



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 AM GMT

PDB ID : 3BMO  
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 Full wwPDB X-ray Structure Validation 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

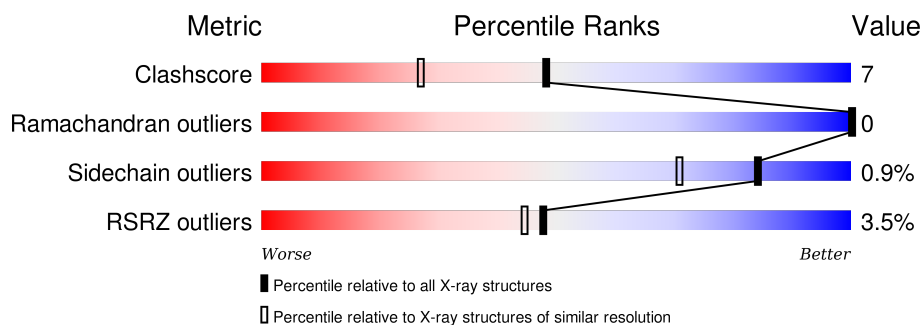
# 1 Overall quality at a glance

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	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	C	288	
1	D	288	
2	B	288	

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
3	ACT	A	270	-	-	-	X
3	ACT	A	271	-	-	-	X
3	ACT	B	269	-	-	-	X
3	ACT	C	269	-	-	-	X
3	ACT	D	269	-	-	-	X
6	AX4	C	272[A]	-	-	X	-
7	DTT	A	275	X	-	-	X
7	DTT	B	272	-	-	-	X
8	D1D	A	276[B]	-	-	-	X
8	D1D	B	273[B]	-	-	X	-
8	D1D	C	274[B]	-	-	-	X
8	D1D	D	273[B]	-	-	-	X
9	GOL	B	274[C]	-	-	X	X
9	GOL	B	275	-	-	-	X

## 2 Entry composition

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

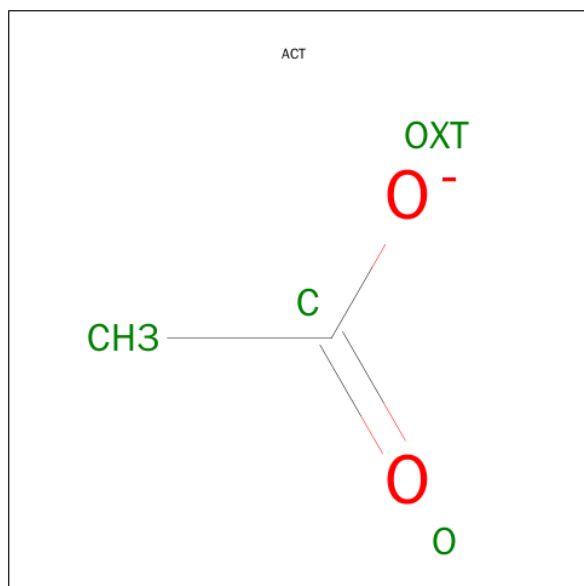
- Molecule 2 is a protein called Pteridine reductase.

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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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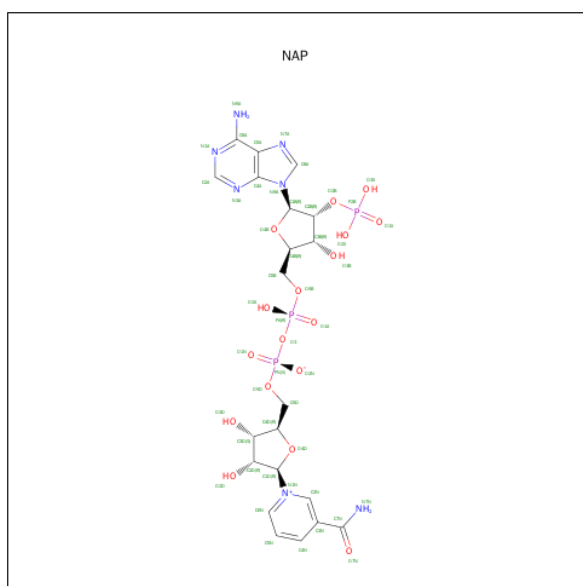
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



