



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 06:20 PM EDT

PDB ID : 3BMO / pdb\_00003bmo  
Title : Structure of Pteridine Reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor (Compound AX4)  
Authors : Martini, V.P.; Iulek, J.; Hunter, W.N.; Tulloch, L.B.  
Deposited on : 2007-12-13  
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

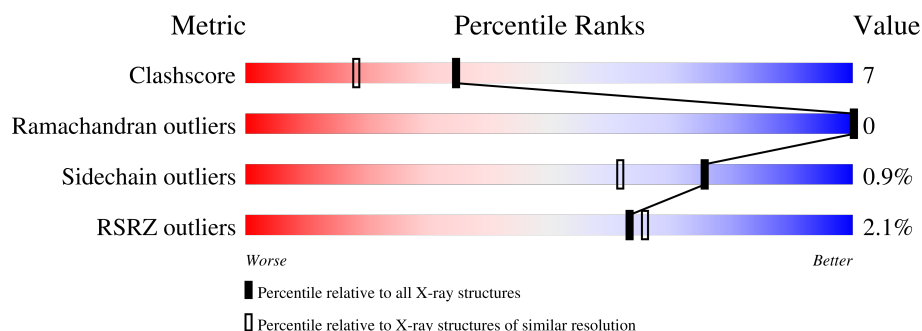
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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  $\geq 3$ , 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	288	<div> <div>2%</div> <div>78%</div> <div>10%</div> <div>11%</div> </div>
1	C	288	<div> <div>2%</div> <div>78%</div> <div>8%</div> <div>12%</div> </div>
1	D	288	<div> <div>2%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
2	B	288	<div> <div>%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AX4	C	272[A]	-	-	X	-
7	DTT	A	275	X	-	-	-
8	D1D	B	273[B]	-	-	X	-
9	GOL	B	274[C]	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9481 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 Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	23	0
			2013	1276	346	378	13			
1	C	252	Total	C	N	O	S	0	16	0
			1962	1241	344	365	12			
1	D	251	Total	C	N	O	S	0	21	0
			1981	1266	341	362	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O76290
A	-18	GLY	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	SER	-	expression tag	UNP O76290
A	-15	HIS	-	expression tag	UNP O76290
A	-14	HIS	-	expression tag	UNP O76290
A	-13	HIS	-	expression tag	UNP O76290
A	-12	HIS	-	expression tag	UNP O76290
A	-11	HIS	-	expression tag	UNP O76290
A	-10	HIS	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	SER	-	expression tag	UNP O76290
A	-7	GLY	-	expression tag	UNP O76290
A	-6	LEU	-	expression tag	UNP O76290
A	-5	VAL	-	expression tag	UNP O76290
A	-4	PRO	-	expression tag	UNP O76290
A	-3	ARG	-	expression tag	UNP O76290
A	-2	GLY	-	expression tag	UNP O76290
A	-1	SER	-	expression tag	UNP O76290
A	0	HIS	-	expression tag	UNP O76290
C	-19	MET	-	expression tag	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag	UNP O76290
C	-12	HIS	-	expression tag	UNP O76290
C	-11	HIS	-	expression tag	UNP O76290
C	-10	HIS	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	SER	-	expression tag	UNP O76290
C	-7	GLY	-	expression tag	UNP O76290
C	-6	LEU	-	expression tag	UNP O76290
C	-5	VAL	-	expression tag	UNP O76290
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	expression tag	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	SER	-	expression tag	UNP O76290
D	-7	GLY	-	expression tag	UNP O76290
D	-6	LEU	-	expression tag	UNP O76290
D	-5	VAL	-	expression tag	UNP O76290
D	-4	PRO	-	expression tag	UNP O76290
D	-3	ARG	-	expression tag	UNP O76290
D	-2	GLY	-	expression tag	UNP O76290
D	-1	SER	-	expression tag	UNP O76290
D	0	HIS	-	expression tag	UNP O76290

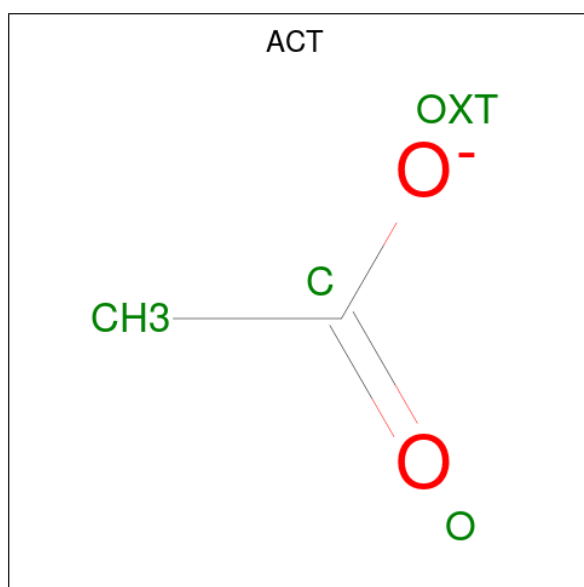
- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	17	0
			1947	1237	336	361	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP O76290
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 1        | Total Na<br>1 1 | 0       | 0       |

- # NAP
- 
- The chemical structure of Naproxen (NAP) is shown, featuring a naproxen core with a propionic acid side chain. The stereochemistry is indicated by wedges and dashes at the chiral centers. The atom numbering is provided for each atom in the structure.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

