



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:24 am BST

PDB ID : 4COL
Title : Crystal structure of the anaerobic ribonucleotide reductase from *Thermotoga maritima* with dATP bound in the specificity site
Authors : Aurelius, O.; Johansson, R.; Bagenholm, V.; Beck, T.; Balhuizen, A.; Lundin, D.; Sjöberg, B.M.; Mulliez, E.; Logan, D.T.
Deposited on : 2014-01-29
Resolution : 1.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

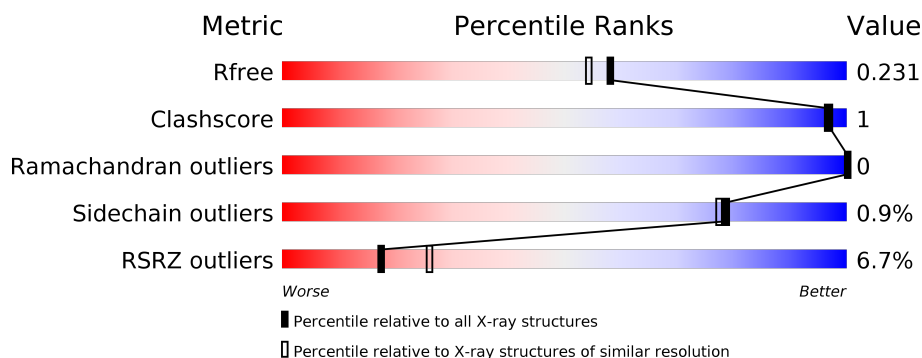
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	651	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	651	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10105 atoms, of which 30 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 ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4795	3104	784	882	25			
1	B	593	Total	C	N	O	S	0	1	0
			4854	3138	796	893	27			

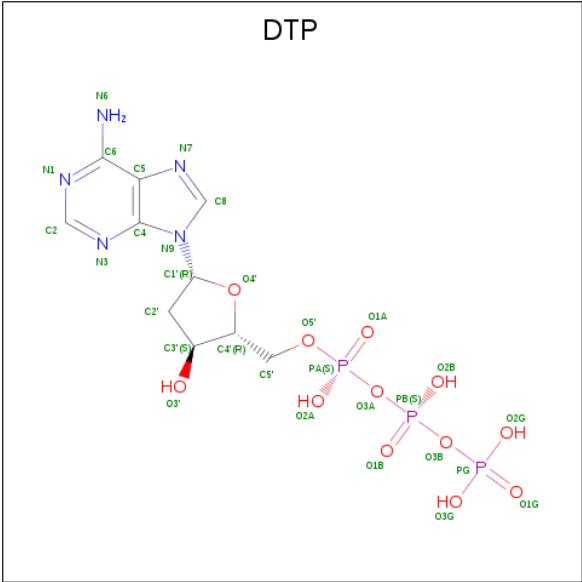
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

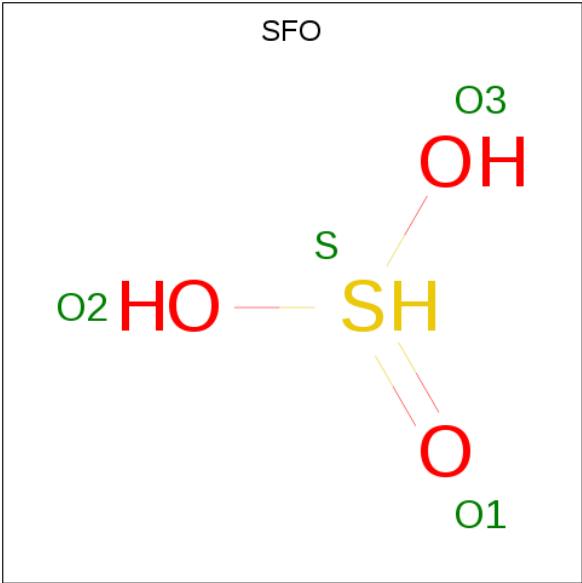
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	P	0	0
			42	10	12	5	12	3		
4	B	1	Total	C	H	N	O	P	0	0
			42	10	12	5	12	3		

