



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:38 AM UTC

PDB ID : 3EGI / pdb_00003egi
Title : Methyltransferase domain of human trimethylguanosine synthase TGS1 bound to m7GpppA (inactive form)
Authors : Monecke, T.; Dickmanns, A.; Ficner, R.
Deposited on : 2008-09-10
Resolution : 2.21 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

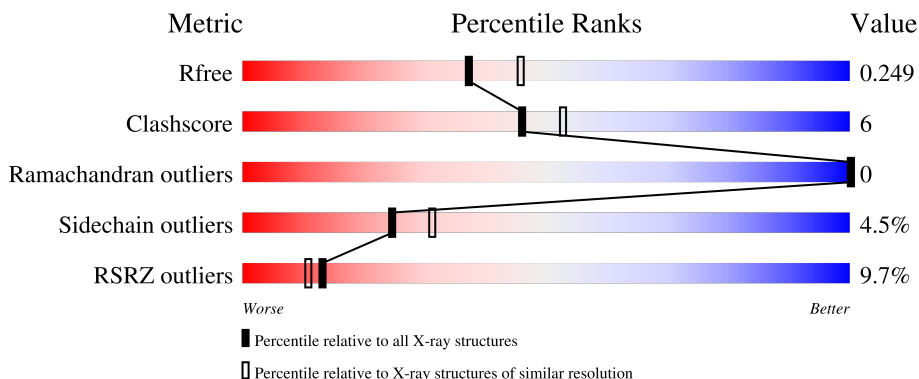
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	206	 6% 82% 11% • 5%
1	B	206	 10% 78% 14% • 7%
1	C	206	 9% 84% 8% • 7%
1	D	206	 10% 81% 9% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6769 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.

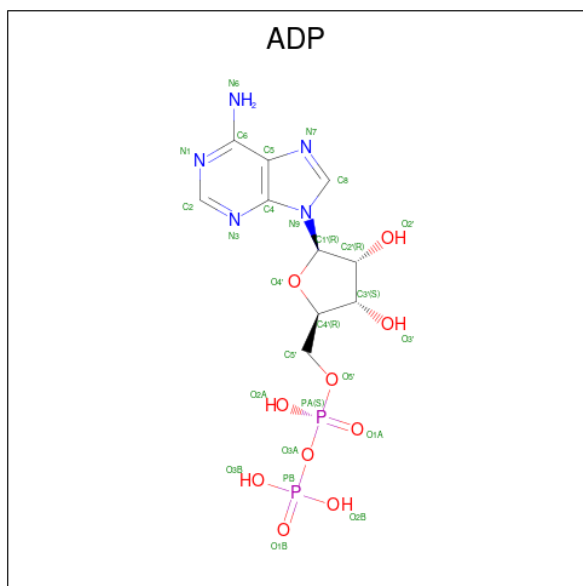
- Molecule 1 is a protein called Trimethylguanosine synthase homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	3	0
			1540	995	257	282	3	3			
1	B	192	Total	C	N	O	S	Se	0	2	0
			1514	979	251	278	3	3			
1	C	192	Total	C	N	O	S	Se	0	1	0
			1505	974	250	275	3	3			
1	D	189	Total	C	N	O	S	Se	0	0	0
			1471	949	246	270	3	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	648	GLY	-	expression tag	UNP Q96RS0
A	649	PRO	-	expression tag	UNP Q96RS0
A	650	LEU	-	expression tag	UNP Q96RS0
A	651	GLY	-	expression tag	UNP Q96RS0
A	652	SER	-	expression tag	UNP Q96RS0
B	648	GLY	-	expression tag	UNP Q96RS0
B	649	PRO	-	expression tag	UNP Q96RS0
B	650	LEU	-	expression tag	UNP Q96RS0
B	651	GLY	-	expression tag	UNP Q96RS0
B	652	SER	-	expression tag	UNP Q96RS0
C	648	GLY	-	expression tag	UNP Q96RS0
C	649	PRO	-	expression tag	UNP Q96RS0
C	650	LEU	-	expression tag	UNP Q96RS0
C	651	GLY	-	expression tag	UNP Q96RS0
C	652	SER	-	expression tag	UNP Q96RS0
D	648	GLY	-	expression tag	UNP Q96RS0
D	649	PRO	-	expression tag	UNP Q96RS0
D	650	LEU	-	expression tag	UNP Q96RS0
D	651	GLY	-	expression tag	UNP Q96RS0
D	652	SER	-	expression tag	UNP Q96RS0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

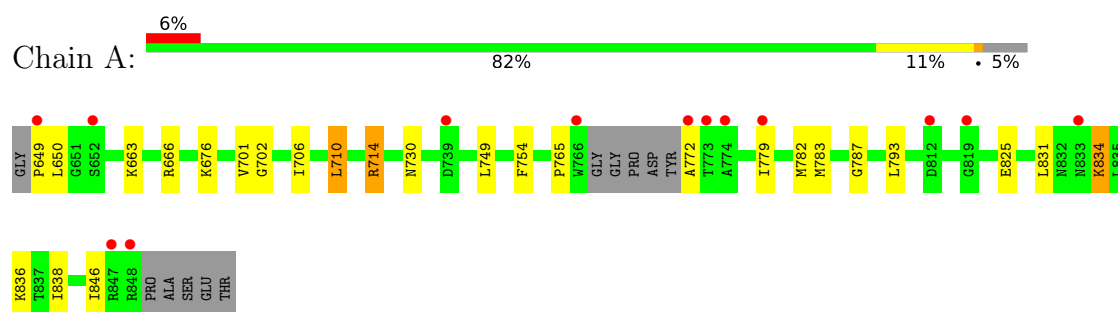
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total	O	0	0
			186	186		
3	B	141	Total	O	0	0
			141	141		
3	C	152	Total	O	0	0
			152	152		
3	D	152	Total	O	0	0
			152	152		