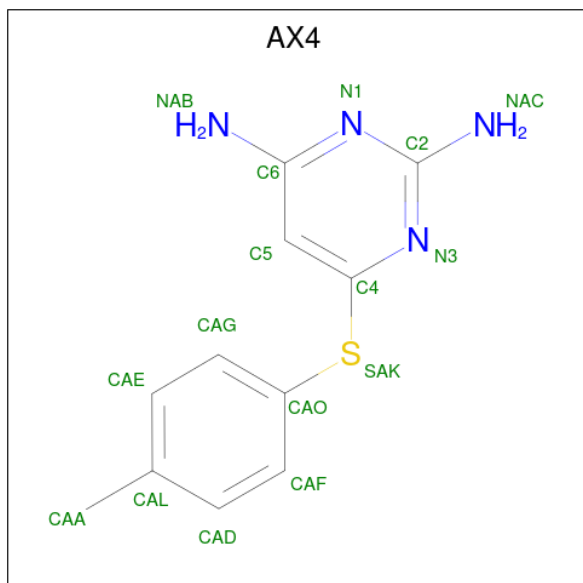


WORLD WIDE  
**PDB**  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

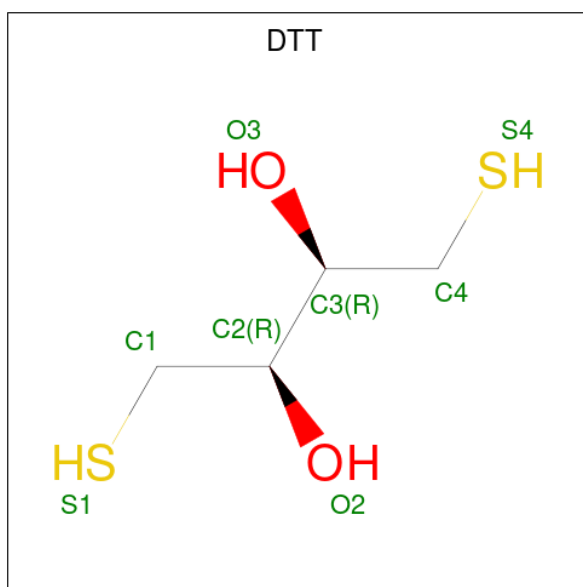
- Molecule 6 is 6-[(4-methylphenyl)sulfanyl]pyrimidine-2,4-diamine (CCD ID: AX4) (formula:  $C_{11}H_{12}N_4S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	1
			16	11	4	1		
6	B	1	Total	C	N	S	0	1
			16	11	4	1		
6	C	1	Total	C	N	S	0	1
			16	11	4	1		
6	D	1	Total	C	N	S	0	1
			16	11	4	1		

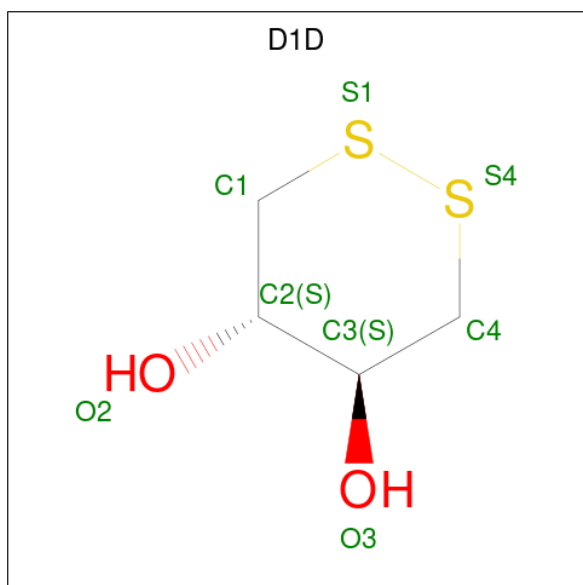
- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula:  $C_4H_{10}O_2S_2$ ).





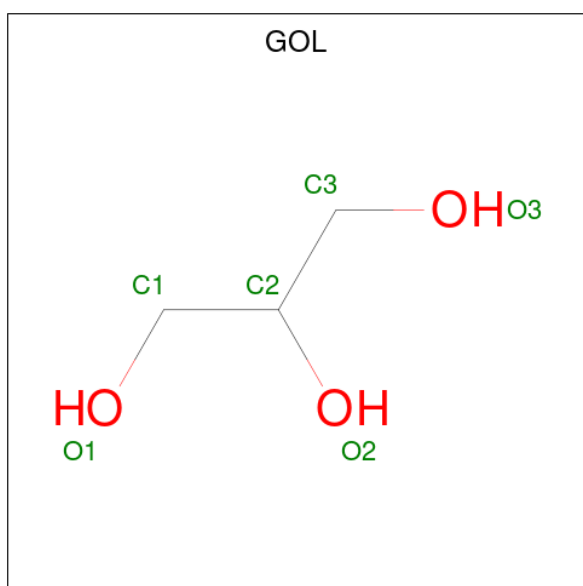
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			8	4	2	2		
7	B	1	Total	C	O	S	0	0
			8	4	2	2		
7	C	1	Total	C	O	S	0	0
			8	4	2	2		
7	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 8 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (CCD ID: D1D) (formula:  $C_4H_8O_2S_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 8 4 2 2	0	1
8	B	1	Total C O S 8 4 2 2	0	1
8	C	1	Total C O S 8 4 2 2	0	1
8	D	1	Total C O S 8 4 2 2	0	1

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	1
9	B	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	309	Total O 309 309	0	0
10	B	304	Total O 304 304	0	0
10	C	298	Total O 298 298	0	0

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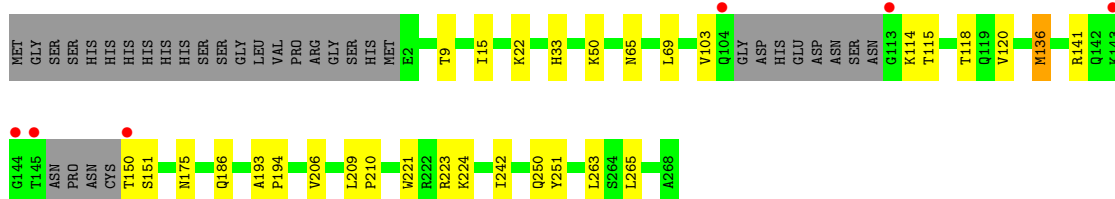
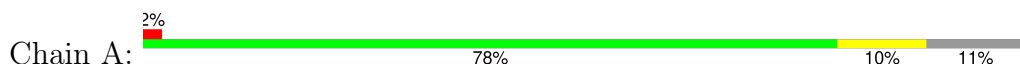
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	300	Total 300	O 300	0	0