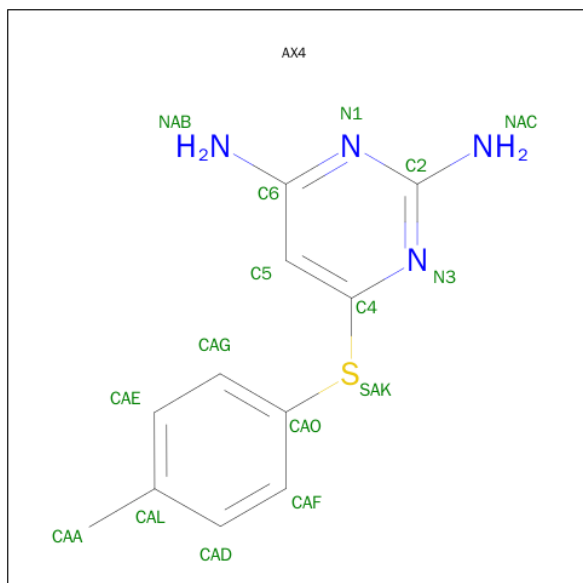
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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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		

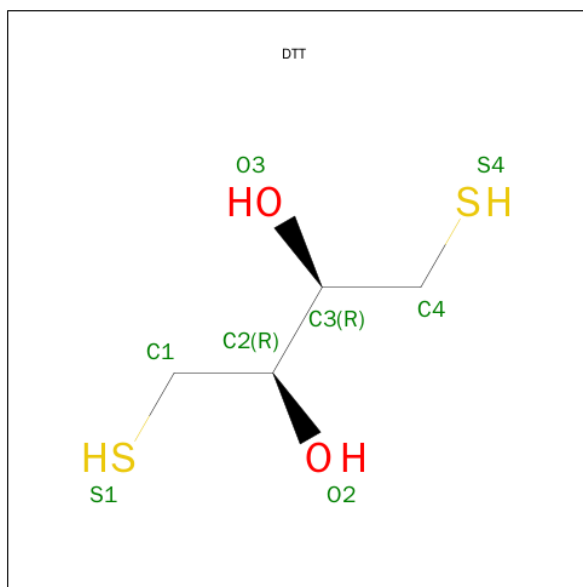
- Molecule 6 is 6-[(4-METHYLPHENYL)SULFANYL]PYRIMIDINE-2,4-DIAMINE (three-letter code: AX4) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>4</sub>S).



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		

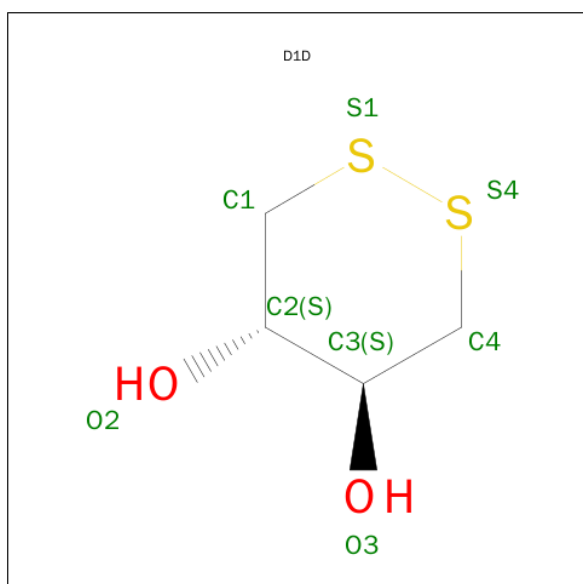
- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).





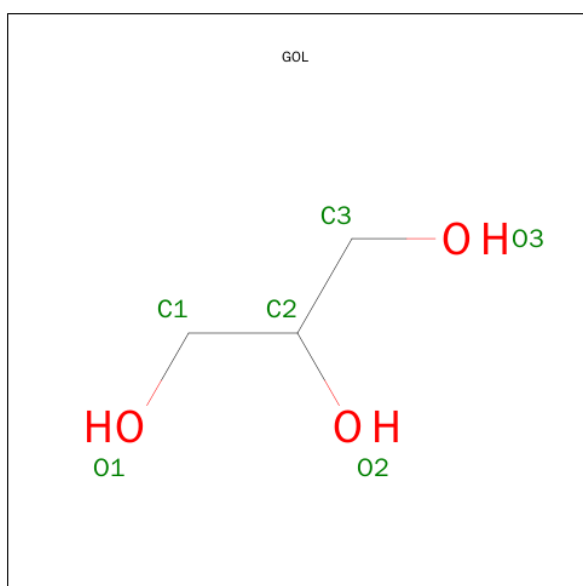
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			8	4	2	2		
7	B	1	Total	C	O	S	0	0
			8	4	2	2		
7	C	1	Total	C	O	S	0	0
			8	4	2	2		
7	D	1	Total	C	O	S	0	0
			8	4	2	2		

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



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 10 is water.