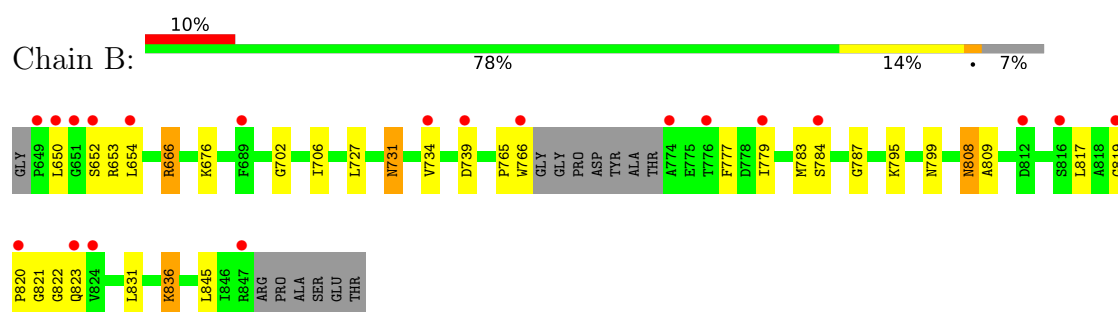
3 Residue-property plots [i](#)

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.

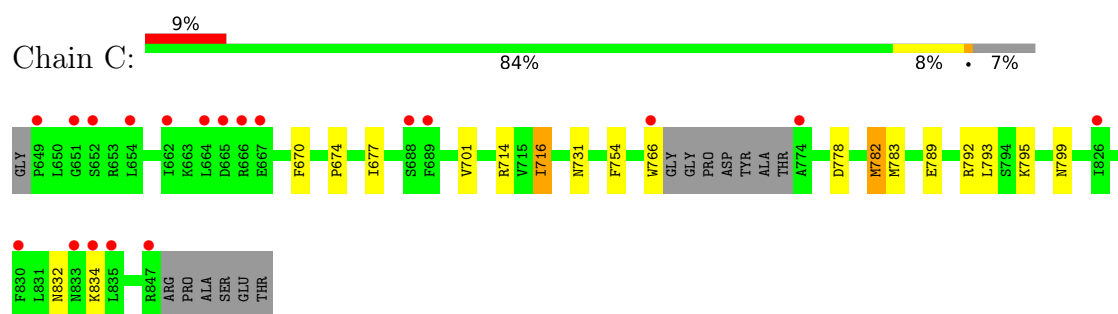
- Molecule 1: Trimethylguanosine synthase homolog



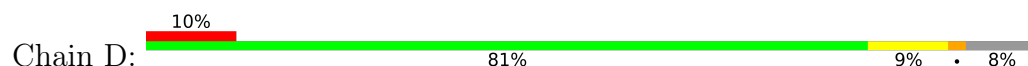
- Molecule 1: Trimethylguanosine synthase homolog

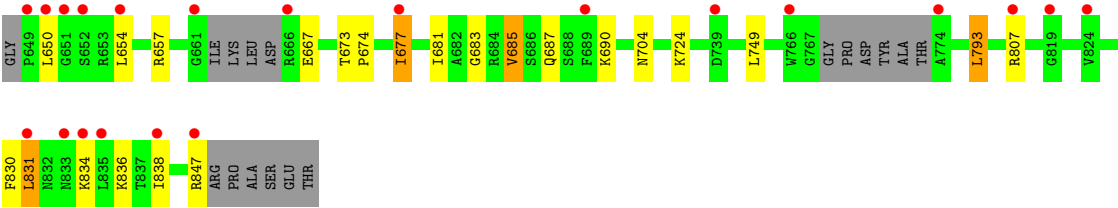


- Molecule 1: Trimethylguanosine synthase homolog



- Molecule 1: Trimethylguanosine synthase homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	213.89Å 213.89Å 62.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.21 39.90 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.90-2.21) 97.4 (39.90-2.21)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.210 , 0.252 0.211 , 0.249	Depositor DCC
R_{free} test set	3610 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6769	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1110e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.66	0/1576	0.85	0/2125
1	B	0.64	0/1544	0.84	0/2082
1	C	0.64	1/1535 (0.1%)	0.81	0/2070
1	D	0.64	0/1497	0.87	0/2017
All	All	0.64	1/6152 (0.0%)	0.84	0/8294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	782	MSE	SE-CE	-5.32	1.79	1.95

There are no bond angle outliers.

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	1540	0	1555	20	1
1	B	1514	0	1521	27	0
1	C	1505	0	1516	11	0
1	D	1471	0	1468	20	0
2	A	27	0	12	2	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	186	0	0	0	0
3	B	141	0	0	2	0
3	C	152	0	0	0	1
3	D	152	0	0	1	0
All	All	6769	0	6108	71	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 6.