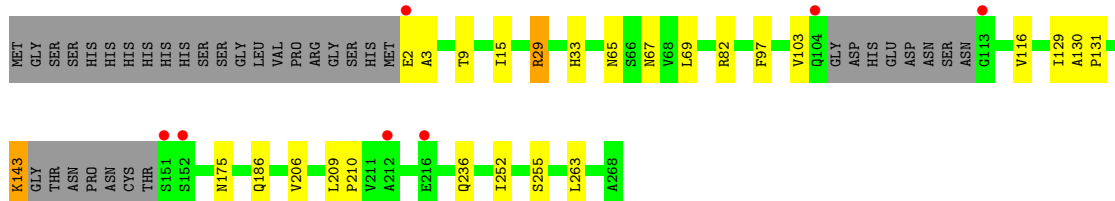
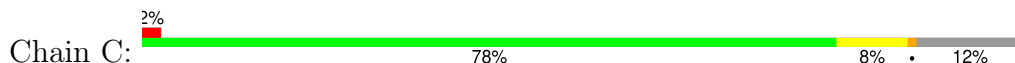
### 3 Residue-property plots [i](#)

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.

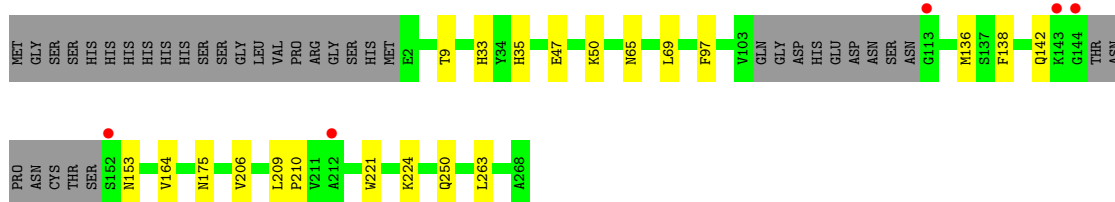
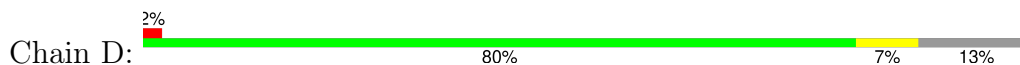
- Molecule 1: Pteridine reductase



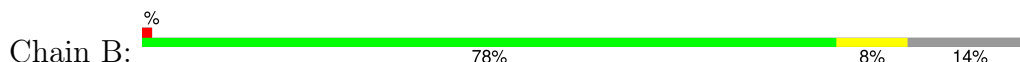
- Molecule 1: Pteridine reductase



- Molecule 1: Pteridine reductase



- Molecule 2: Pteridine reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73Å 90.99Å 82.82Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	22.38 – 1.60 22.38 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (22.38-1.60) 95.4 (22.38-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.118 , 0.150 0.135 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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 20.13 % 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 9.2899e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AX4, NAP, D1D, DTT, CSX, ACT, GOL, NA

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	0.89	0/2109	0.87	0/2853
1	C	0.88	0/2037	0.87	0/2756
1	D	0.85	0/2074	0.82	0/2803
2	B	0.91	0/2017	0.86	0/2728
All	All	0.89	0/8237	0.86	0/11140

There are no bond length outliers.

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	2013	0	2109	38	0
1	C	1962	0	2045	32	0
1	D	1981	0	2101	21	0
2	B	1947	0	2040	25	0
3	A	12	0	9	1	0
3	B	4	0	3	0	0
3	C	8	0	6	0	0
3	D	4	0	3	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	48	0	25	1	0
5	B	48	0	25	2	0
5	C	48	0	25	1	0
5	D	48	0	25	1	0
6	A	16	0	7	3	0
6	B	16	0	7	0	0
6	C	16	0	7	7	0
6	D	16	0	7	4	0
7	A	8	0	9	2	0
7	B	8	0	9	3	0
7	C	8	0	9	0	0
7	D	8	0	9	0	0
8	A	8	0	8	3	0
8	B	8	0	8	7	0
8	C	8	0	8	2	0
8	D	8	0	8	2	0
9	A	6	0	8	0	0
9	B	12	0	16	6	0
10	A	309	0	0	8	0
10	B	304	0	0	16	0
10	C	298	0	0	8	0
10	D	300	0	0	4	0
All	All	9481	0	8536	124	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 7.

The worst 5 of 124 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:223[B]:ARG:NH1	1:A:224[B]:LYS:HG3	1.43	1.32
1:A:223[B]:ARG:NH1	1:A:224[B]:LYS:CG	1.99	1.26
1:A:223[B]:ARG:HH12	1:A:224[B]:LYS:CG	1.48	1.26
2:B:168:CSX:SG	2:B:168:CSX:OD	2.14	1.04
1:A:223[B]:ARG:HH22	1:A:224[B]:LYS:HZ1	1.08	1.00

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	271/288 (94%)	261 (96%)	10 (4%)	0	100	100
1	C	262/288 (91%)	251 (96%)	11 (4%)	0	100	100
1	D	266/288 (92%)	256 (96%)	10 (4%)	0	100	100
2	B	259/288 (90%)	251 (97%)	8 (3%)	0	100	100
All	All	1058/1152 (92%)	1019 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	225/231 (97%)	222 (99%)	3 (1%)	65	46
1	C	216/231 (94%)	211 (98%)	5 (2%)	45	21
1	D	220/231 (95%)	220 (100%)	0	100	100
2	B	213/230 (93%)	211 (99%)	2 (1%)	75	62
All	All	874/923 (95%)	864 (99%)	10 (1%)	75	53