- Molecule 5 is SULFONIC ACID (three-letter code: SFO) (formula: $\text{H}_3\text{O}_3\text{S}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	H	O	S	0	0
			7	3	3	1		
5	B	1	Total	H	O	S	0	0
			7	3	3	1		

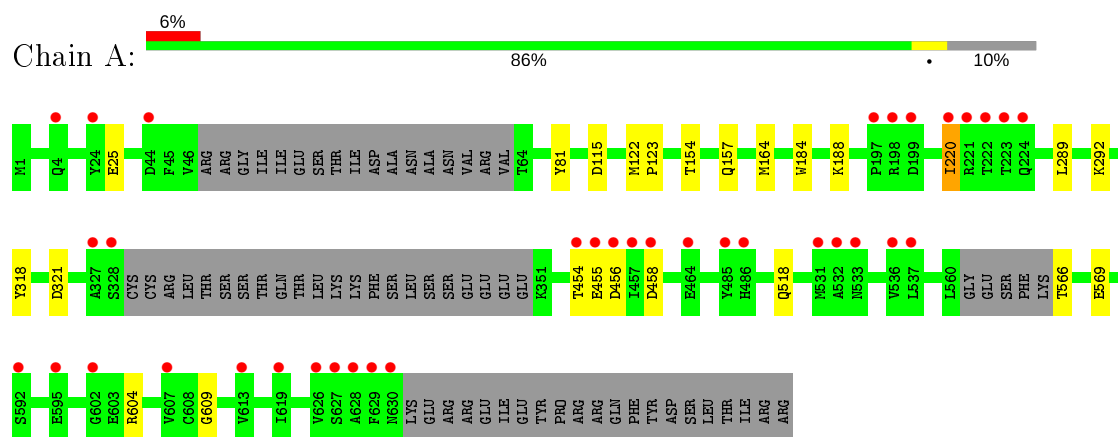
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total 192	O 192	0	0
6	B	162	Total 162	O 162	0	0

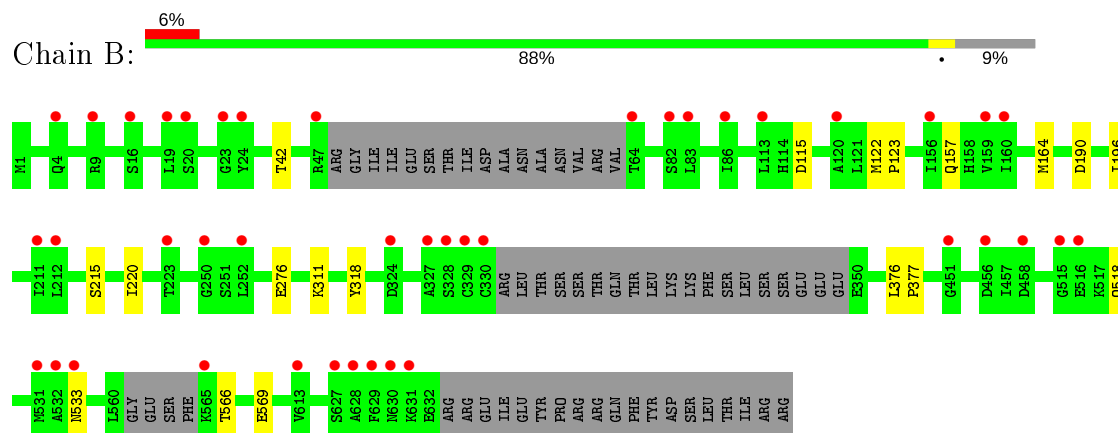
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE



