7	2.39	136.70	132.09
5	A	1103	ADP	C2'-C3'-C4'	2.29	107.04	102.61
5	A	1103	ADP	C4-N9-C8	2.15	108.00	105.74
5	A	1103	ADP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

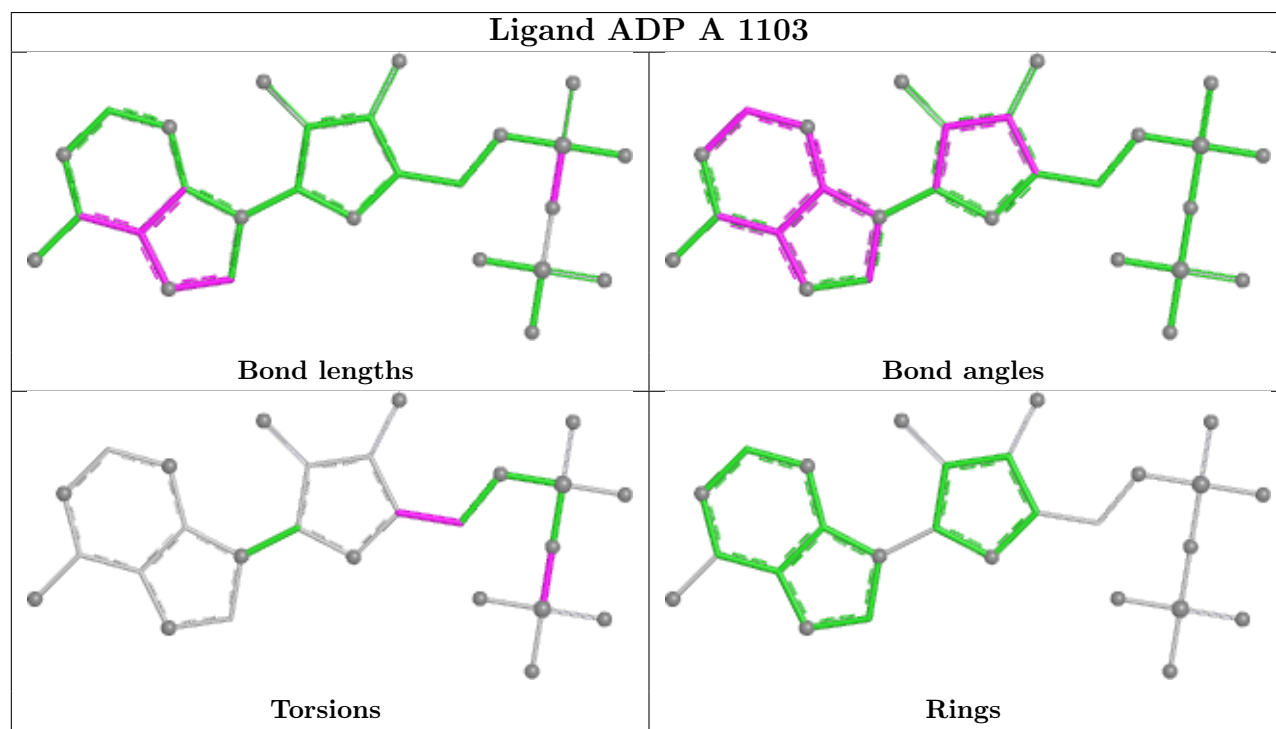
Mol	Chain	Res	Type	Atoms
5	A	1103	ADP	O4'-C4'-C5'-O5'
5	A	1103	ADP	C3'-C4'-C5'-O5'
5	A	1103	ADP	PA-O3A-PB-O3B
5	A	1103	ADP	PA-O3A-PB-O2B

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	1051/1059 (99%)	0.45	82 (7%)	19 21	27, 57, 122, 160	0
2	B	15/15 (100%)	1.69	6 (40%)	1 0	63, 96, 150, 158	0
All	All	1066/1074 (99%)	0.47	88 (8%)	17 19	27, 57, 123, 160	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	VAL	5.6
1	A	26	LEU	5.3
1	A	20	ALA	4.9
2	B	15	DA	4.8
1	A	507	PRO	4.6
1	A	417	ALA	4.6
1	A	245	GLY	4.4
1	A	1	MET	4.2
1	A	115	PHE	4.1
1	A	24	VAL	4.1
1	A	557	ALA	4.1
1	A	569	HIS	4.1
1	A	0	HIS	4.0
1	A	108	PRO	3.9
1	A	396	TYR	3.9
1	A	542	ALA	3.9
1	A	514	MET	3.8
1	A	520	ILE	3.8
1	A	492	VAL	3.7
1	A	105	THR	3.6
1	A	152	PRO	3.6
1	A	31	ALA	3.4
1	A	902	PRO	3.3
1	A	488	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	989	ASP	3.2
1	A	375	PRO	3.2
1	A	873	LEU	3.2
1	A	33	ALA	3.2
1	A	374	ALA	3.1
1	A	27	LEU	3.1
1	A	22	PRO	3.1
1	A	110	ILE	3.0
1	A	480	VAL	3.0
1	A	149	GLY	2.9
1	A	239	LEU	2.8
1	A	61	GLY	2.7
2	B	8	DC	2.7
1	A	373	ALA	2.7
1	A	467	LEU	2.7
1	A	121	TYR	2.7
1	A	34	LEU	2.7
1	A	558	THR	2.6
1	A	249	SER	2.6
1	A	392	LYS	2.6
1	A	879	ASP	2.6
1	A	109	TRP	2.5
1	A	-2	GLY	2.5
1	A	506	GLY	2.5
1	A	50	VAL	2.5
1	A	148	ARG	2.5
1	A	877	TYR	2.5
1	A	11	LEU	2.5
1	A	548	LEU	2.4
1	A	106	SER	2.4
1	A	882	TRP	2.4
1	A	544	VAL	2.4
1	A	563	LEU	2.4
1	A	150	SER	2.4
1	A	100	LEU	2.4
1	A	-1	GLY	2.3
2	B	7	DC	2.3
1	A	102	GLY	2.3
1	A	414	GLY	2.3
1	A	538	LYS	2.2
1	A	12	LEU	2.2
1	A	521	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	494	ASP	2.2
1	A	2	GLU	2.2
1	A	504	LYS	2.2
1	A	529	PHE	2.2
1	A	376	GLY	2.2
1	A	535	TYR	2.1
1	A	490	SER	2.1
1	A	874	TYR	2.1
1	A	80	LEU	2.1
1	A	878	SER	2.1
2	B	11	DG	2.1
1	A	3	PRO	2.1
1	A	44	VAL	2.1
2	B	13	DG	2.1
1	A	267	TRP	2.1
1	A	537	LYS	2.0
1	A	515	ALA	2.0
2	B	12	DA	2.0
1	A	49	LEU	2.0
1	A	151	ASP	2.0
1	A	82	ILE	2.0
1	A	478	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.