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29[B]	ARG
1	C	67	ASN
1	C	143	LYS

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Mol	Chain	Res	Type
2	B	67[A]	ASN
2	B	67[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	119	GLN
1	D	92	ASN
1	C	67	ASN
1	C	236	GLN
1	C	60	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSX	B	168	2	3,6,7	0.82	0	1,6,8	2.54	1 (100%)

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	CSX	B	168	2	-	0/2/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	CSX	CA-CB-SG	2.54	119.15	113.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	168	CSX	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	ACT	A	271	-	3,3,3	1.12	0	3,3,3	0.90	0
5	NAP	A	273	-	46,52,52	1.51	5 (10%)	61,80,80	1.52	9 (14%)
8	D1D	B	273[B]	-	8,8,8	0.90	0	6,10,10	0.98	0
3	ACT	A	269	-	3,3,3	0.79	0	3,3,3	1.42	0
3	ACT	C	270	-	3,3,3	0.84	0	3,3,3	1.19	0
5	NAP	B	270	-	46,52,52	1.59	8 (17%)	61,80,80	1.66	11 (18%)
3	ACT	A	270	-	3,3,3	0.53	0	3,3,3	1.41	0
9	GOL	B	274[C]	-	5,5,5	0.64	0	5,5,5	0.27	0
7	DTT	B	272	-	7,7,7	0.72	0	4,8,8	1.12	0
8	D1D	D	273[B]	-	8,8,8	1.03	1 (12%)	6,10,10	0.87	0
3	ACT	D	269	-	3,3,3	0.90	0	3,3,3	1.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DTT	D	272	-	7,7,7	0.57	0	4,8,8	0.90	0
8	D1D	C	274[B]	-	8,8,8	1.46	1 (12%)	6,10,10	2.04	2 (33%)
5	NAP	C	271	-	46,52,52	1.41	2 (4%)	61,80,80	1.65	9 (14%)
7	DTT	C	273	-	7,7,7	0.67	0	4,8,8	0.73	0
5	NAP	D	270	-	46,52,52	1.47	3 (6%)	61,80,80	1.71	10 (16%)
8	D1D	A	276[B]	-	8,8,8	1.40	1 (12%)	6,10,10	0.84	0
7	DTT	A	275	-	7,7,7	0.54	0	4,8,8	0.71	0
9	GOL	B	275	-	5,5,5	0.38	0	5,5,5	0.67	0
9	GOL	A	277	-	5,5,5	0.70	0	5,5,5	1.15	0
3	ACT	C	269	-	3,3,3	0.72	0	3,3,3	1.25	0
3	ACT	B	269	-	3,3,3	0.65	0	3,3,3	1.32	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
9	GOL	B	275	-	-	1/4/4/4	-
8	D1D	C	274[B]	-	-	-	0/1/1/1
5	NAP	A	273	-	-	0/31/67/67	0/5/5/5
9	GOL	B	274[C]	-	-	2/4/4/4	-
7	DTT	B	272	-	-	7/8/8/8	-
5	NAP	C	271	-	-	0/31/67/67	0/5/5/5
8	D1D	B	273[B]	-	-	-	0/1/1/1
7	DTT	C	273	-	-	3/8/8/8	-
9	GOL	A	277	-	-	0/4/4/4	-
8	D1D	D	273[B]	-	-	-	0/1/1/1
5	NAP	D	270	-	-	0/31/67/67	0/5/5/5
7	DTT	D	272	-	-	2/8/8/8	-
8	D1D	A	276[B]	-	-	-	0/1/1/1
5	NAP	B	270	-	-	0/31/67/67	0/5/5/5
7	DTT	A	275	-	2/2/2/2	2/8/8/8	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	270	NAP	O7N-C7N	6.82	1.36	1.24
5	C	271	NAP	O7N-C7N	6.14	1.35	1.24
5	A	273	NAP	O7N-C7N	5.26	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	270	NAP	O7N-C7N	5.18	1.33	1.24
5	C	271	NAP	C2A-N3A	4.45	1.39	1.32

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	270	NAP	N3A-C2A-N1A	-6.81	119.42	128.67
5	C	271	NAP	C4B-O4B-C1B	-6.30	104.16	109.92
5	D	270	NAP	C4B-O4B-C1B	-5.68	104.72	109.92
5	A	273	NAP	C4B-O4B-C1B	-5.21	105.15	109.92
5	C	271	NAP	N3A-C2A-N1A	-5.14	121.70	128.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	275	DTT	C2
7	A	275	DTT	C3

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	275	DTT	C1-C2-C3-C4
7	A	275	DTT	O3-C3-C4-S4
7	B	272	DTT	S1-C1-C2-O2
7	B	272	DTT	C1-C2-C3-O3
7	B	272	DTT	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 31 short contacts:

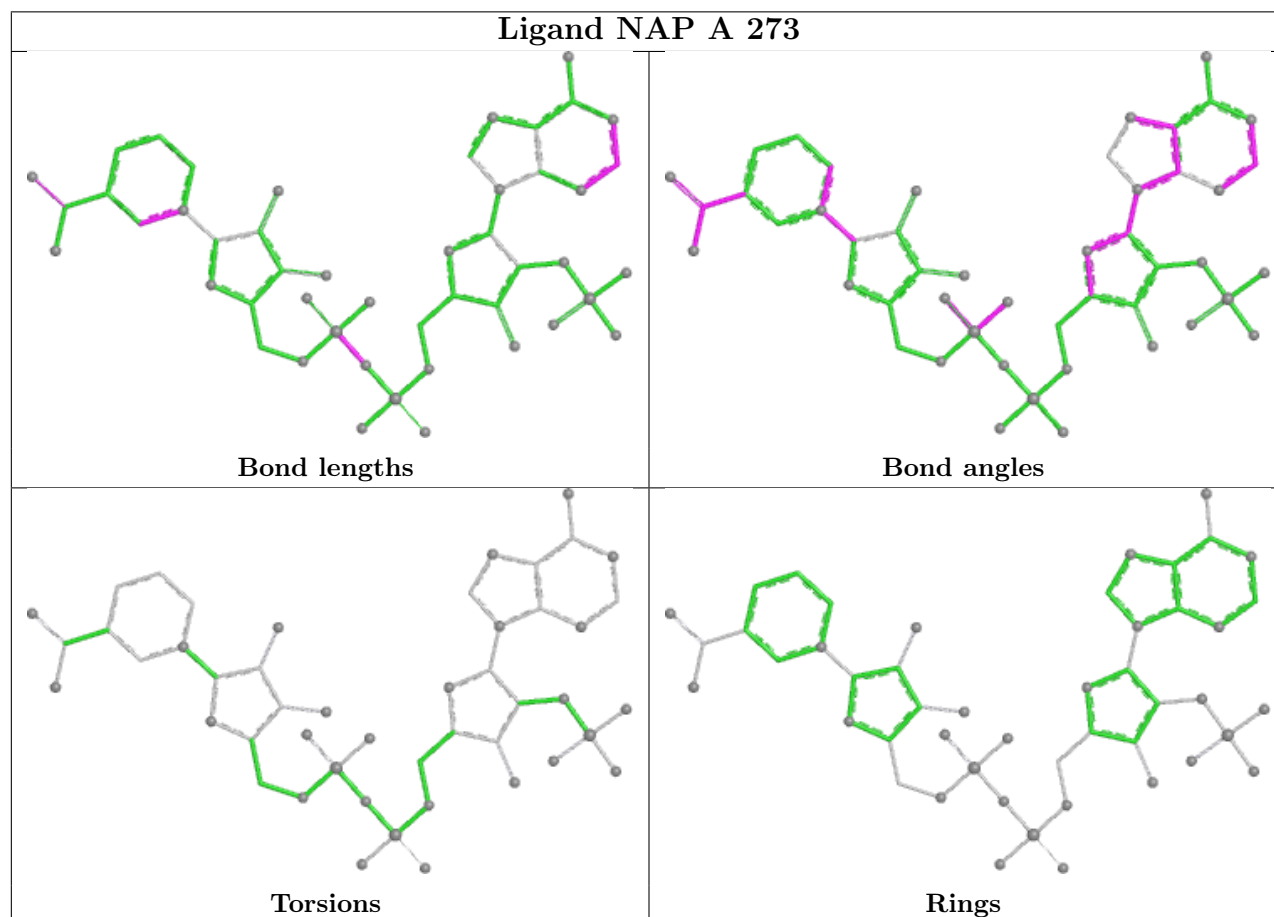
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	271	ACT	1	0
5	A	273	NAP	1	0
8	B	273[B]	D1D	7	0
5	B	270	NAP	2	0
9	B	274[C]	GOL	5	0
7	B	272	DTT	3	0
8	D	273[B]	D1D	2	0
8	C	274[B]	D1D	2	0
5	C	271	NAP	1	0
5	D	270	NAP	1	0