• Molecule 1: ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.00Å 94.12Å 86.71Å 90.00° 112.03° 90.00°	Depositor
Resolution (Å)	29.14 – 1.96 29.14 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.14-1.96) 99.3 (29.14-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.191 , 0.226 0.204 , 0.231	Depositor DCC
R_{free} test set	2078 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10105	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: SFO, ZN, DTP, 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	0.35	0/4914	0.52	0/6634
1	B	0.33	0/4973	0.50	0/6710
All	All	0.34	0/9887	0.51	0/13344

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ILE	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	4795	0	4724	11	0
1	B	4854	0	4785	8	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	12	12	0	0
4	B	30	12	12	0	0
5	A	4	3	3	0	0
5	B	4	3	3	0	0
6	A	192	0	0	0	0
6	B	162	0	0	0	1
All	All	10075	30	9539	17	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 1.

All (17) 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:164[B]:MET:SD	1:A:220:ILE:HG21	2.42	0.59
1:A:456:ASP:OD1	1:A:458:ASP:N	2.39	0.54
1:B:276:GLU:OE2	1:B:311:LYS:NZ	2.42	0.53
1:A:157:GLN:NE2	1:B:157:GLN:OE1	2.46	0.48
1:B:566:THR:HG23	1:B:569:GLU:H	1.80	0.46
1:B:164[B]:MET:SD	1:B:220:ILE:HD13	2.56	0.45
1:A:81:TYR:CE2	1:B:42:THR:HG21	2.51	0.45
1:A:292:LYS:NZ	1:A:321:ASP:O	2.41	0.45
1:A:454:THR:OG1	1:A:455:GLU:N	2.50	0.45
1:B:122:MET:HB2	1:B:123:PRO:HD2	1.99	0.44
1:A:566:THR:HG23	1:A:569:GLU:H	1.84	0.43
1:A:122:MET:HB2	1:A:123:PRO:HD2	1.99	0.42
1:B:190:ASP:HB3	1:B:196:ILE:HG13	2.01	0.42
1:A:25:GLU:N	1:A:25:GLU:OE1	2.44	0.42
1:A:604:ARG:NH1	1:A:609:GLY:O	2.54	0.41
1:B:376:LEU:HB2	1:B:377:PRO:HD3	2.02	0.41
1:A:184:TRP:CH2	1:A:188:LYS:HD2	2.55	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:B:533:ASN:OD1	6:B:2009:HOH:O[2_555]	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	579/651 (89%)	565 (98%)	14 (2%)	0	100	100
1	B	586/651 (90%)	574 (98%)	12 (2%)	0	100	100
All	All	1165/1302 (90%)	1139 (98%)	26 (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	517/577 (90%)	512 (99%)	5 (1%)	76	74
1	B	524/577 (91%)	520 (99%)	4 (1%)	81	80
All	All	1041/1154 (90%)	1032 (99%)	9 (1%)	78	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASP
1	A	154	THR
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	318	TYR
1	A	518	GLN
1	B	115	ASP
1	B	215	SER
1	B	318	TYR
1	B	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z > 2$
4	DTP	A	702	3	26,32,32	0.83	1 (3%)	30,50,50	1.35	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SFO	A	1631	-	1,3,3	0.05	0	0,3,3	0.00	-
4	DTP	B	702	3	26,32,32	0.84	1 (3%)	30,50,50	1.43	5 (16%)
5	SFO	B	1633	-	1,3,3	0.03	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	B	702	3	-	3/18/34/34	0/3/3/3
4	DTP	A	702	3	-	2/18/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	DTP	C5-C4	2.27	1.46	1.40
4	B	702	DTP	C5-C4	2.19	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	DTP	N3-C2-N1	-3.80	122.74	128.68
4	B	702	DTP	N3-C2-N1	-3.57	123.09	128.68
4	B	702	DTP	PB-O3B-PG	-3.17	121.95	132.83
4	A	702	DTP	PB-O3B-PG	-2.88	122.93	132.83
4	B	702	DTP	PA-O3A-PB	-2.71	123.51	132.83
4	B	702	DTP	C4-C5-N7	-2.67	106.62	109.40
4	A	702	DTP	C4-C5-N7	-2.26	107.05	109.40
4	A	702	DTP	PA-O3A-PB	-2.25	125.12	132.83
4	B	702	DTP	O2B-PB-O1B	2.17	122.99	112.24
4	A	702	DTP	C2-N1-C6	2.08	122.31	118.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	DTP	PA-O3A-PB-O1B
4	B	702	DTP	PA-O3A-PB-O2B
4	B	702	DTP	PG-O3B-PB-O2B