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

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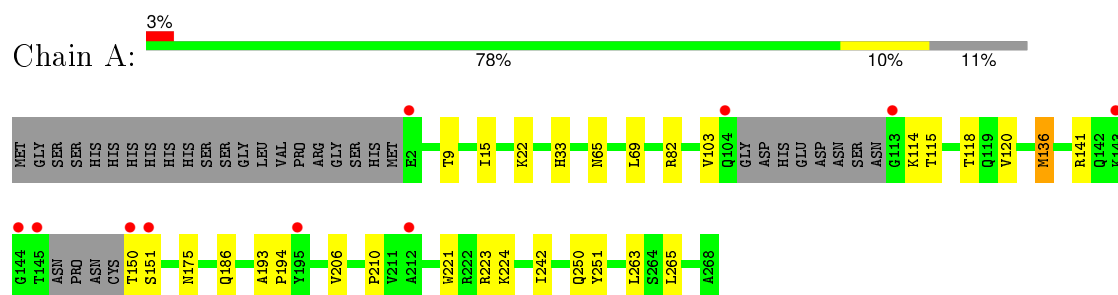
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	300	Total	O	0	0
			300	300		

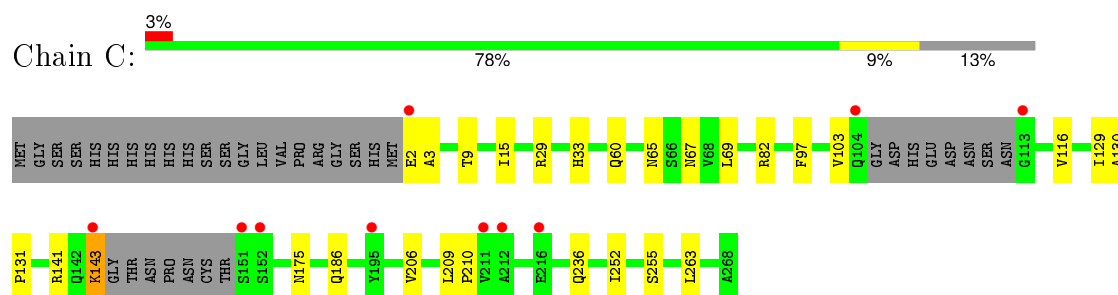
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

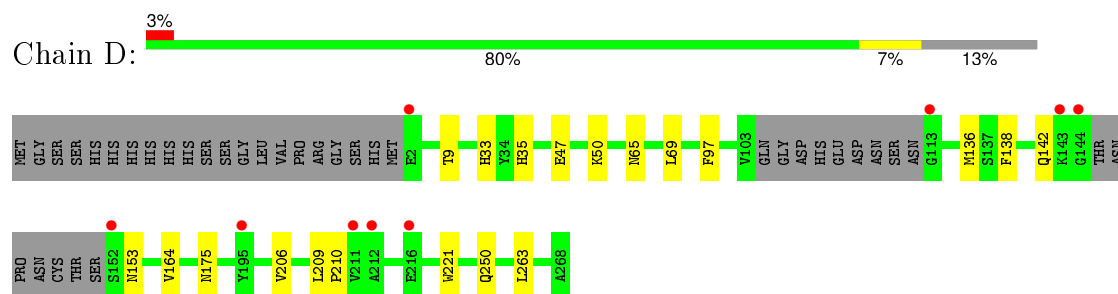
#### ● Molecule 1: Pteridine reductase



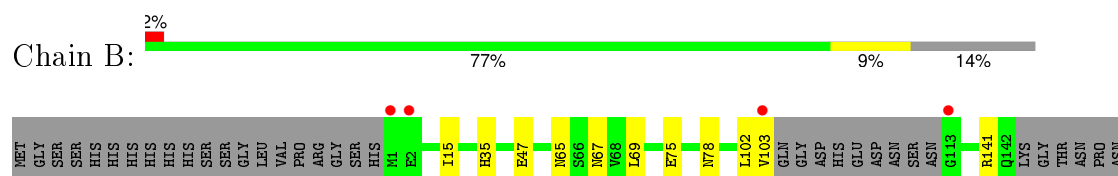
#### ● Molecule 1: Pteridine reductase

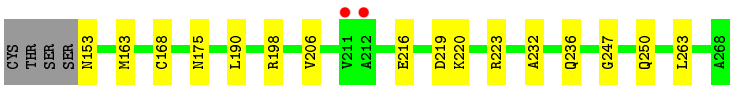


#### ● Molecule 1: Pteridine reductase



#### ● Molecule 2: Pteridine reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73 Å 90.99 Å 82.82 Å 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) 95.5 (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 1.60 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.118 , 0.150 0.135 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
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 , 58.5	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 125368 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, AX4, NA, D1D, NAP, CSX, ACT, DTT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.72	0/2109	0.81	1/2853 (0.0%)
1	C	0.73	0/2037	0.76	0/2756
1	D	0.69	0/2074	0.77	0/2803
2	B	0.75	0/2017	0.79	2/2728 (0.1%)
All	All	0.72	0/8237	0.78	3/11140 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	B	198	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	B	198	ARG	NE-CZ-NH2	-5.48	117.56	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2013	0	2109	37	0
1	C	1962	0	2045	32	0
1	D	1981	0	2101	20	0
2	B	1947	0	2040	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	7	0
10	B	304	0	0	17	0
10	C	298	0	0	8	0
10	D	300	0	0	3	0
All	All	9481	0	8536	123	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.