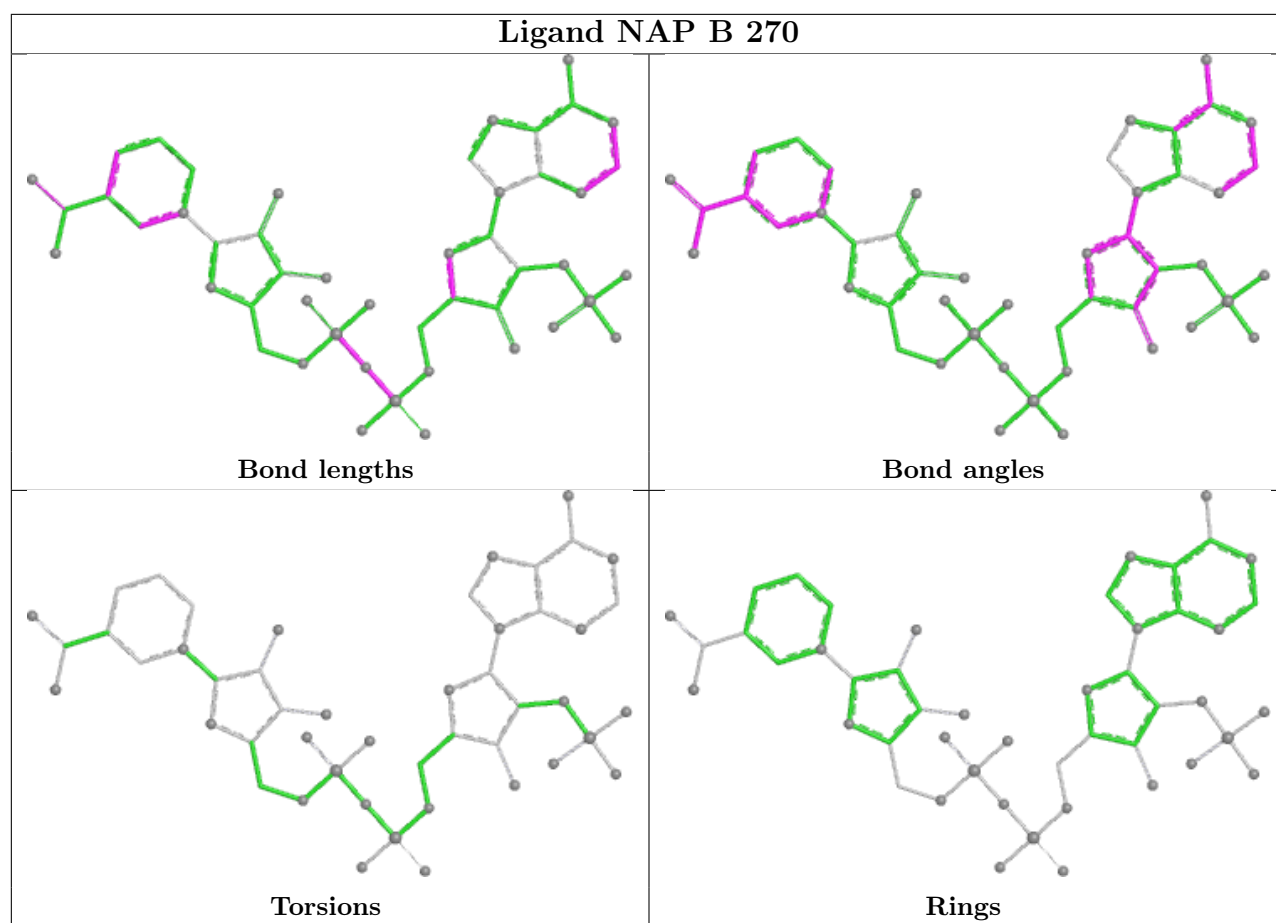
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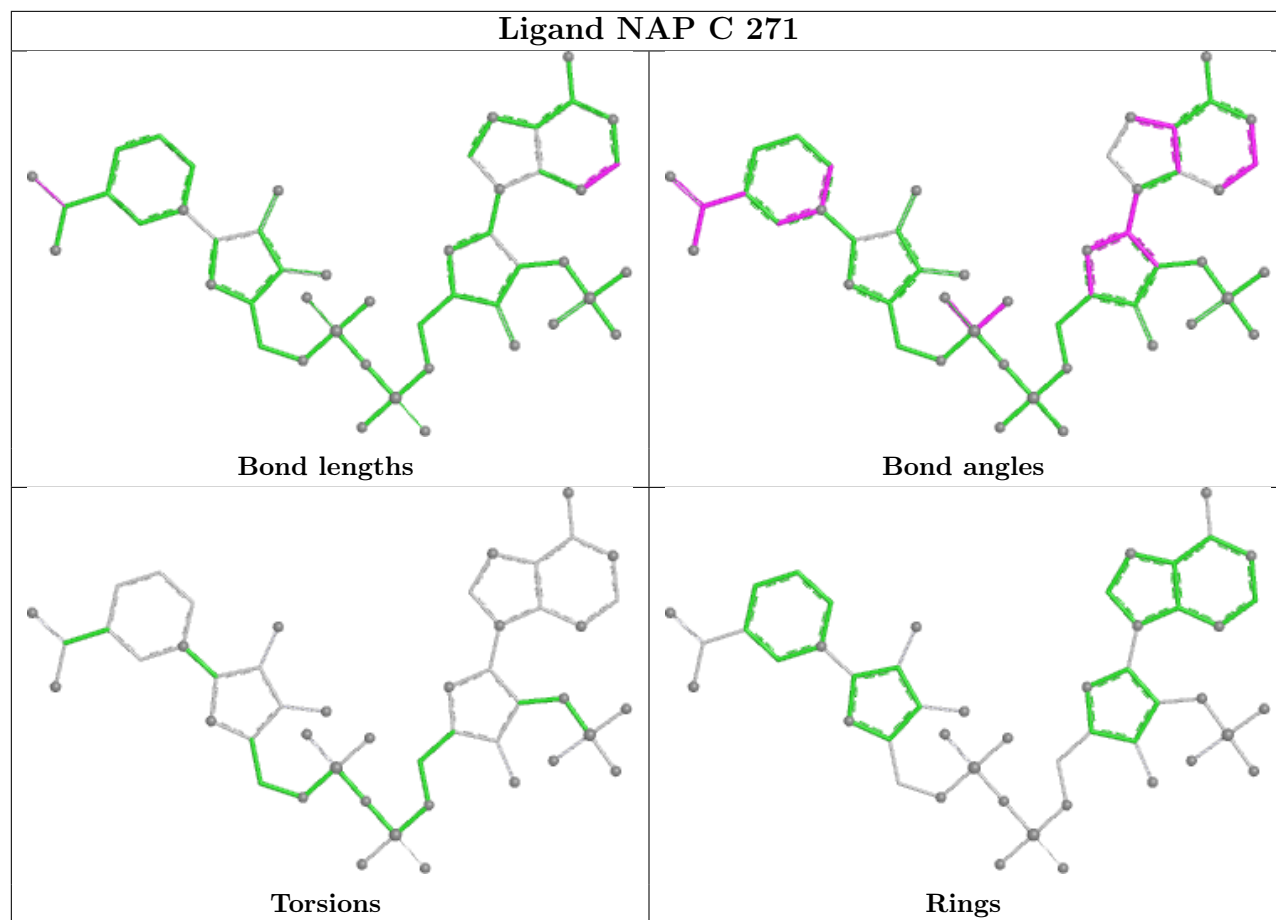
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	276[B]	D1D	3	0
7	A	275	DTT	2	0
9	B	275	GOL	1	0