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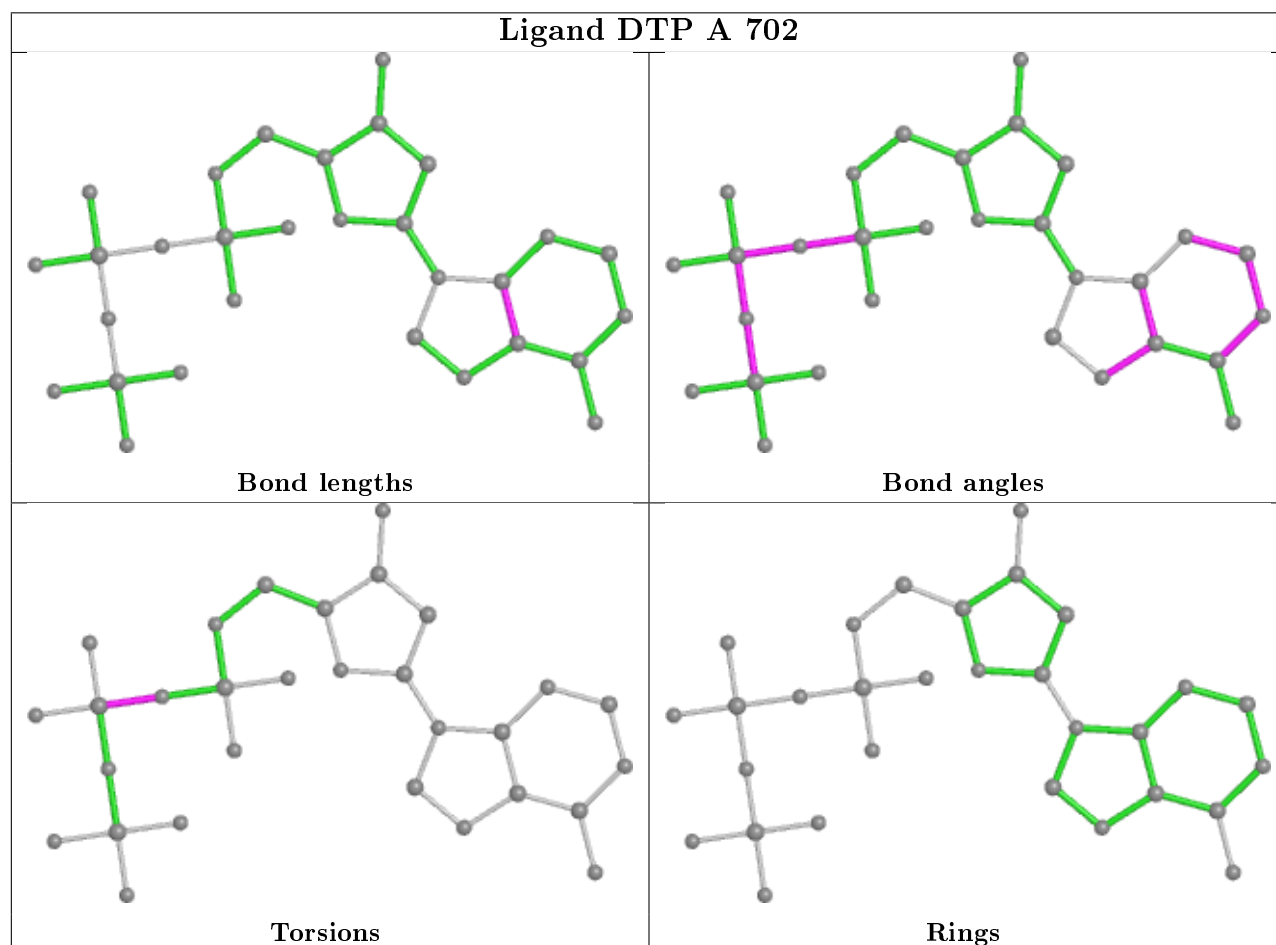
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