All (71) 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:666:ARG:HH11	1:B:666:ARG:HG3	1.18	1.08
1:C:766:TRP:CD1	1:C:783:MSE:HE2	2.11	0.85
1:D:673:THR:HG23	1:D:677:ILE:HD11	1.61	0.83
1:A:730:ASN:HD22	1:B:731:ASN:ND2	1.86	0.74
1:B:831:LEU:HB3	1:B:836:LYS:HD2	1.70	0.74
1:D:673:THR:HG23	1:D:677:ILE:CD1	2.18	0.74
1:B:808:ASN:H	1:B:808:ASN:HD22	1.37	0.73
1:A:749:LEU:HD22	1:A:793:LEU:HD12	1.72	0.70
1:A:765:PRO:HG3	2:A:3:ADP:H5'1	1.72	0.70
1:B:666:ARG:HG3	1:B:666:ARG:NH1	1.98	0.69
1:B:666:ARG:HH11	1:B:666:ARG:CG	2.05	0.66
1:D:674:PRO:HD2	1:D:677:ILE:HD12	1.78	0.65
1:D:683:GLY:O	1:D:687:GLN:HG2	1.96	0.65
1:B:795:LYS:NZ	1:B:799:ASN:OD1	2.30	0.64
1:D:681:ILE:O	1:D:685:VAL:HG13	1.98	0.62
1:B:766:TRP:HD1	1:B:783:MSE:CE	2.13	0.61
1:D:673:THR:CG2	1:D:677:ILE:CD1	2.80	0.60
1:A:730:ASN:HD22	1:B:731:ASN:HD22	1.50	0.59
1:B:766:TRP:HD1	1:B:783:MSE:HE3	1.67	0.59
1:D:673:THR:HB	1:D:704:ASN:HD21	1.68	0.59
1:D:673:THR:HG22	1:D:677:ILE:HD13	1.88	0.56
1:D:673:THR:CG2	1:D:677:ILE:HD13	2.36	0.55
1:D:807:ARG:NH2	1:D:836:LYS:HA	2.22	0.55
1:A:714:ARG:HD3	1:C:754:PHE:HZ	1.73	0.54
1:A:754:PHE:CD1	1:C:716[A]:ILE:HD11	2.43	0.54
1:B:808:ASN:HD22	1:B:808:ASN:N	2.00	0.54
1:B:777:PHE:HB3	1:B:809:ALA:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:LEU:HD22	1:D:793:LEU:HD13	1.90	0.53
1:D:834:LYS:HE3	1:D:836:LYS:HE2	1.91	0.52
1:B:779[B]:ILE:HG23	1:B:787:GLY:HA3	1.91	0.52
1:B:766:TRP:HA	1:B:783:MSE:HE3	1.92	0.52
1:D:724:LYS:NZ	3:D:40:HOH:O	2.43	0.51
1:B:676:LYS:HE2	3:B:621:HOH:O	2.11	0.51
1:B:666:ARG:HB3	1:D:667:GLU:HG3	1.94	0.49
1:B:765:PRO:O	1:B:783:MSE:HE2	2.13	0.48
1:A:702:GLY:O	1:A:706:ILE:HG12	2.13	0.48
1:B:808:ASN:H	1:B:808:ASN:ND2	2.08	0.48
1:B:836:LYS:HE2	1:B:836:LYS:HA	1.96	0.47
1:C:795:LYS:NZ	1:C:799:ASN:OD1	2.46	0.47
1:C:670:PHE:HB3	1:C:701:VAL:HG23	1.96	0.47
1:A:779[B]:ILE:HG23	1:A:787:GLY:HA3	1.96	0.46
1:A:649:PRO:O	1:A:650:LEU:HD23	2.16	0.46
1:B:820:PRO:HA	1:B:821:GLY:HA2	1.67	0.45
1:D:690:LYS:HA	1:D:690:LYS:HE2	1.99	0.45
1:D:831:LEU:HB2	1:D:836:LYS:HG3	1.98	0.45
1:A:714:ARG:HB3	1:A:714:ARG:HH11	1.81	0.45
1:A:706:ILE:HG22	1:A:710:LEU:HD22	1.98	0.44
1:A:676:LYS:HB2	1:A:676:LYS:HE2	1.66	0.44
1:D:657:ARG:HG3	1:D:830:PHE:CD2	2.52	0.44
1:A:834:LYS:HE2	1:A:834:LYS:HB3	1.80	0.43
1:B:766:TRP:CD1	1:B:783:MSE:HE3	2.49	0.43
1:C:778:ASP:H	1:C:782:MSE:SE	2.51	0.43
1:A:754:PHE:HZ	1:C:714:ARG:HE	1.66	0.43
1:B:819:GLY:O	1:B:822:GLY:N	2.48	0.43
1:A:765:PRO:O	1:A:783:MSE:HG2	2.19	0.42
1:C:789:GLU:OE2	1:C:792:ARG:NH2	2.41	0.42
1:D:681:ILE:O	1:D:685:VAL:CG1	2.65	0.42
1:A:765:PRO:HG3	2:A:3:ADP:C5'	2.47	0.42
1:B:702:GLY:O	1:B:706:ILE:HG12	2.20	0.42
1:D:807:ARG:HH21	1:D:836:LYS:HA	1.84	0.42
1:A:831:LEU:HB3	1:A:836:LYS:HE3	2.02	0.41
1:C:674:PRO:HD2	1:C:677:ILE:HD12	2.02	0.41
1:D:834:LYS:HE2	1:D:834:LYS:HB3	1.89	0.41
1:C:731:ASN:HD22	1:C:731:ASN:HA	1.69	0.41
1:A:772:ALA:N	1:A:782:MSE:HE3	2.36	0.41
1:B:739:ASP:OD1	3:B:606:HOH:O	2.22	0.41
1:A:701:VAL:HG21	1:B:727:LEU:HD11	2.03	0.40
1:B:731:ASN:HD22	1:B:731:ASN:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:GLU:HB2	1:A:846:ILE:HG23	2.03	0.40
1:B:652:SER:OG	1:B:823:GLN:HG3	2.22	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)
1:A:676:LYS:NZ	3:C:48:HOH:O[1_556]	2.09	0.11