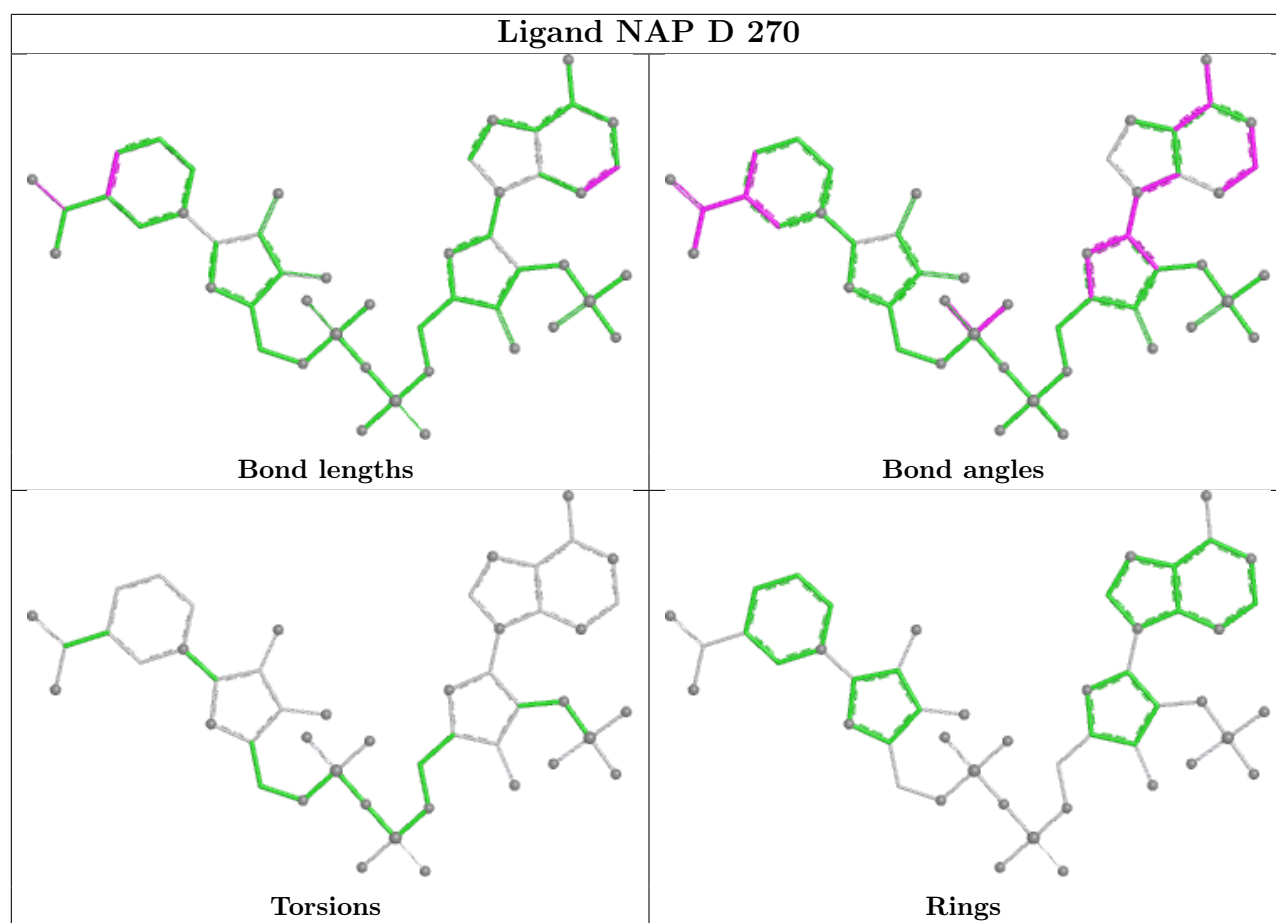
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	255/288 (88%)	-0.39	6 (2%) 59 62	5, 10, 23, 54	23 (9%)
1	C	252/288 (87%)	-0.25	7 (2%) 55 56	6, 11, 27, 45	16 (6%)
1	D	251/288 (87%)	-0.17	5 (1%) 64 67	5, 11, 25, 53	21 (8%)
2	B	248/288 (86%)	-0.51	3 (1%) 76 79	5, 9, 18, 48	17 (6%)
All	All	1006/1152 (87%)	-0.33	21 (2%) 63 66	5, 10, 24, 54	77 (7%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	THR	4.4
1	D	113	GLY	3.4
1	C	212	ALA	3.3
1	D	144	GLY	3.2
2	B	1	MET	3.0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CSX	B	168	7/8	0.91	0.10	11,13,26,28	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

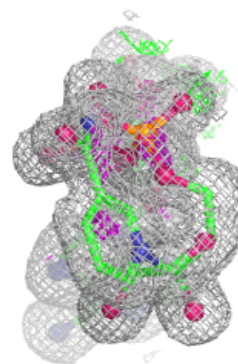
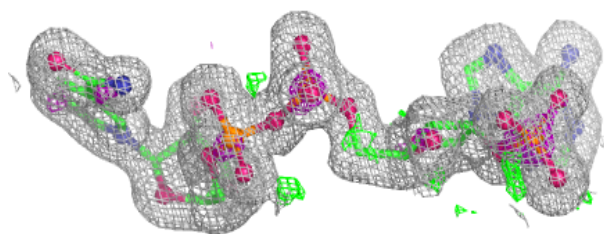
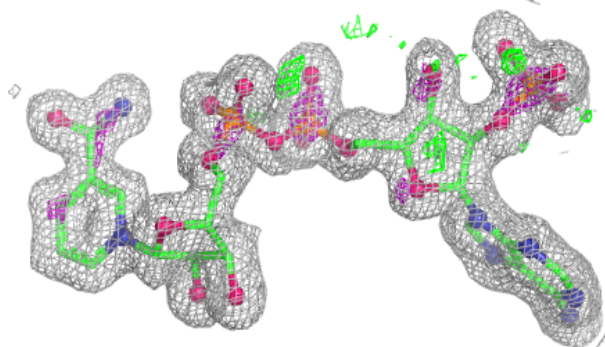
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	GOL	B	275	6/6	0.75	0.14	25,29,30,34	0
3	ACT	A	271	4/4	0.81	0.14	21,26,28,29	0
3	ACT	B	269	4/4	0.84	0.17	23,23,24,26	0
8	D1D	D	273[B]	8/8	0.86	0.15	26,28,30,31	8
8	D1D	A	276[B]	8/8	0.89	0.14	27,31,34,34	8
3	ACT	A	270	4/4	0.90	0.18	24,24,25,27	0
9	GOL	B	274[C]	6/6	0.91	0.11	15,23,28,31	6
7	DTT	A	275	8/8	0.92	0.13	29,46,52,59	0
7	DTT	B	272	8/8	0.92	0.14	25,45,53,57	0
3	ACT	D	269	4/4	0.92	0.16	23,23,23,26	0
8	D1D	C	274[B]	8/8	0.93	0.10	17,21,25,27	8
7	DTT	D	272	8/8	0.93	0.13	27,46,52,58	0
7	DTT	C	273	8/8	0.93	0.13	27,42,49,56	0
8	D1D	B	273[B]	8/8	0.93	0.13	16,18,20,21	8
3	ACT	C	269	4/4	0.94	0.14	21,21,22,24	0
9	GOL	A	277	6/6	0.94	0.11	15,18,19,23	0
4	NA	A	272	1/1	0.96	0.08	28,28,28,28	0
3	ACT	C	270	4/4	0.97	0.06	15,17,18,18	0
6	AX4	A	274[A]	16/16	0.97	0.09	7,10,11,14	7
6	AX4	B	271[A]	16/16	0.97	0.07	7,10,15,18	7
6	AX4	D	271[A]	16/16	0.97	0.10	10,13,15,15	7
3	ACT	A	269	4/4	0.97	0.08	11,12,12,16	0
5	NAP	D	270	48/48	0.98	0.05	8,10,12,13	0
5	NAP	A	273	48/48	0.98	0.04	6,9,10,13	0
5	NAP	C	271	48/48	0.98	0.04	7,10,11,12	0
6	AX4	C	272[A]	16/16	0.98	0.08	9,13,17,18	7
5	NAP	B	270	48/48	0.99	0.04	5,8,10,11	0