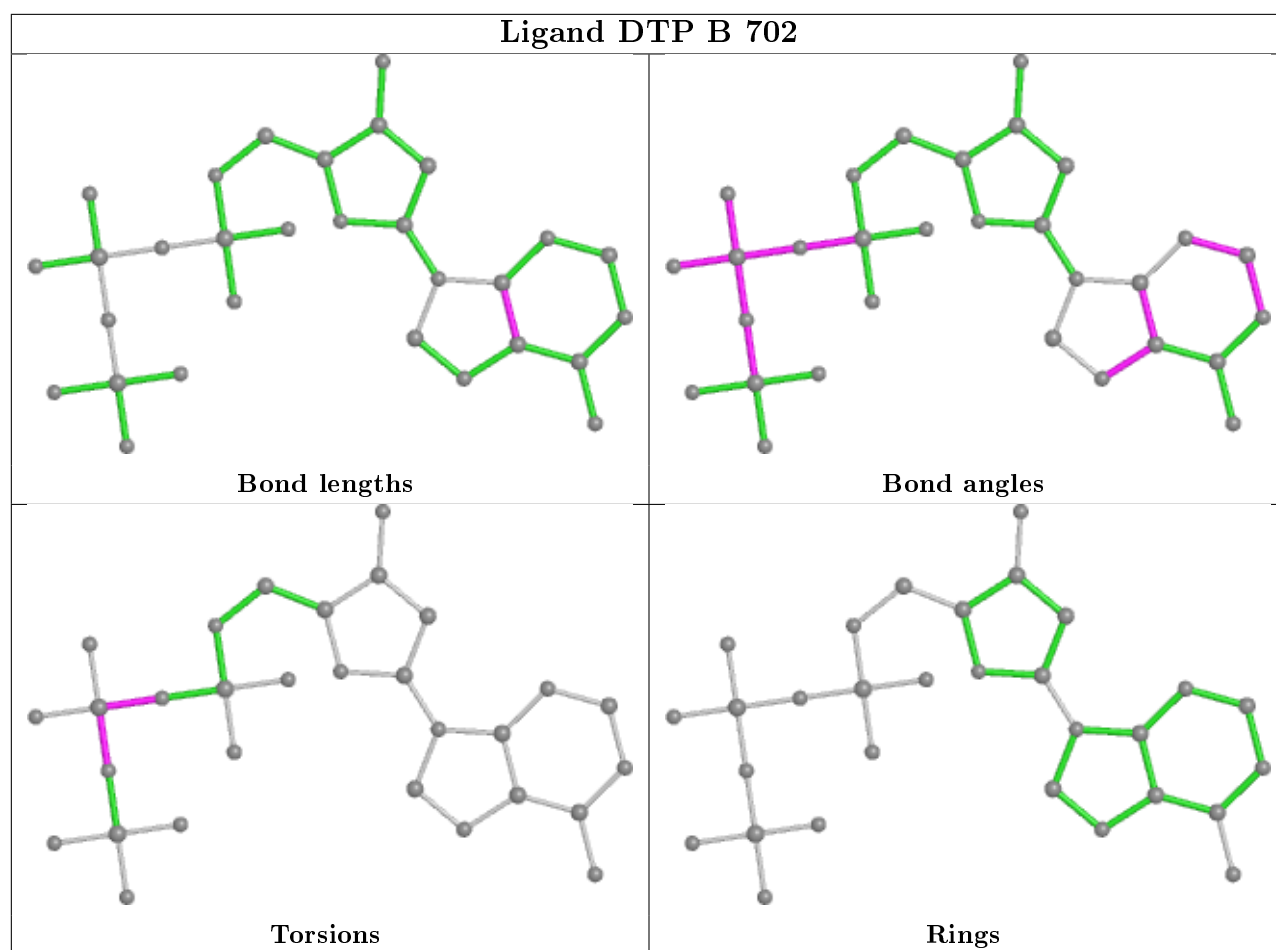
Mol	Chain	Res	Type	Atoms
4	B	702	DTP	PA-O3A-PB-O1B
4	A	702	DTP	PA-O3A-PB-O2B