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	194/206 (94%)	191 (98%)	3 (2%)	0	100	100
1	B	190/206 (92%)	185 (97%)	5 (3%)	0	100	100
1	C	189/206 (92%)	182 (96%)	7 (4%)	0	100	100
1	D	183/206 (89%)	177 (97%)	6 (3%)	0	100	100
All	All	756/824 (92%)	735 (97%)	21 (3%)	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	166/167 (99%)	160 (96%)	6 (4%)	31	40
1	B	163/167 (98%)	152 (93%)	11 (7%)	15	16
1	C	162/167 (97%)	157 (97%)	5 (3%)	35	46
1	D	157/167 (94%)	149 (95%)	8 (5%)	21	26
All	All	648/668 (97%)	618 (95%)	30 (5%)	24	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	LYS
1	A	666	ARG
1	A	710	LEU
1	A	714	ARG
1	A	834	LYS
1	A	838	ILE
1	B	650	LEU
1	B	653	ARG
1	B	654	LEU
1	B	666	ARG
1	B	731	ASN
1	B	734	VAL
1	B	784	SER
1	B	808	ASN
1	B	817	LEU
1	B	836	LYS
1	B	845	LEU
1	C	716[A]	ILE
1	C	716[B]	ILE
1	C	793	LEU
1	C	832	ASN
1	C	834	LYS
1	D	650	LEU
1	D	654	LEU
1	D	677	ILE
1	D	685	VAL
1	D	793	LEU
1	D	831	LEU
1	D	838	ILE
1	D	847	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	ASN
1	A	828	GLN
1	A	832	ASN
1	B	687	GLN
1	B	731	ASN
1	B	808	ASN
1	B	829	ASN
1	C	687	GLN
1	C	731	ASN
1	C	800	ASN
1	C	832	ASN
1	D	704	ASN
1	D	731	ASN

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](#)

4 ligands 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	$\# Z > 2$
2	ADP	C	1	-	28,29,29	1.84	6 (21%)	43,45,45	2.04	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	4	-	28,29,29	1.83	6 (21%)	43,45,45	1.99	12 (27%)
2	ADP	A	3	-	28,29,29	1.85	7 (25%)	43,45,45	1.97	12 (27%)
2	ADP	D	2	-	28,29,29	1.97	7 (25%)	43,45,45	1.86	12 (27%)

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	C	1	-	-	1/16/32/32	0/3/3/3
2	ADP	B	4	-	-	2/16/32/32	0/3/3/3
2	ADP	A	3	-	-	6/16/32/32	0/3/3/3
2	ADP	D	2	-	-	0/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	ADP	PA-O3A	-4.59	1.54	1.59
2	B	4	ADP	C5-N7	-4.45	1.31	1.39
2	A	3	ADP	C5-N7	-4.14	1.31	1.39
2	D	2	ADP	C5-N7	-4.11	1.31	1.39
2	C	1	ADP	C5-N7	-3.90	1.32	1.39
2	A	3	ADP	C4-N9	-3.89	1.29	1.37
2	C	1	ADP	C8-N9	-3.77	1.31	1.37
2	B	4	ADP	C4-N9	-3.73	1.29	1.37
2	C	1	ADP	C4-N9	-3.60	1.30	1.37
2	D	2	ADP	C8-N9	-3.42	1.31	1.37
2	C	1	ADP	PA-O3A	-3.31	1.55	1.59
2	A	3	ADP	C8-N9	-3.28	1.32	1.37
2	B	4	ADP	C5-C4	3.27	1.44	1.39
2	D	2	ADP	C4-N9	-3.14	1.31	1.37
2	B	4	ADP	C8-N9	-3.10	1.32	1.37
2	A	3	ADP	C5-C4	3.05	1.44	1.39
2	D	2	ADP	C5-C4	3.01	1.44	1.39
2	C	1	ADP	C5-C4	2.62	1.43	1.39
2	A	3	ADP	O4'-C4'	-2.57	1.39	1.45
2	D	2	ADP	PB-O2B	-2.20	1.46	1.54
2	B	4	ADP	PA-O3A	-2.18	1.57	1.59
2	C	1	ADP	PA-O2A	-2.14	1.45	1.55
2	A	3	ADP	PA-O1A	-2.13	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ADP	PA-O2A	-2.10	1.45	1.55
2	D	2	ADP	PA-O2A	-2.09	1.45	1.55
2	A	3	ADP	PA-O2A	-2.04	1.45	1.55