All (123) 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
8:B:273[B]:D1D:H4C2	10:B:433:HOH:O	1.61	1.00
1:A:223[B]:ARG:HH12	1:A:224[B]:LYS:HG2	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223[B]:ARG:HH22	1:A:224[B]:LYS:HZ1	1.20	0.90
1:A:223[B]:ARG:NH1	1:A:224[B]:LYS:HG2	1.80	0.89
1:A:223[B]:ARG:HH22	1:A:224[B]:LYS:NZ	1.71	0.89
2:B:168:CSX:OD	7:B:272:DTT:S1	2.35	0.85
1:D:175:ASN:HB2	10:D:491:HOH:O	1.77	0.83
2:B:206[B]:VAL:HG12	8:B:273[B]:D1D:H3	1.61	0.82
1:C:175:ASN:HB2	10:C:487:HOH:O	1.80	0.80
1:A:223[B]:ARG:HH11	1:A:224[B]:LYS:HG3	1.47	0.80
8:B:273[B]:D1D:H2	10:B:433:HOH:O	1.83	0.78
2:B:175:ASN:HB2	10:B:470:HOH:O	1.83	0.77
7:B:272:DTT:H12	10:B:433:HOH:O	1.86	0.76
1:C:82[B]:ARG:HD2	10:C:398:HOH:O	1.87	0.75
1:C:175:ASN:ND2	10:C:393:HOH:O	1.94	0.74
9:B:274[C]:GOL:H11	10:B:328:HOH:O	1.87	0.74
1:C:210:PRO:HG3	6:C:272[A]:AX4:CAG	2.19	0.73
1:C:3:ALA:HB3	1:C:29[A]:ARG:HD2	1.71	0.72
1:D:210:PRO:HG3	6:D:271[A]:AX4:CAF	2.20	0.72
1:C:82[B]:ARG:CD	10:C:398:HOH:O	2.36	0.72
1:A:175[A]:ASN:OD1	10:A:430:HOH:O	2.09	0.71
1:C:82[B]:ARG:CG	10:C:398:HOH:O	2.39	0.71
2:B:153:ASN:ND2	10:B:513:HOH:O	2.26	0.68
1:A:223[B]:ARG:HH11	1:A:224[B]:LYS:CG	2.01	0.68
1:A:206[B]:VAL:HG23	1:A:263:LEU:HD22	1.77	0.65
1:C:236:GLN:HE21	1:D:250[B]:GLN:CG	2.11	0.64
1:A:250[B]:GLN:NE2	10:A:389:HOH:O	2.27	0.63
2:B:206[A]:VAL:HG23	2:B:263:LEU:HD22	1.79	0.62
2:B:168:CSX:OD	9:B:274[C]:GOL:H12	1.99	0.62
1:C:236:GLN:HE21	1:D:250[B]:GLN:CD	2.03	0.62
1:A:115:THR:O	1:A:118[B]:THR:HG22	2.00	0.62
6:A:274[A]:AX4:HAD	7:A:275:DTT:H42	1.82	0.61
2:B:220[B]:LYS:HG2	2:B:223[B]:ARG:HH21	1.65	0.61
2:B:219:ASP:O	2:B:223[B]:ARG:HG3	2.03	0.58
1:C:210:PRO:CG	6:C:272[A]:AX4:CAG	2.82	0.57
10:A:430:HOH:O	1:C:186:GLN:NE2	2.27	0.57
1:A:265:LEU:HB2	2:B:190[B]:LEU:HD21	1.86	0.57
1:C:97:PHE:CE2	6:C:272[A]:AX4:HAG	2.39	0.56
8:B:273[B]:D1D:C4	10:B:433:HOH:O	2.34	0.55
1:D:206[B]:VAL:HG23	1:D:263:LEU:HD22	1.87	0.55
1:C:210:PRO:HD3	6:C:272[A]:AX4:CAO	2.37	0.55
9:B:274[C]:GOL:H31	10:B:433:HOH:O	2.07	0.55
1:A:250[B]:GLN:NE2	2:B:236:GLN:HE21	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:272:DTT:C1	10:B:433:HOH:O	2.47	0.55
1:D:209:LEU:HD23	6:D:271[A]:AX4:CAE	2.38	0.54
1:A:250[B]:GLN:CD	2:B:236:GLN:HE21	2.09	0.54
1:D:97:PHE:CE2	6:D:271[A]:AX4:HAF	2.44	0.53
2:B:206[A]:VAL:HG23	2:B:263:LEU:CD2	2.39	0.53
1:A:250[B]:GLN:CD	10:A:485:HOH:O	2.46	0.52
10:A:484:HOH:O	1:C:103:VAL:HG22	2.09	0.52
1:A:206[B]:VAL:HG23	1:A:263:LEU:CD2	2.40	0.52
1:D:210:PRO:CG	6:D:271[A]:AX4:CAF	2.89	0.51
1:A:103:VAL:HG11	1:C:143:LYS:HG2	1.93	0.51
1:C:209:LEU:HD23	6:C:272[A]:AX4:CAD	2.41	0.51
1:A:210:PRO:HG3	6:A:274[A]:AX4:CAF	2.41	0.49
1:C:210:PRO:HG3	6:C:272[A]:AX4:HAG	1.94	0.49
3:A:271:ACT:H3	10:A:514:HOH:O	2.13	0.49