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	586/651 (90%)	0.34	37 (6%)	20 28	24, 44, 72, 93	0
1	B	593/651 (91%)	0.44	42 (7%)	16 24	24, 46, 75, 93	0
All	All	1179/1302 (90%)	0.39	79 (6%)	17 26	24, 45, 74, 93	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ARG	7.6
1	A	223	THR	7.0
1	B	24	TYR	6.6
1	A	457	ILE	6.3
1	B	531	MET	5.5
1	B	533	ASN	5.5
1	A	627	SER	5.1
1	B	629	PHE	4.8
1	B	328	SER	4.7
1	B	223	THR	4.5
1	A	628	ALA	4.4
1	B	628	ALA	4.3
1	A	629	PHE	4.0
1	B	329	CYS	4.0
1	B	627	SER	3.9
1	A	458	ASP	3.9
1	B	630	ASN	3.6
1	A	220	ILE	3.6
1	A	222	THR	3.6
1	B	160	ILE	3.4
1	A	536	VAL	3.4
1	A	221	ARG	3.3
1	B	458	ASP	3.3
1	A	533	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	607	VAL	3.2
1	B	19	LEU	3.1
1	B	9	ARG	3.1
1	B	47	ARG	3.0
1	A	199	ASP	3.0
1	A	532	ALA	2.9
1	B	212	LEU	2.9
1	B	516	GLU	2.8
1	A	485	TYR	2.8
1	B	156	ILE	2.7
1	B	613	VAL	2.7
1	B	330	CYS	2.7
1	B	515	GLY	2.7
1	A	454	THR	2.7
1	A	626	VAL	2.7
1	B	64	THR	2.7
1	B	631	LYS	2.6
1	A	456	ASP	2.6
1	B	211	ILE	2.6
1	A	613	VAL	2.5
1	A	630	ASN	2.5
1	A	531	MET	2.5
1	A	464	GLU	2.5
1	A	4	GLN	2.4
1	B	83	LEU	2.4
1	A	486	HIS	2.4
1	A	537	LEU	2.4
1	A	602	GLY	2.4
1	A	44	ASP	2.3
1	B	86	ILE	2.3
1	B	565	LYS	2.3
1	B	120	ALA	2.3
1	B	23	GLY	2.3
1	A	619	ILE	2.3
1	B	532	ALA	2.3
1	A	224	GLN	2.3
1	A	592	SER	2.3
1	A	24	TYR	2.3
1	A	197	PRO	2.3
1	B	451	GLY	2.2
1	B	250	GLY	2.2
1	B	16	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	455	GLU	2.2
1	A	327	ALA	2.2
1	B	82	SER	2.1
1	B	4	GLN	2.1
1	A	595	GLU	2.1
1	B	327	ALA	2.1
1	B	159	VAL	2.1
1	B	252	LEU	2.1
1	B	324	ASP	2.0
1	B	456	ASP	2.0
1	A	328	SER	2.0
1	B	113	LEU	2.0
1	B	20	SER	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 carbohydrates in this entry.

