



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:04 AM UTC

PDB ID : 9TL1 / pdb_00009tl1
Title : Structure of duck RIG-I (delta CARDS) bound to 31-mer RNA mismatched hairpin with 5'ppA-U blunt end mimicking the influenza B virus vRNA promoter (panhandle) and to ADP.
Authors : Cusack, S.; Ivanov, I.
Deposited on : 2025-12-10
Resolution : 1.70 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

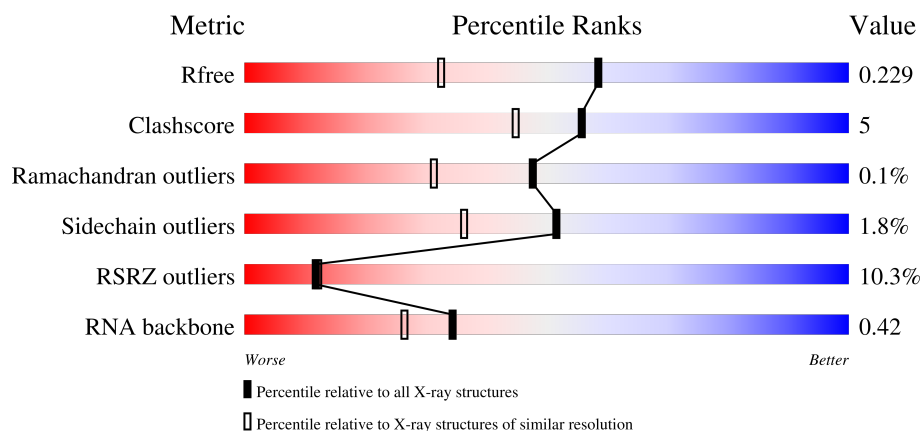
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)
RNA backbone	3983	1094 (2.20-1.20)

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	692	10% 87% 11% .
2	R	30	20% 63% 17% . 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6747 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 RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	39	0
			5748	3606	1012	1090	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	GLN	GLU	engineered mutation	UNP D3TI84

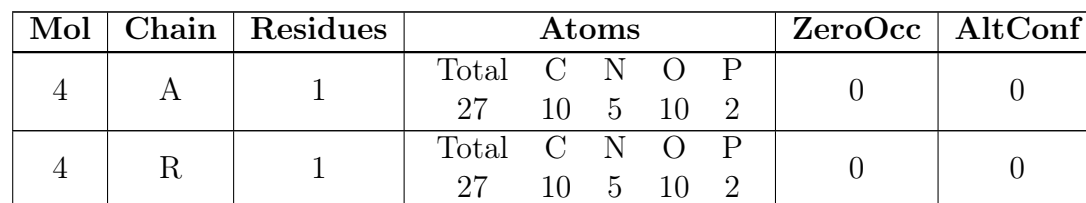
- Molecule 2 is a RNA chain called 31-mer RNA hairpin with 5'ppA-U blunt end mimicking the influenza B virus vRNA promoter (panhandle)..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	25	Total	C	N	O	P	0	3	0
			597	267	106	196	28			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



- GOL
-
- The diagram shows the skeletal structure of 1,2,3-propanetriol (glycerol). It consists of a three-carbon chain. The first carbon (left) is bonded to a hydroxyl group (HO) labeled O1. The second carbon (middle) is bonded to a hydroxyl group (OH) labeled O2. The third carbon (right) is bonded to a hydroxyl group (OH) labeled O3. The carbons are labeled C1, C2, and C3 in green. The hydroxyl groups are labeled HO and OH in red. The oxygen atoms are labeled O1, O2, and O3 in green.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	R	1	Total Mg 1 1	0	0