2:B:247:GLY:HA2	2:B:250:GLN:HG3	1.94	0.48
1:C:252:ILE:CG2	1:C:255[B]:SER:OG	2.60	0.48
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.96	0.48
1:A:136[A]:MET:HE1	1:C:116:VAL:HG21	1.96	0.48
2:B:206[B]:VAL:HG12	8:B:273[B]:D1D:C3	2.37	0.48
1:D:221:TRP:CZ3	8:D:273[B]:D1D:H4C1	2.48	0.48
1:C:206[A]:VAL:HG23	1:C:263:LEU:HD22	1.96	0.48
9:B:275:GOL:H11	10:B:356:HOH:O	2.14	0.48
1:C:82[B]:ARG:HG2	10:C:398:HOH:O	2.10	0.47
2:B:75[B]:GLU:HG2	10:B:430:HOH:O	2.14	0.47
1:C:143:LYS:HZ3	1:C:143:LYS:C	2.16	0.47
6:A:274[A]:AX4:HAD	7:A:275:DTT:C4	2.43	0.47
1:D:138:PHE:O	1:D:142:GLN:HG2	2.15	0.47
1:D:206[B]:VAL:HG23	1:D:263:LEU:CD2	2.45	0.47
1:D:47:GLU:HA	1:D:50[A]:LYS:HE2	1.95	0.47
1:A:22:LYS:HG2	1:A:242:ILE:HG12	1.97	0.47
1:C:210:PRO:HD3	6:C:272[A]:AX4:CAF	2.44	0.47
9:B:274[C]:GOL:C3	10:B:433:HOH:O	2.63	0.46
1:C:206[A]:VAL:HG23	1:C:263:LEU:CD2	2.46	0.46
1:A:120:VAL:HG11	1:C:129[B]:ILE:HD13	1.98	0.46
1:C:9:THR:HA	1:C:33:HIS:HB3	1.98	0.46
1:A:114:LYS:HB3	1:A:118[B]:THR:CG2	2.46	0.46
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.97	0.45
1:C:236:GLN:NE2	1:D:250[B]:GLN:HG3	2.31	0.45
2:B:65:ASN:HA	2:B:69:LEU:HD22	1.99	0.45
2:B:103:VAL:HG22	10:D:493:HOH:O	2.18	0.44
1:D:153:ASN:CG	1:D:250[A]:GLN:HE22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:LEU:O	1:D:136[A]:MET:HG3	2.17	0.44
1:A:15:ILE:HB	5:A:273:NAP:H51N	1.99	0.44
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.99	0.43
1:C:130:ALA:HB3	1:C:131:PRO:HD3	2.00	0.43
2:B:47[B]:GLU:HG3	10:B:371:HOH:O	2.18	0.43
1:A:141:ARG:HG2	10:A:424:HOH:O	2.19	0.43
1:D:9:THR:HA	1:D:33:HIS:HB3	2.00	0.43
1:A:186:GLN:NE2	10:C:393:HOH:O	2.41	0.43
1:D:35:HIS:HB2	5:D:270:NAP:C2A	2.49	0.42
1:C:206[B]:VAL:HG12	8:C:274[B]:D1D:H3	2.01	0.42
9:B:274[C]:GOL:H2	10:B:433:HOH:O	2.19	0.42
2:B:78:ASN:OD1	2:B:141:ARG:NH1	2.48	0.42
2:B:163:MET:HE2	10:B:559:HOH:O	2.19	0.42
1:A:193:ALA:HB3	1:A:194:PRO:HD3	2.00	0.42
1:D:164:VAL:HG12	10:D:574:HOH:O	2.18	0.42
1:C:82[B]:ARG:NH2	10:C:458:HOH:O	2.53	0.41
1:A:9:THR:HA	1:A:33:HIS:HB3	2.02	0.41
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.56	0.41
1:A:221:TRP:CE3	1:A:224[B]:LYS:HD2	2.55	0.41
2:B:15:ILE:HB	5:B:270:NAP:H51N	2.02	0.41
2:B:216[A]:GLU:CD	10:B:508:HOH:O	2.58	0.41
1:A:221:TRP:CZ3	8:A:276[B]:D1D:H4C1	2.55	0.41
1:A:150:THR:HG23	1:A:151:SER:N	2.36	0.41
8:B:273[B]:D1D:C2	10:B:433:HOH:O	2.56	0.40
1:D:47:GLU:HA	1:D:50[A]:LYS:CE	2.51	0.40
1:A:223[B]:ARG:NH2	1:A:224[B]:LYS:NZ	2.53	0.40
2:B:35:HIS:HB2	5:B:270:NAP:C2A	2.51	0.40
1:C:15:ILE:HB	5:C:271:NAP:H51N	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	223 (99%)	2 (1%)	84	71
1	C	216/231 (94%)	211 (98%)	5 (2%)	58	29
1	D	220/231 (95%)	220 (100%)	0	100	100
2	B	213/230 (93%)	211 (99%)	2 (1%)	84	71
All	All	874/923 (95%)	865 (99%)	9 (1%)	84	67