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	ADP	C5-C4-N3	-5.93	118.55	126.72
2	D	2	ADP	C5-C4-N3	-5.74	118.81	126.72
2	C	1	ADP	C5-C4-N3	-5.39	119.30	126.72
2	A	3	ADP	C5-C4-N3	-5.27	119.46	126.72
2	A	3	ADP	N3-C4-N9	4.81	135.35	127.17
2	D	2	ADP	N3-C4-N9	4.76	135.26	127.17
2	B	4	ADP	N3-C4-N9	4.70	135.16	127.17
2	C	1	ADP	N3-C4-N9	4.36	134.58	127.17
2	C	1	ADP	C4-C5-N7	-4.33	105.63	110.58
2	B	4	ADP	C2-N3-C4	4.12	121.89	111.83
2	C	1	ADP	C4-N9-C8	4.11	110.06	105.74
2	B	4	ADP	N3-C2-N1	-3.85	122.76	128.58
2	A	3	ADP	O3A-PA-O1A	-3.81	99.24	110.70
2	D	2	ADP	C4-C5-N7	-3.65	106.41	110.58
2	A	3	ADP	C4-N9-C8	3.58	109.50	105.74
2	C	1	ADP	C2-N3-C4	3.54	120.48	111.83
2	D	2	ADP	C2-N3-C4	3.50	120.38	111.83
2	C	1	ADP	C5-N7-C8	3.46	108.89	103.45
2	A	3	ADP	C2-N3-C4	3.46	120.29	111.83
2	C	1	ADP	N9-C8-N7	-3.25	109.32	113.94
2	B	4	ADP	C4-C5-N7	-3.21	106.92	110.58
2	C	1	ADP	N3-C2-N1	-3.20	123.74	128.58
2	C	1	ADP	O3B-PB-O3A	-3.09	94.26	104.64
2	C	1	ADP	C6-C5-N7	3.07	138.01	132.09
2	A	3	ADP	C4-C5-N7	-2.89	107.28	110.58
2	D	2	ADP	C5-N7-C8	2.87	107.96	103.45
2	D	2	ADP	N3-C2-N1	-2.86	124.25	128.58
2	B	4	ADP	O3A-PA-O1A	-2.79	102.30	110.70
2	D	2	ADP	C4-N9-C8	2.79	108.67	105.74
2	A	3	ADP	O2A-PA-O3A	2.66	114.47	107.27
2	A	3	ADP	N3-C2-N1	-2.61	124.62	128.58
2	B	4	ADP	C6-C5-N7	2.61	137.12	132.09
2	B	4	ADP	C2'-C1'-N9	2.48	119.45	113.30
2	D	2	ADP	C6-C5-N7	2.40	136.71	132.09
2	A	3	ADP	C5-N7-C8	2.31	107.08	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3	ADP	C6-C5-N7	2.27	136.47	132.09
2	C	1	ADP	O2A-PA-O1A	2.25	122.93	112.44
2	D	2	ADP	O2A-PA-O1A	2.25	122.93	112.44
2	A	3	ADP	C4-N9-C1'	-2.23	121.42	126.63
2	B	4	ADP	C5-N7-C8	2.21	106.92	103.45
2	B	4	ADP	C2-N1-C6	2.18	122.31	118.73
2	B	4	ADP	O2A-PA-O1A	2.15	122.45	112.44
2	D	2	ADP	C2-N1-C6	2.13	122.22	118.73
2	B	4	ADP	C4-N9-C8	2.10	107.94	105.74
2	A	3	ADP	N9-C8-N7	-2.09	110.97	113.94
2	D	2	ADP	N9-C8-N7	-2.04	111.04	113.94
2	D	2	ADP	O4'-C1'-C2'	-2.02	102.28	106.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	ADP	C5'-O5'-PA-O1A
2	A	3	ADP	C5'-O5'-PA-O2A
2	A	3	ADP	C5'-O5'-PA-O3A
2	A	3	ADP	PB-O3A-PA-O2A
2	B	4	ADP	PB-O3A-PA-O2A
2	C	1	ADP	C2'-C1'-N9-C8
2	A	3	ADP	PB-O3A-PA-O1A
2	B	4	ADP	PB-O3A-PA-O1A
2	A	3	ADP	C2'-C1'-N9-C8