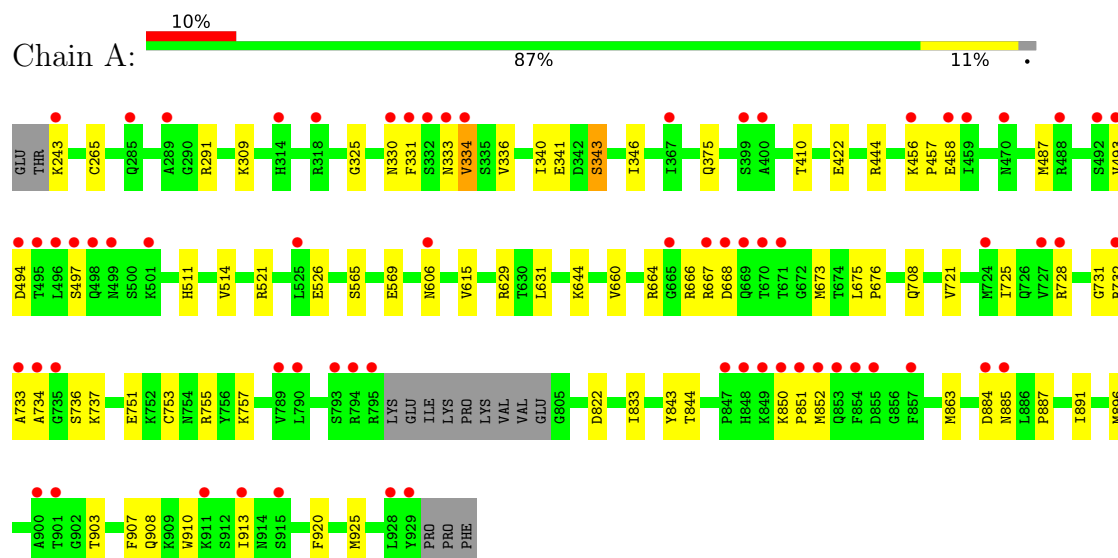
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	300	Total O 300 300	0	0
8	R	33	Total O 33 33	0	0

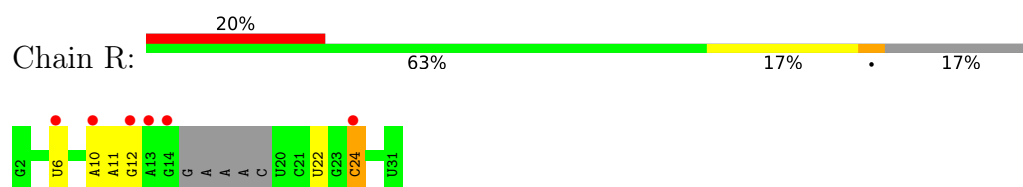
3 Residue-property plots

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: RNA helicase



• Molecule 2: 31-mer RNA hairpin with 5'ppA-U blunt end mimicking the influenza B virus vRNA promoter (panhandle).



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.88Å 100.03Å 190.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.06 – 1.70 95.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	77.0 (95.06-1.70) 77.0 (95.06-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.185 , 0.225 0.193 , 0.229	Depositor DCC
R_{free} test set	3472 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.2	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	0.96	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: ZN, ADP, GOL, CSO, K, 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	0.56	0/5825	1.01	1/7841 (0.0%)
2	R	0.56	0/666	1.02	3/1033 (0.3%)
All	All	0.56	0/6491	1.01	4/8874 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	6	U	O3'-P-O5'	-8.15	91.77	104.00
1	A	331	PHE	CA-CB-CG	6.44	120.24	113.80
2	R	22	U	O3'-P-O5'	-5.50	95.76	104.00
2	R	24	C	O3'-P-O5'	-5.35	95.97	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	ARG	Sidechain

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	5748	0	5760	57	0
2	R	597	0	302	4	0
3	A	1	0	0	0	0
4	A	27	0	12	0	0
4	R	27	0	11	3	0
5	A	6	0	8	1	0
5	R	6	0	8	1	0
6	A	1	0	0	0	0
7	R	1	0	0	0	0
8	A	300	0	0	7	1
8	R	33	0	0	0	0
All	All	6747	0	6101	59	1

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 5.