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

Mol	Chain	Res	Type
1	A	136[A]	MET
1	A	136[B]	MET
2	B	67[A]	ASN
2	B	67[B]	ASN
1	C	2	GLU
1	C	60	GLN
1	C	67	ASN
1	C	141	ARG
1	C	143	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
2	B	236	GLN
1	C	25	GLN
1	C	60	GLN
1	C	67	ASN
1	C	104	GLN
1	C	186	GLN
1	C	236	GLN
1	C	250	GLN
1	D	236	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	0.73	0	3,6,8	1.63	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
2	CSX	B	168	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 carbohydrates 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	269	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
3	ACT	A	270	-	1,3,3	0.67	0	0,3,3	0.00	-
3	ACT	A	271	-	1,3,3	0.71	0	0,3,3	0.00	-
5	NAP	A	273	-	42,52,52	1.24	3 (7%)	54,80,80	1.94	10 (18%)
6	AX4	A	274[A]	-	17,17,17	1.20	1 (5%)	20,23,23	1.93	3 (15%)
7	DTT	A	275	-	7,7,7	0.56	0	4,8,8	0.98	0
8	D1D	A	276[B]	-	6,8,8	0.62	0	6,10,10	0.86	0
9	GOL	A	277	-	5,5,5	0.63	0	5,5,5	1.04	0
3	ACT	B	269	-	1,3,3	0.83	0	0,3,3	0.00	-
5	NAP	B	270	-	42,52,52	1.37	5 (11%)	54,80,80	1.96	12 (22%)
6	AX4	B	271[A]	-	17,17,17	1.69	2 (11%)	20,23,23	2.00	8 (40%)
7	DTT	B	272	-	7,7,7	0.75	0	4,8,8	1.67	1 (25%)
8	D1D	B	273[B]	-	6,8,8	0.90	0	6,10,10	1.01	1 (16%)
9	GOL	B	274[C]	-	5,5,5	0.61	0	5,5,5	0.21	0
9	GOL	B	275	-	5,5,5	0.35	0	5,5,5	0.63	0
3	ACT	C	269	-	1,3,3	1.53	0	0,3,3	0.00	-
3	ACT	C	270	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAP	C	271	-	42,52,52	1.27	2 (4%)	54,80,80	1.98	11 (20%)
6	AX4	C	272[A]	-	17,17,17	1.64	4 (23%)	20,23,23	2.12	5 (25%)
7	DTT	C	273	-	7,7,7	0.69	0	4,8,8	0.94	0
8	D1D	C	274[B]	-	6,8,8	0.74	0	6,10,10	1.99	2 (33%)
3	ACT	D	269	-	1,3,3	0.52	0	0,3,3	0.00	-
5	NAP	D	270	-	42,52,52	1.33	2 (4%)	54,80,80	2.26	8 (14%)
6	AX4	D	271[A]	-	17,17,17	1.08	2 (11%)	20,23,23	2.20	5 (25%)
7	DTT	D	272	-	7,7,7	0.60	0	4,8,8	1.06	0
8	D1D	D	273[B]	-	6,8,8	0.40	0	6,10,10	0.89	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
3	ACT	A	269	-	-	0/0/0/0	0/0/0/0
3	ACT	A	270	-	-	0/0/0/0	0/0/0/0
3	ACT	A	271	-	-	0/0/0/0	0/0/0/0
5	NAP	A	273	-	-	0/27/67/67	0/5/5/5
6	AX4	A	274[A]	-	-	0/4/4/4	0/2/2/2
7	DTT	A	275	-	2/2/2/2	0/8/8/8	0/0/0/0
8	D1D	A	276[B]	-	-	0/0/11/11	0/0/1/1
9	GOL	A	277	-	-	0/4/4/4	0/0/0/0
3	ACT	B	269	-	-	0/0/0/0	0/0/0/0
5	NAP	B	270	-	-	0/27/67/67	0/5/5/5
6	AX4	B	271[A]	-	-	0/4/4/4	0/2/2/2