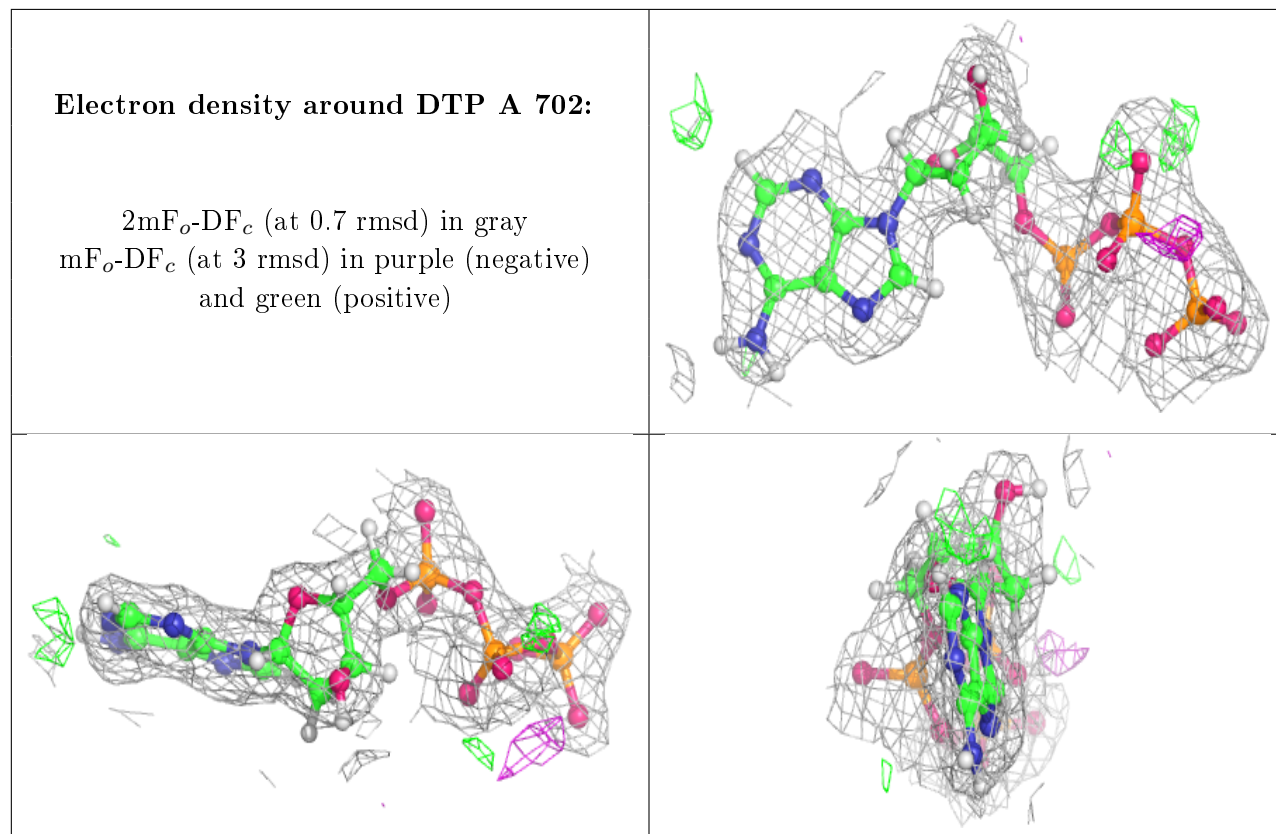
6.4 Ligands [i](#)