All (59) 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:667:ARG:HA	4:R:103:ADP:O3B	1.44	1.15
2:R:10[B]:A:H2'	2:R:11[B]:A:O4'	1.56	1.06
1:A:456[B]:LYS:HE2	1:A:457[B]:PRO:O	1.66	0.94
1:A:667:ARG:CA	4:R:103:ADP:O3B	2.20	0.90
1:A:732[A]:ARG:O	1:A:733[A]:ALA:HB3	1.78	0.81
1:A:606[B]:ASN:OD1	8:A:1101:HOH:O	2.03	0.77
1:A:732[A]:ARG:O	1:A:733[A]:ALA:CB	2.36	0.74
1:A:511:HIS:ND1	2:R:10[B]:A:H1'	2.04	0.71
1:A:733[A]:ALA:O	1:A:734[A]:ALA:CB	2.41	0.68
1:A:456[B]:LYS:HD3	1:A:456[B]:LYS:O	1.95	0.66
1:A:733[A]:ALA:O	1:A:734[A]:ALA:HB2	1.99	0.61
1:A:920:PHE:CE1	1:A:925:MET:HG3	2.36	0.61
1:A:606[A]:ASN:O	1:A:606[A]:ASN:CG	2.44	0.60
1:A:666[B]:ARG:O	1:A:666[B]:ARG:HG3	2.03	0.59
1:A:907:PHE:CD2	1:A:913:ILE:HD11	2.39	0.58
1:A:309:LYS:HD3	1:A:325:GLY:HA3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456[B]:LYS:CE	1:A:457[B]:PRO:O	2.47	0.57
1:A:375[B]:GLN:OE1	8:A:1102:HOH:O	2.16	0.55
1:A:341:GLU:OE2	8:A:1103:HOH:O	2.17	0.55
1:A:494:ASP:HA	1:A:497:SER:O	2.07	0.54
1:A:456[B]:LYS:HD3	1:A:456[B]:LYS:C	2.33	0.54
1:A:343:SER:HB2	1:A:346:ILE:HD13	1.88	0.54
2:R:10[B]:A:H2'	2:R:11[B]:A:C1'	2.37	0.54
1:A:753[B]:CYS:SG	1:A:757:LYS:HE3	2.50	0.52
1:A:891:ILE:HB	1:A:910:TRP:CE2	2.44	0.52
1:A:644[B]:LYS:HD3	1:A:660:VAL:HG23	1.92	0.52
1:A:664:ARG:HA	1:A:673:MET:O	2.11	0.51
1:A:884:ASP:OD1	1:A:885:ASN:HB2	2.10	0.51
1:A:487:MET:HE2	1:A:493:VAL:HG21	1.93	0.50
1:A:731[B]:GLY:O	1:A:736:SER:OG	2.26	0.50
1:A:521:ARG:HD2	8:A:1364:HOH:O	2.12	0.49
1:A:751[B]:GLU:OE1	1:A:755:ARG:NH2	2.45	0.49
1:A:850:LYS:O	1:A:852:MET:N	2.46	0.48
1:A:721[A]:VAL:HG21	1:A:757:LYS:CB	2.43	0.48
1:A:708:GLN:NE2	1:A:731[A]:GLY:O	2.47	0.48
1:A:822:ASP:OD1	8:A:1104:HOH:O	2.19	0.48
1:A:458[A]:GLU:CD	1:A:737:LYS:HG2	2.40	0.47
1:A:725:ILE:O	1:A:728[B]:ARG:HB3	2.15	0.47
1:A:615:VAL:HG21	5:A:1003:GOL:H12	1.97	0.46
1:A:343:SER:HB2	1:A:346:ILE:CD1	2.46	0.46
1:A:721[A]:VAL:HG21	1:A:757:LYS:HB2	1.96	0.45
1:A:896:MET:HG3	1:A:907:PHE:CD2	2.51	0.45
1:A:751[B]:GLU:OE1	1:A:755:ARG:NE	2.49	0.45
1:A:330:ASN:O	1:A:334:VAL:HB	2.18	0.44
1:A:833:ILE:HA	1:A:887:PRO:O	2.19	0.43
1:A:908:GLN:NE2	2:R:24:C:OP1	2.51	0.42
1:A:708:GLN:HB3	1:A:732[A]:ARG:HA	2.01	0.42
1:A:265[B]:CSO:HA	1:A:410:THR:O	2.20	0.42
1:A:336:VAL:O	1:A:340:ILE:HG12	2.19	0.42
1:A:606[A]:ASN:ND2	8:A:1126:HOH:O	2.53	0.42
1:A:667:ARG:CB	4:R:103:ADP:O3B	2.68	0.41
1:A:843:TYR:CD1	1:A:863[B]:MET:HG3	2.55	0.41
1:A:340:ILE:HA	1:A:346:ILE:HD11	2.02	0.41
1:A:514:VAL:CG1	5:R:101:GOL:H31	2.51	0.41
1:A:675:LEU:N	1:A:676:PRO:CD	2.84	0.41
1:A:896:MET:HE2	1:A:913:ILE:HD13	2.01	0.41
1:A:629:ARG:NE	8:A:1109:HOH:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:MET:HG3	1:A:907:PHE:HD2	1.86	0.41
1:A:565[A]:SER:O	1:A:569[A]:GLU:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1333:HOH:O	8:A:1389:HOH:O[5_545]	2.19	0.01