7	DTT	B	272	-	-	0/8/8/8	0/0/0/0
8	D1D	B	273[B]	-	-	0/0/11/11	0/0/1/1
9	GOL	B	274[C]	-	-	0/4/4/4	0/0/0/0
9	GOL	B	275	-	-	0/4/4/4	0/0/0/0
3	ACT	C	269	-	-	0/0/0/0	0/0/0/0
3	ACT	C	270	-	-	0/0/0/0	0/0/0/0
5	NAP	C	271	-	-	0/27/67/67	0/5/5/5
6	AX4	C	272[A]	-	-	0/4/4/4	0/2/2/2
7	DTT	C	273	-	-	0/8/8/8	0/0/0/0
8	D1D	C	274[B]	-	-	0/0/11/11	0/0/1/1
3	ACT	D	269	-	-	0/0/0/0	0/0/0/0
5	NAP	D	270	-	-	0/27/67/67	0/5/5/5
6	AX4	D	271[A]	-	-	0/4/4/4	0/2/2/2
7	DTT	D	272	-	-	0/8/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D1D	D	273[B]	-	-	0/0/11/11	0/0/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	271[A]	AX4	CAO-SAK	-5.66	1.66	1.77
6	D	271[A]	AX4	CAO-SAK	-2.80	1.72	1.77
6	A	274[A]	AX4	CAO-SAK	-2.73	1.72	1.77
6	C	272[A]	AX4	C5-C4	-2.37	1.35	1.38
6	C	272[A]	AX4	CAO-SAK	-2.27	1.73	1.77
5	B	270	NAP	O4B-C4B	-2.08	1.40	1.45
3	C	270	ACT	CH3-C	2.01	1.51	1.48
5	A	273	NAP	C2A-N1A	2.02	1.37	1.33
6	D	271[A]	AX4	C4-N3	2.08	1.35	1.34
5	B	270	NAP	C2A-N1A	2.13	1.37	1.33
6	C	272[A]	AX4	C2-N3	2.30	1.39	1.35
3	A	269	ACT	CH3-C	2.31	1.52	1.48
6	B	271[A]	AX4	C4-SAK	2.40	1.80	1.77
5	B	270	NAP	C4N-C3N	2.42	1.43	1.39
5	B	270	NAP	C2A-N3A	2.98	1.37	1.32
5	D	270	NAP	C2A-N3A	3.55	1.38	1.32
5	A	273	NAP	C2A-N3A	3.56	1.38	1.32
5	C	271	NAP	C2A-N3A	3.84	1.39	1.32
5	B	270	NAP	O7N-C7N	4.50	1.33	1.24
5	A	273	NAP	O7N-C7N	4.57	1.33	1.24
6	C	272[A]	AX4	C4-N3	4.90	1.38	1.34
5	C	271	NAP	O7N-C7N	5.34	1.35	1.24
5	D	270	NAP	O7N-C7N	5.93	1.36	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	270	NAP	N3A-C2A-N1A	-12.37	119.42	128.89
5	C	271	NAP	N3A-C2A-N1A	-9.40	121.70	128.89
5	A	273	NAP	N3A-C2A-N1A	-9.30	121.78	128.89
5	B	270	NAP	N3A-C2A-N1A	-8.44	122.43	128.89
6	C	272[A]	AX4	C5-C4-SAK	-6.53	115.23	124.19
6	D	271[A]	AX4	C5-C4-SAK	-6.46	115.34	124.19
6	A	274[A]	AX4	C5-C4-SAK	-6.27	115.59	124.19
5	C	271	NAP	C4B-O4B-C1B	-5.06	104.16	109.72
6	D	271[A]	AX4	N3-C2-N1	-4.57	118.04	125.53
5	D	270	NAP	C4B-O4B-C1B	-4.55	104.72	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	271[A]	AX4	C5-C4-SAK	-4.21	118.42	124.19
5	A	273	NAP	C4B-O4B-C1B	-4.15	105.15	109.72
5	B	270	NAP	C3N-C2N-N1N	-4.11	115.63	120.36
5	C	271	NAP	O7N-C7N-C3N	-4.03	115.19	119.59
6	B	271[A]	AX4	N3-C2-N1	-3.91	119.12	125.53
5	A	273	NAP	O7N-C7N-C3N	-3.83	115.40	119.59
6	C	272[A]	AX4	N3-C2-N1	-3.74	119.40	125.53