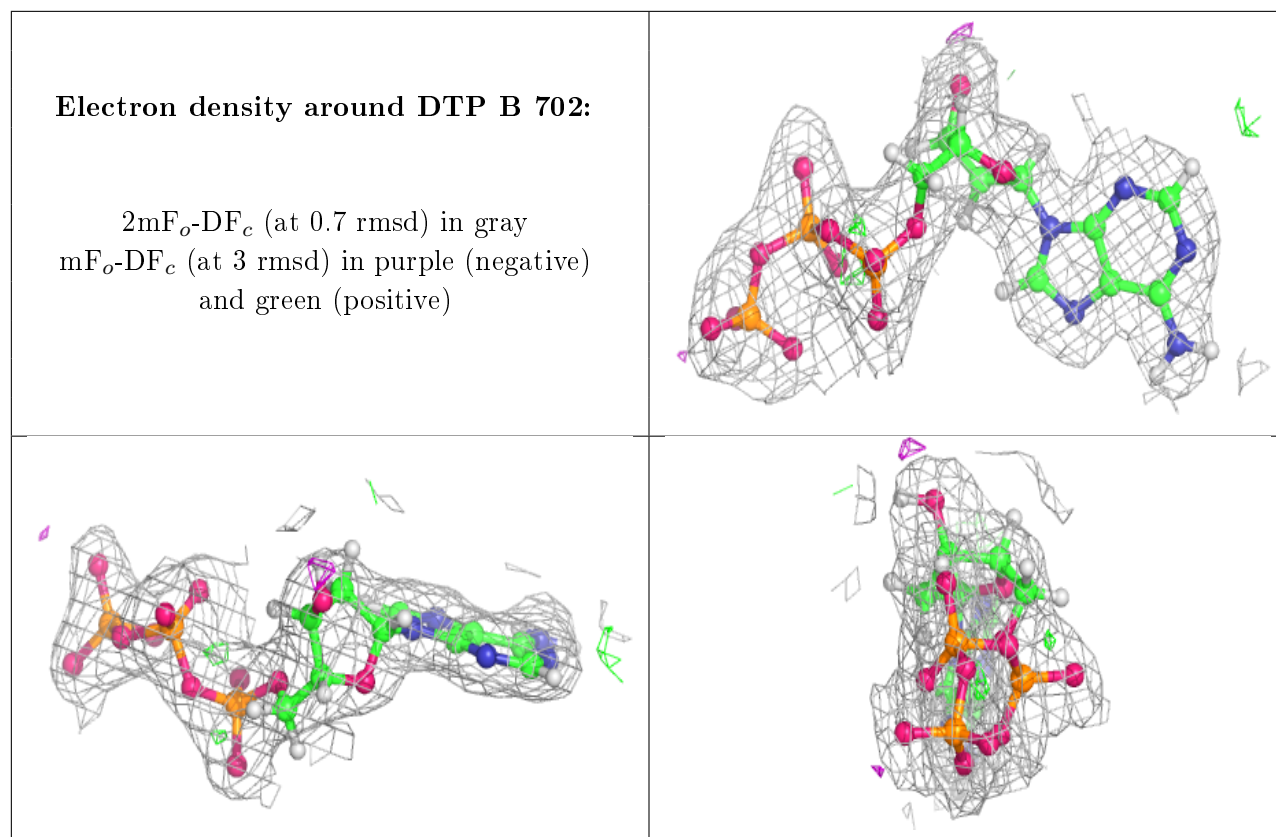
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SFO	A	1631	4/4	0.95	0.10	41,47,64,77	0
3	MG	A	701	1/1	0.96	0.06	38,38,38,38	0
4	DTP	A	702	30/30	0.96	0.08	33,41,48,49	0
5	SFO	B	1633	4/4	0.96	0.09	39,51,75,90	0
3	MG	B	701	1/1	0.97	0.03	39,39,39,39	0
4	DTP	B	702	30/30	0.97	0.10	34,41,49,56	0
2	ZN	B	700	1/1	0.98	0.04	53,53,53,53	0
2	ZN	A	700	1/1	0.98	0.03	60,60,60,60	0

The following is a graphical depiction of the model fit to experimental electron density of all

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





6.5 Other polymers [i](#)

There are no such residues in this entry.