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	711/692 (103%)	691 (97%)	19 (3%)	1 (0%)	48 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	851	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	644/625 (103%)	632 (98%)	12 (2%)	50 34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	LYS
1	A	291	ARG
1	A	333	ASN
1	A	334	VAL
1	A	343	SER
1	A	422	GLU
1	A	526	GLU
1	A	631	LEU
1	A	668	ASP
1	A	844[A]	THR
1	A	844[B]	THR
1	A	903	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	A	378	ASN
1	A	417	ASN
1	A	650	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	20/30 (66%)	1 (5%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	12	G

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSO	A	265[B]	1	4,5,7	0.89	0	1,5,8	0.27	0
1	CSO	A	265[A]	1	3,6,7	0.71	0	1,6,8	0.29	0

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
1	CSO	A	265[B]	1	-	1/1/4/7	-
1	CSO	A	265[A]	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	265[B]	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	265[B]	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
5	GOL	A	1003	-	5,5,5	0.06	0	5,5,5	0.21	0
4	ADP	R	103	2	28,29,29	1.49	5 (17%)	43,45,45	1.75	7 (16%)
4	ADP	A	1002	-	28,29,29	0.50	0	43,45,45	0.57	0
5	GOL	R	101	-	5,5,5	0.14	0	5,5,5	0.52	0

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
5	GOL	A	1003	-	-	4/4/4/4	-
4	ADP	R	103	2	-	0/16/32/32	0/3/3/3
4	ADP	A	1002	-	-	1/16/32/32	0/3/3/3
5	GOL	R	101	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	103	ADP	C5-C4	4.49	1.47	1.39
4	R	103	ADP	C5-N7	-3.01	1.33	1.39
4	R	103	ADP	C4-N9	-2.99	1.31	1.37
4	R	103	ADP	C8-N7	2.11	1.35	1.31
4	R	103	ADP	PA-O3A	2.06	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	103	ADP	C5-C4-N3	-5.83	118.68	126.72
4	R	103	ADP	N3-C4-N9	4.71	135.18	127.17
4	R	103	ADP	C2-N3-C4	3.77	121.04	111.83
4	R	103	ADP	N3-C2-N1	-3.41	123.42	128.58
4	R	103	ADP	O2B-PB-O1B	2.51	120.63	110.83
4	R	103	ADP	C4-N9-C8	2.32	108.18	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	103	ADP	C4-C5-N7	-2.26	107.99	110.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