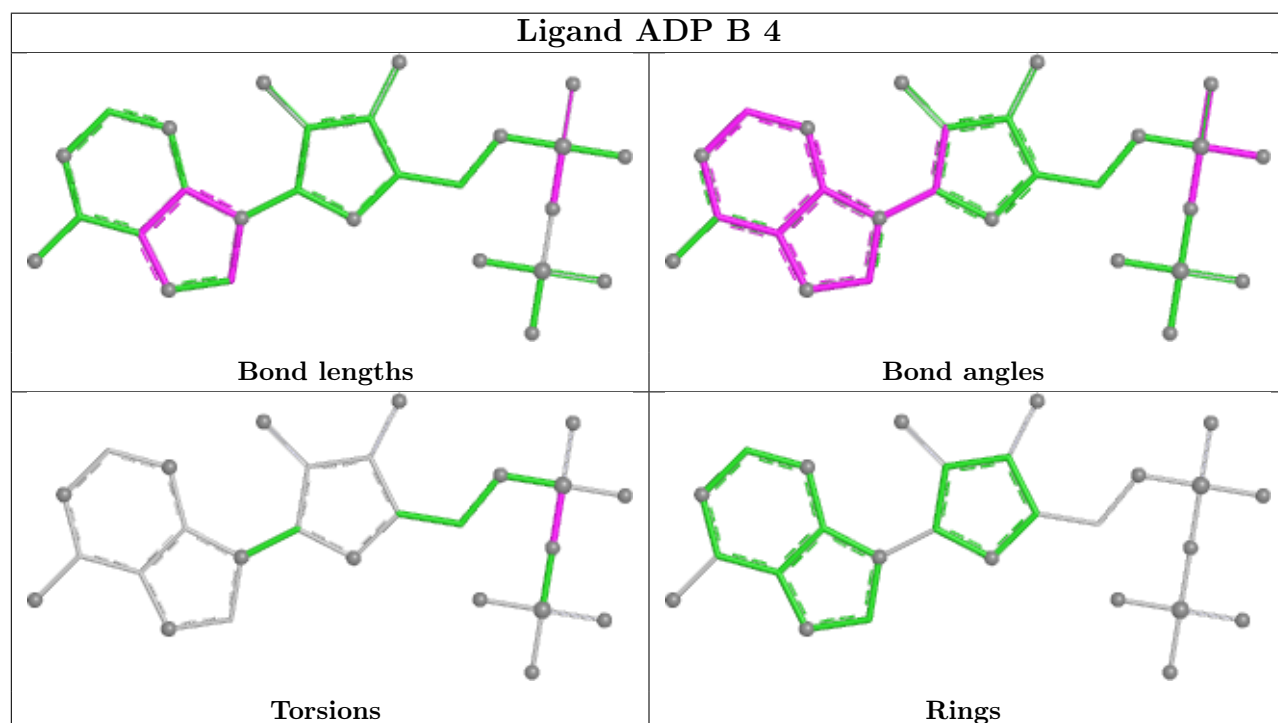
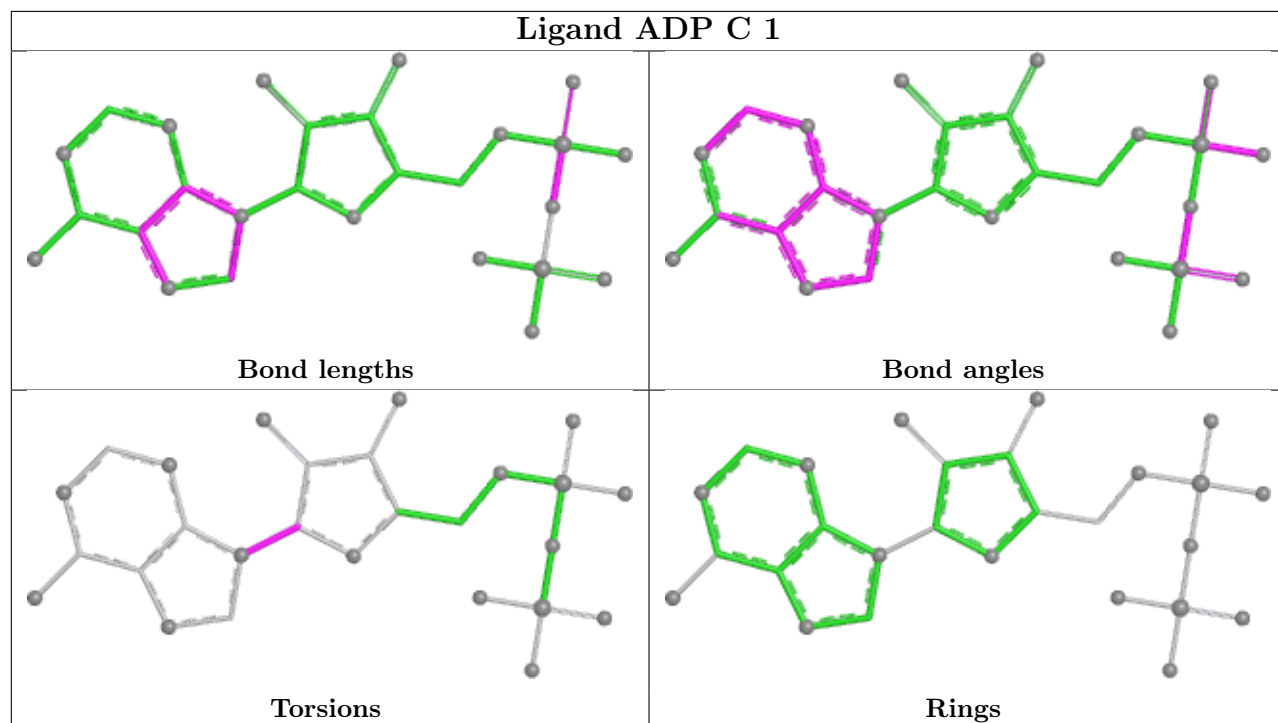
There are no ring outliers.