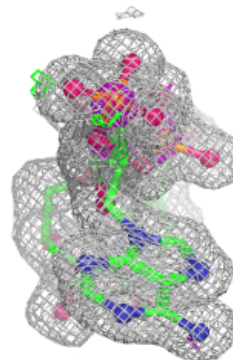
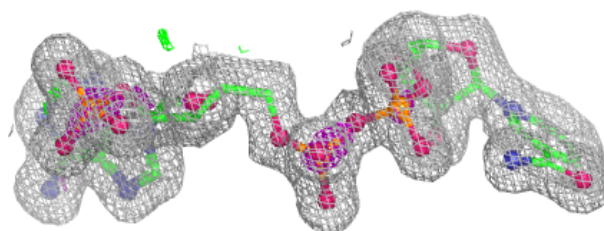
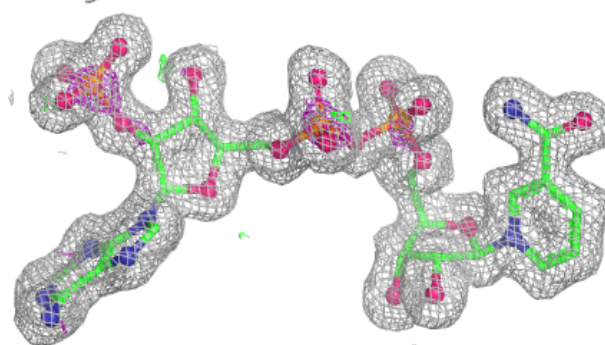
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP D 270:**

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

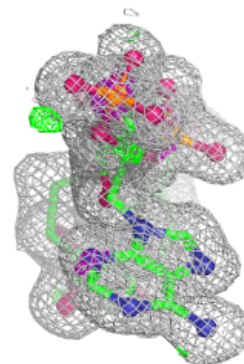
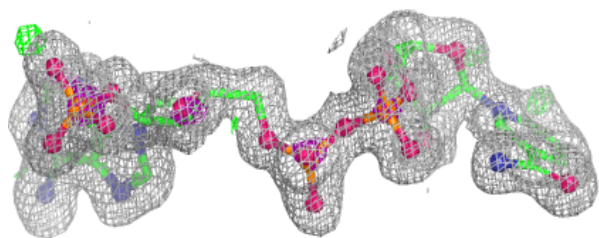
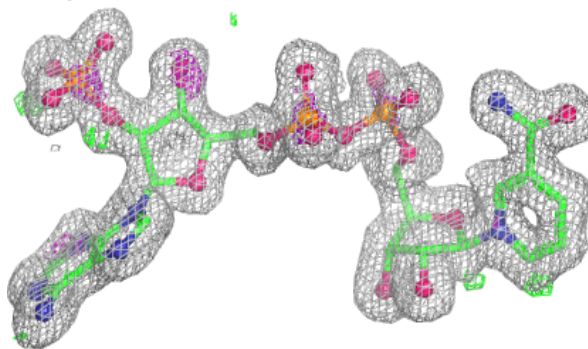
**Electron density around NAP A 273:**

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

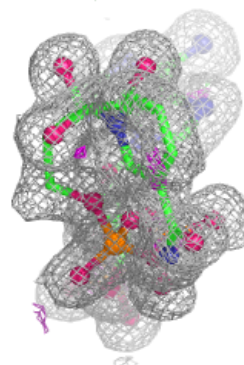
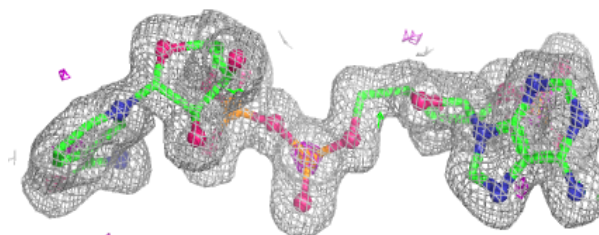


**Electron density around NAP C 271:**

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

**Electron density around NAP B 270:**

$2mF_o-DF_c$  (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.