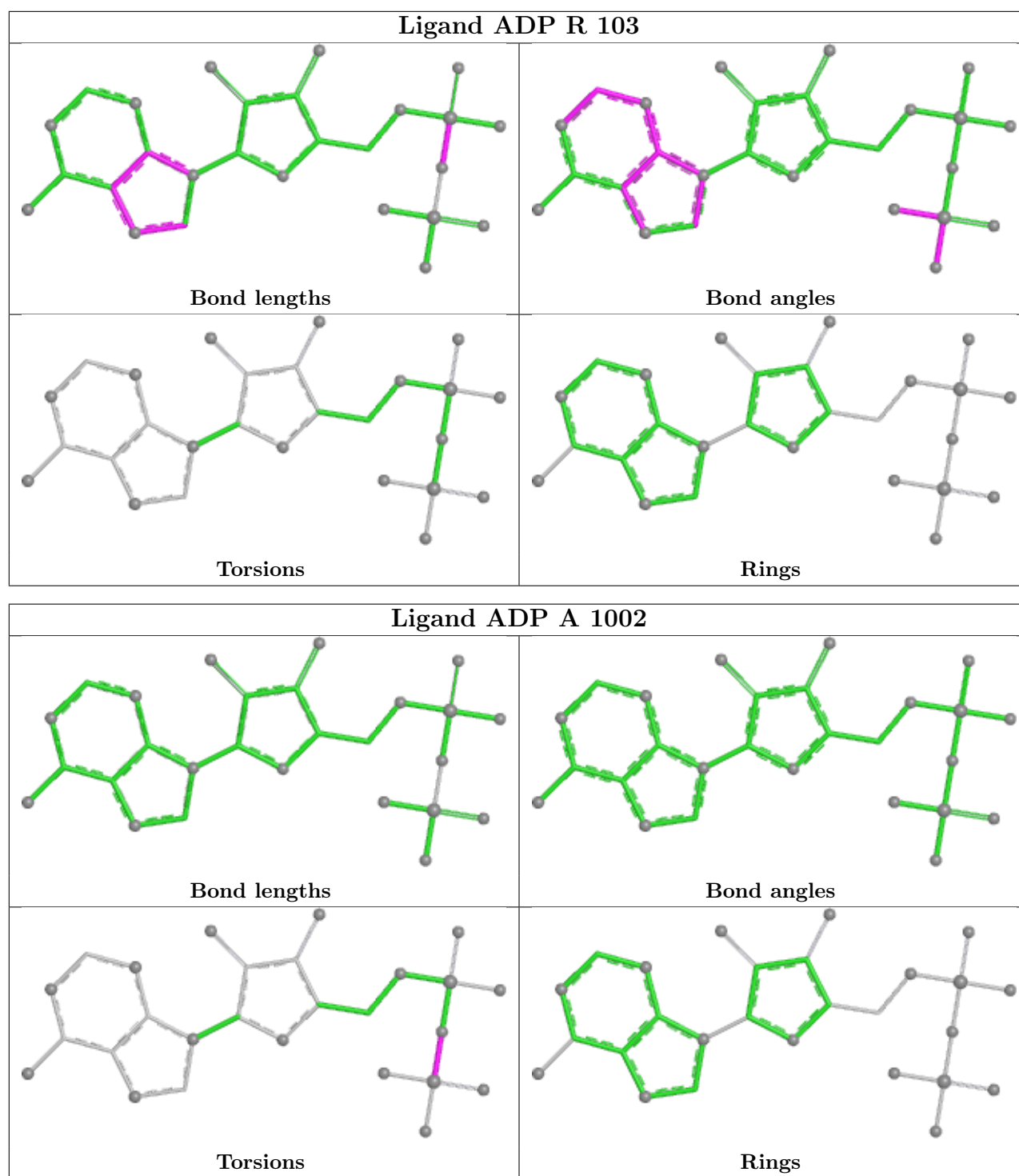
Mol	Chain	Res	Type	Atoms
5	A	1003	GOL	C1-C2-C3-O3
5	R	101	GOL	C1-C2-C3-O3
5	A	1003	GOL	O1-C1-C2-C3
5	A	1003	GOL	O1-C1-C2-O2
5	A	1003	GOL	O2-C2-C3-O3
5	R	101	GOL	O2-C2-C3-O3
4	A	1002	ADP	PA-O3A-PB-O2B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	GOL	1	0
4	R	103	ADP	3	0
5	R	101	GOL	1	0