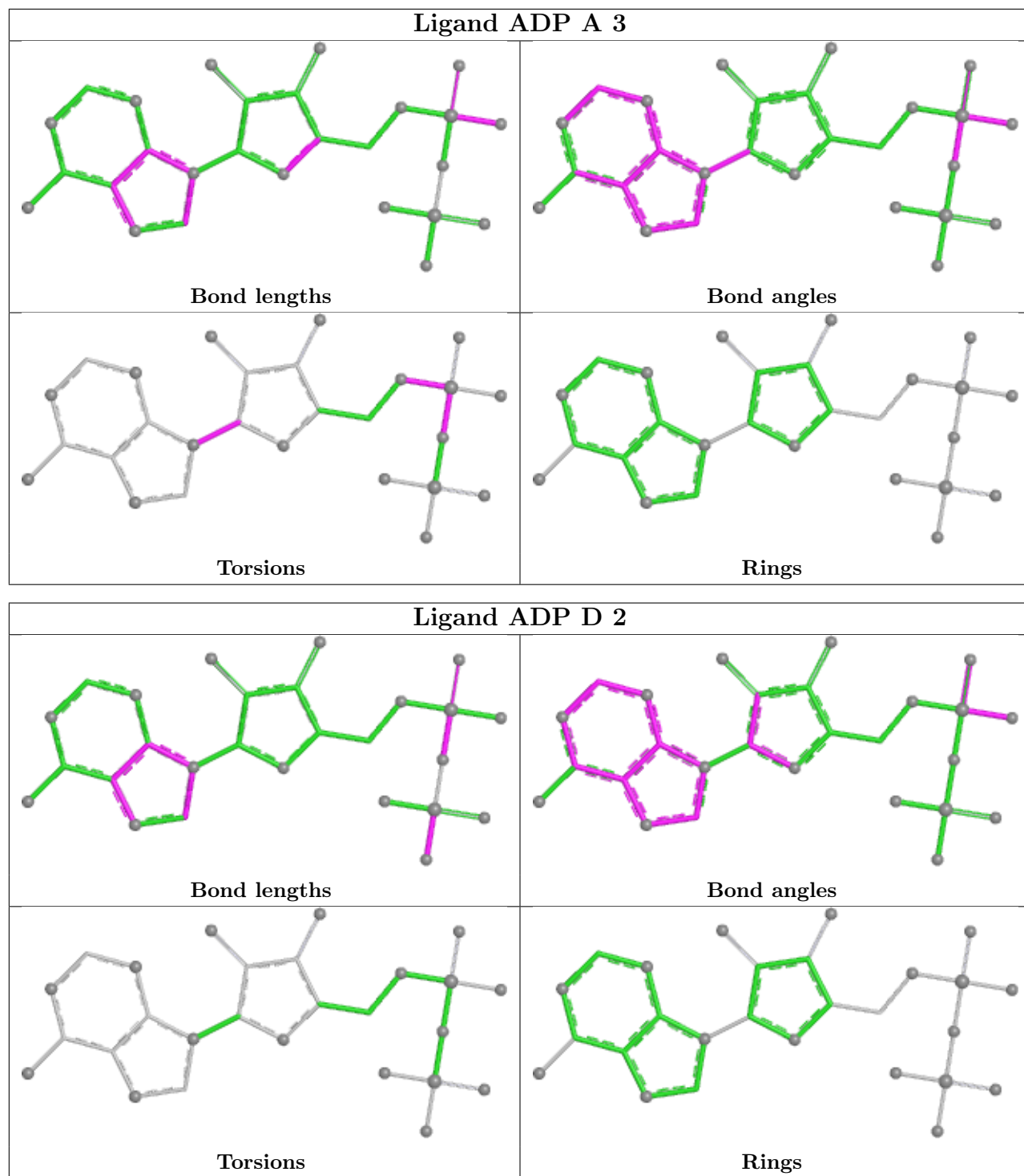
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	ADP	2	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	192/206 (93%)	0.22	13 (6%) 23 20	17, 32, 49, 67	3 (1%)
1	B	189/206 (91%)	0.53	20 (10%) 11 9	16, 34, 55, 63	2 (1%)
1	C	189/206 (91%)	0.77	19 (10%) 12 10	15, 39, 59, 66	1 (0%)
1	D	186/206 (90%)	0.66	21 (11%) 10 8	22, 38, 57, 64	0
All	All	756/824 (91%)	0.54	73 (9%) 13 11	15, 35, 57, 67	6 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	774	ALA	6.7
1	B	651	GLY	6.5
1	C	766	TRP	5.4
1	B	649	PRO	5.0
1	A	772	ALA	4.8
1	C	651	GLY	4.5
1	C	649	PRO	4.5
1	B	650	LEU	4.2
1	D	650	LEU	4.2
1	C	665	ASP	4.1
1	C	666	ARG	4.1
1	D	649	PRO	4.1
1	B	820	PRO	4.0
1	D	834	LYS	3.9
1	C	834	LYS	3.7
1	D	835	LEU	3.6
1	D	831	LEU	3.5
1	B	774	ALA	3.4
1	A	779[A]	ILE	3.4
1	D	833	ASN	3.4
1	A	773	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	774	ALA	3.2
1	A	739	ASP	3.2
1	A	766	TRP	3.2
1	B	819	GLY	3.1
1	D	766	TRP	3.1
1	B	739	ASP	3.1
1	C	654	LEU	3.0
1	D	689	PHE	3.0
1	D	661	GLY	2.9
1	C	689	PHE	2.9
1	A	848	ARG	2.9
1	B	652	SER	2.8
1	D	651	GLY	2.8
1	A	649	PRO	2.8
1	C	664	LEU	2.8
1	A	819	GLY	2.7
1	C	667	GLU	2.7
1	C	847	ARG	2.7
1	C	833	ASN	2.7
1	D	819	GLY	2.6
1	B	766	TRP	2.6
1	B	847	ARG	2.6
1	B	689	PHE	2.6
1	A	812	ASP	2.5
1	D	838	ILE	2.5
1	B	776	THR	2.4
1	D	677	ILE	2.4
1	C	652	SER	2.4
1	B	823	GLN	2.4
1	C	688	SER	2.4
1	D	807	ARG	2.3
1	D	824	VAL	2.3
1	D	654	LEU	2.3
1	B	812	ASP	2.2
1	D	666	ARG	2.2
1	D	652	SER	2.2
1	C	835	LEU	2.2
1	B	784	SER	2.2
1	A	652	SER	2.2
1	B	779[A]	ILE	2.2
1	C	830	PHE	2.2
1	A	774	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	816	SER	2.2
1	A	833	ASN	2.1
1	B	824	VAL	2.1
1	D	739	ASP	2.1
1	D	847	ARG	2.1
1	C	662	ILE	2.1
1	B	734	VAL	2.1
1	C	826	ILE	2.1
1	A	847	ARG	2.0
1	B	654	LEU	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](#)

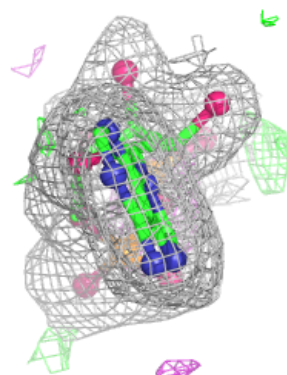
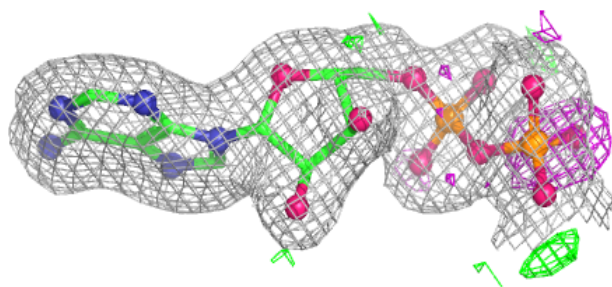
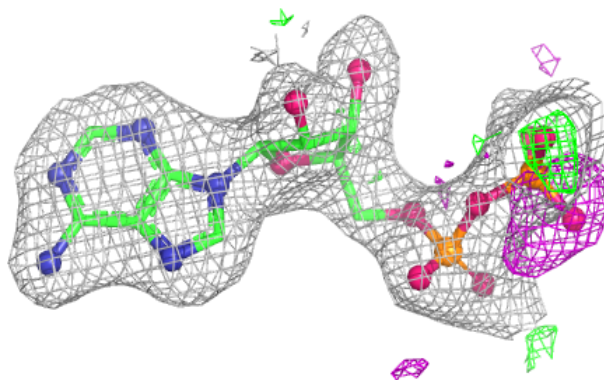
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ADP	A	3	27/27	0.92	0.10	28,32,64,66	0
2	ADP	B	4	27/27	0.92	0.08	28,30,57,59	0
2	ADP	D	2	27/27	0.93	0.09	31,35,63,65	0
2	ADP	C	1	27/27	0.94	0.08	29,32,61,64	0