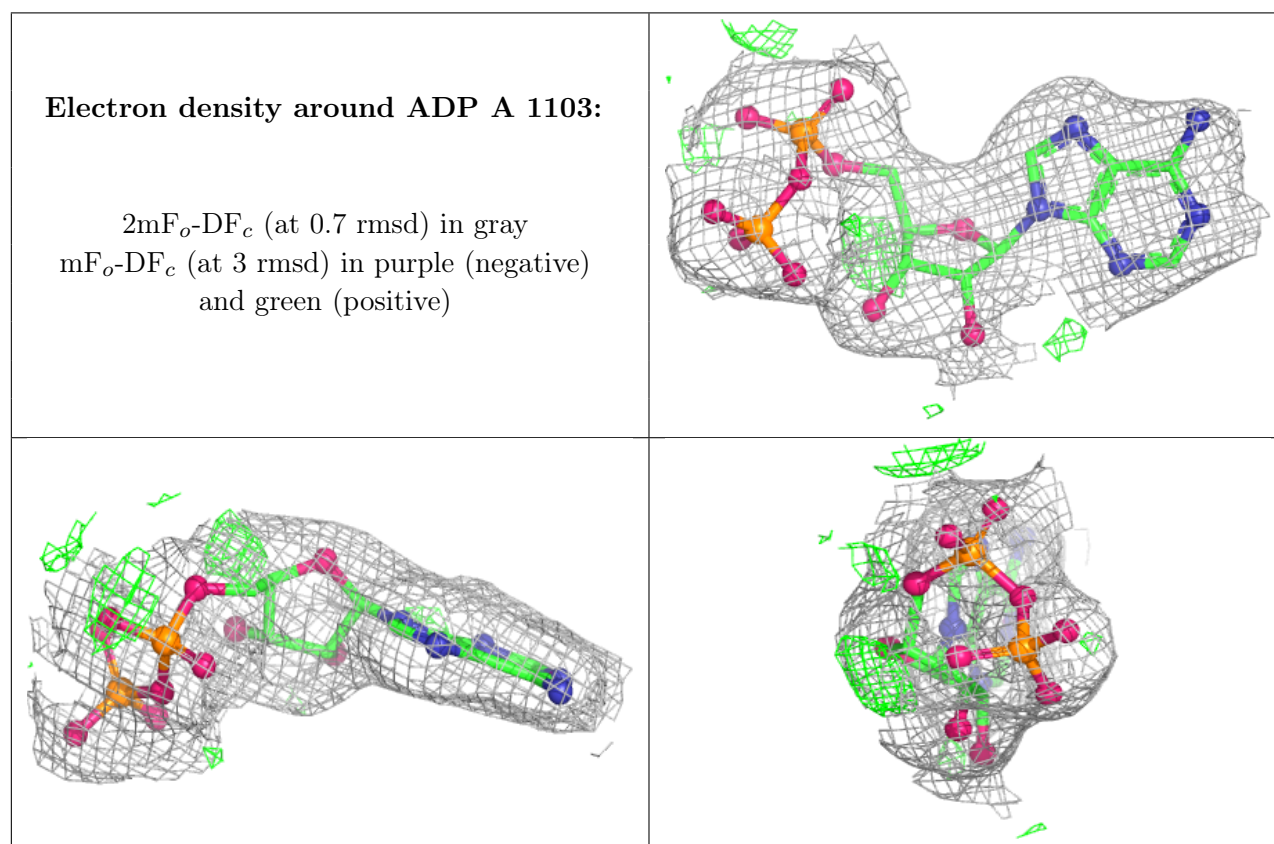
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	A	1103	27/27	0.91	0.10	51,60,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	101	1/1	0.96	0.14	76,76,76,76	0
3	SF4	A	1101	8/8	0.98	0.04	55,60,62,67	0
4	CA	A	1102	1/1	0.99	0.06	43,43,43,43	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.