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 ⓘ

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

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	677/692 (97%)	0.45	66 (9%) 13 14	8, 27, 60, 119	38 (5%)
2	R	25/30 (83%)	0.84	6 (24%) 2 2	13, 29, 112, 139	3 (12%)
All	All	702/722 (97%)	0.47	72 (10%) 12 12	8, 28, 63, 139	41 (5%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LEU	6.5
1	A	851	PRO	6.2
1	A	331	PHE	6.0
1	A	497	SER	5.8
1	A	734[A]	ALA	5.7
1	A	332	SER	5.5
1	A	733[A]	ALA	5.4
1	A	854	PHE	5.1
1	A	732[A]	ARG	5.1
1	A	493	VAL	4.8
1	A	314[A]	HIS	4.7
1	A	852	MET	4.3
1	A	929	TYR	4.1
1	A	857	PHE	4.0
1	A	668	ASP	4.0
1	A	495	THR	3.8
1	A	670	THR	3.8
1	A	795	ARG	3.7
2	R	14	G	3.7
1	A	735	GLY	3.7
1	A	492	SER	3.6
2	R	24	C	3.3
1	A	790	LEU	3.2
1	A	334	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	498	GLN	3.2
1	A	458[A]	GLU	3.2
1	A	665	GLY	3.2
1	A	330	ASN	3.2
1	A	911	LYS	3.1
1	A	849	LYS	3.1
1	A	913	ILE	3.1
1	A	671	THR	3.1
1	A	850	LYS	3.0
1	A	885	ASN	2.9
1	A	333	ASN	2.9
1	A	606[A]	ASN	2.9
2	R	10[A]	A	2.9
1	A	456[A]	LYS	2.8
1	A	243	LYS	2.8
1	A	400	ALA	2.7
1	A	728[A]	ARG	2.7
1	A	289	ALA	2.7
1	A	928	LEU	2.7
1	A	494	ASP	2.5
1	A	669	GLN	2.5
1	A	793	SER	2.5
1	A	789	VAL	2.5
1	A	853	GLN	2.5
2	R	13	A	2.5
1	A	501	LYS	2.4
1	A	488	ARG	2.4
1	A	900	ALA	2.4
2	R	12	G	2.4
1	A	667	ARG	2.4
1	A	499	ASN	2.3
1	A	727	VAL	2.3
1	A	794	ARG	2.3
1	A	847	PRO	2.2
2	R	6	U	2.2
1	A	285	GLN	2.2
1	A	855	ASP	2.2
1	A	884	ASP	2.2
1	A	470	ASN	2.2
1	A	459[A]	ILE	2.1
1	A	724[A]	MET	2.1
1	A	915	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	848	HIS	2.1
1	A	399	SER	2.0
1	A	525	LEU	2.0
1	A	901	THR	2.0
1	A	318	ARG	2.0
1	A	367	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	265[A]	7/8	0.94	0.08	22,23,30,36	7
1	CSO	A	265[B]	6/8	0.94	0.08	18,20,20,21	6

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.