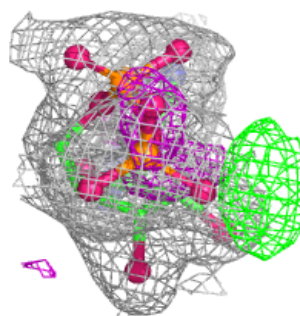
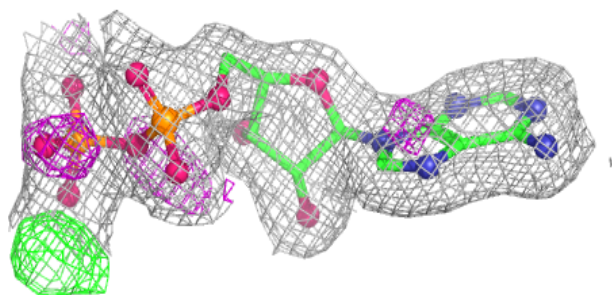
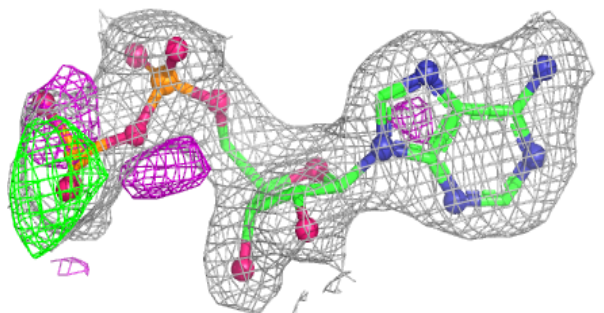
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 3:

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

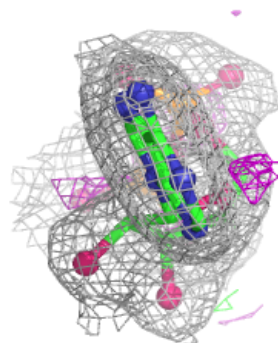
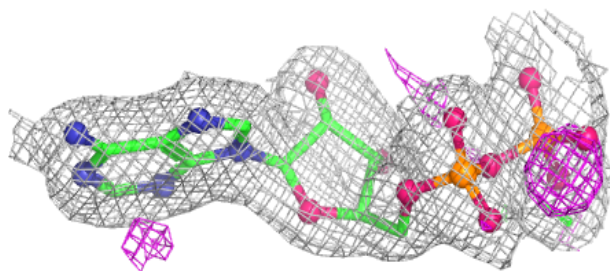
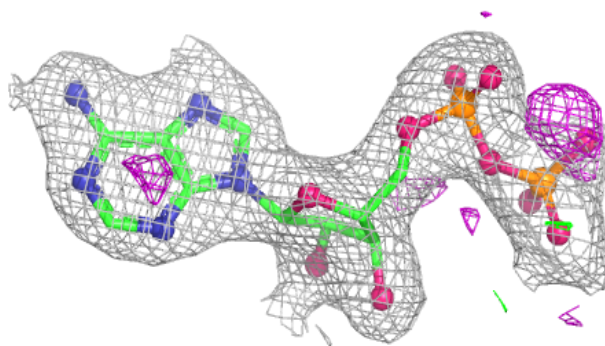
**Electron density around ADP B 4:**

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

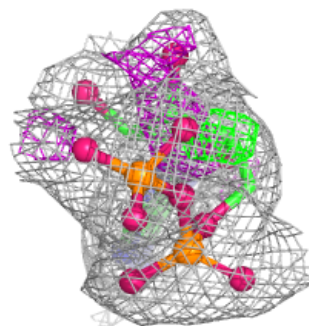
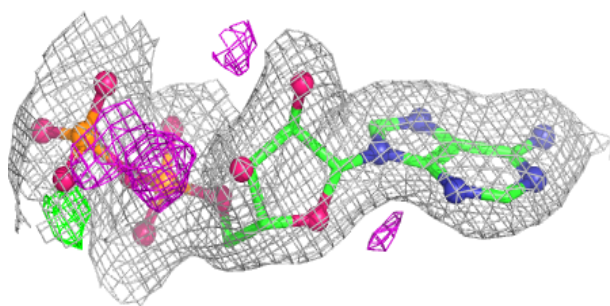
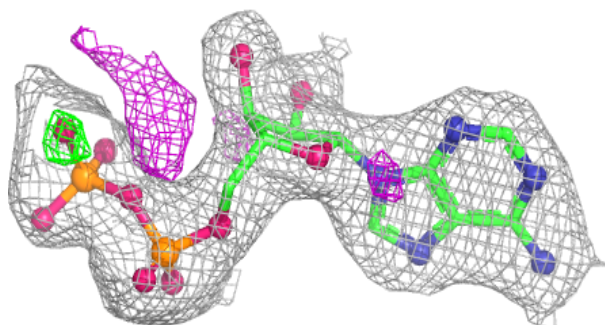


Electron density around ADP D 2:

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

**Electron density around ADP C 1:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.