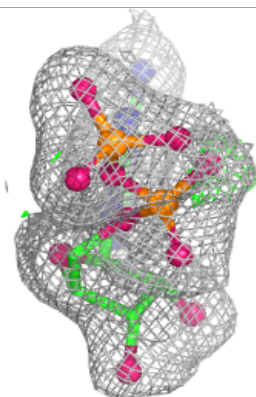
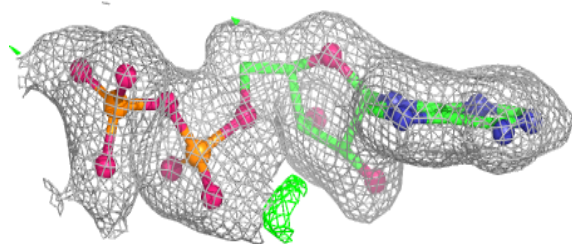
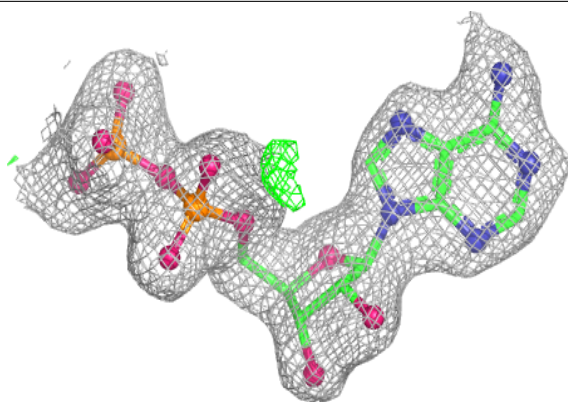
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	R	102	1/1	0.81	0.21	56,56,56,56	0
5	GOL	R	101	6/6	0.90	0.12	45,50,51,53	0
5	GOL	A	1003	6/6	0.90	0.12	40,47,48,48	0
4	ADP	A	1002	27/27	0.95	0.08	26,45,48,50	0
6	K	A	1004	1/1	0.97	0.05	25,25,25,25	1
4	ADP	R	103	27/27	0.97	0.06	19,23,45,49	0
3	ZN	A	1001	1/1	1.00	0.01	17,17,17,17	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.

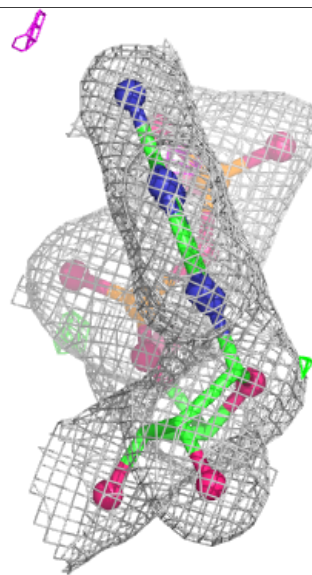
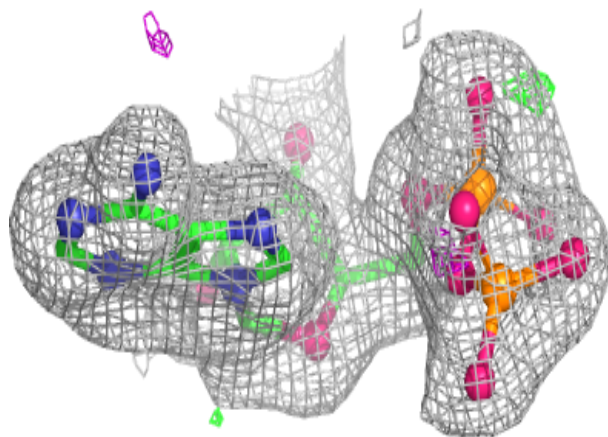
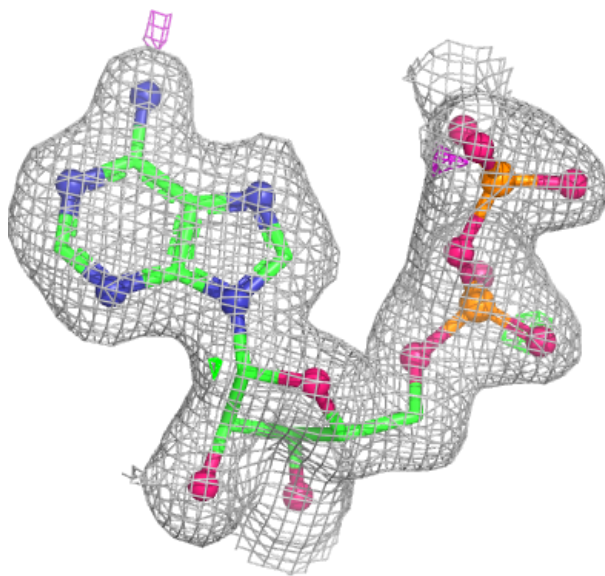
Electron density around ADP A 1002:

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



Electron density around ADP R 103:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.