6	A	274[A]	AX4	N3-C2-N1	-3.63	119.58	125.53
5	B	270	NAP	C4B-O4B-C1B	-3.63	105.73	109.72
8	C	274[B]	D1D	O3-C3-C4	-3.61	103.78	110.05
5	A	273	NAP	C1B-N9A-C4A	-3.28	122.00	126.94
5	D	270	NAP	O7N-C7N-N7N	-2.83	118.61	122.59
5	D	270	NAP	C1B-N9A-C4A	-2.73	122.82	126.94
6	B	271[A]	AX4	CAE-CAG-CAO	-2.64	117.17	120.58
5	B	270	NAP	O7N-C7N-C3N	-2.58	116.77	119.59
5	A	273	NAP	C3N-C2N-N1N	-2.57	117.40	120.36
5	C	271	NAP	C3N-C2N-N1N	-2.53	117.44	120.36
5	A	273	NAP	C4A-C5A-N7A	-2.51	107.17	109.48
5	C	271	NAP	C4A-C5A-N7A	-2.48	107.20	109.48
6	B	271[A]	AX4	CAF-CAD-CAL	-2.43	118.12	121.39
5	C	271	NAP	C1B-N9A-C4A	-2.42	123.30	126.94
5	C	271	NAP	O3-PN-O5D	-2.29	96.86	102.94
5	B	270	NAP	O7N-C7N-N7N	-2.25	119.43	122.59
5	B	270	NAP	C1B-N9A-C4A	-2.15	123.70	126.94
5	B	270	NAP	PN-O3-PA	-2.02	127.07	132.73
8	B	273[B]	D1D	O3-C3-C4	-2.00	106.57	110.05
6	D	271[A]	AX4	NAB-C6-N1	2.05	120.23	116.50
5	B	270	NAP	O4D-C1D-N1N	2.05	110.38	108.13
5	A	273	NAP	C2N-C3N-C4N	2.06	120.58	118.29
5	C	271	NAP	O4D-C1D-N1N	2.11	110.45	108.13
6	B	271[A]	AX4	C5-C4-N3	2.16	125.30	123.66
6	B	271[A]	AX4	NAB-C6-N1	2.26	120.63	116.50
5	B	270	NAP	O3B-C3B-C2B	2.28	117.73	111.16
5	A	273	NAP	O4B-C1B-N9A	2.36	113.03	108.10
5	C	271	NAP	C2A-N1A-C6A	2.40	123.06	118.77
5	D	270	NAP	C2N-C3N-C4N	2.43	120.99	118.29
6	C	272[A]	AX4	CAO-SAK-C4	2.52	106.70	103.40
6	B	271[A]	AX4	CAO-SAK-C4	2.59	106.79	103.40
6	A	274[A]	AX4	NAC-C2-N3	2.62	121.53	117.20
6	C	272[A]	AX4	NAB-C6-N1	2.77	121.55	116.50
6	C	272[A]	AX4	NAC-C2-N3	2.81	121.85	117.20
5	D	270	NAP	O4B-C1B-N9A	2.82	114.01	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	270	NAP	C2A-N1A-C6A	2.83	123.82	118.77
5	C	271	NAP	O4B-C1B-N9A	2.83	114.02	108.10
5	A	273	NAP	O4D-C1D-N1N	2.87	111.28	108.13
7	B	272	DTT	C2-C1-S1	2.87	118.67	113.91
5	B	270	NAP	O4B-C1B-N9A	2.88	114.13	108.10
8	C	274[B]	D1D	O2-C2-C1	3.04	115.32	110.05
5	B	270	NAP	C2N-C3N-C4N	3.13	121.77	118.29
6	D	271[A]	AX4	NAC-C2-N3	3.20	122.50	117.20
6	D	271[A]	AX4	CAO-SAK-C4	3.21	107.61	103.40
5	C	271	NAP	C3N-C7N-N7N	3.29	121.42	117.82
6	B	271[A]	AX4	NAC-C2-N3	3.47	122.95	117.20
5	A	273	NAP	C3N-C7N-N7N	4.06	122.26	117.82
5	D	270	NAP	C3N-C7N-N7N	4.75	123.01	117.82
5	B	270	NAP	C3N-C7N-N7N	5.42	123.75	117.82

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	271	ACT	1	0
5	A	273	NAP	1	0
6	A	274[A]	AX4	3	0
7	A	275	DTT	2	0
8	A	276[B]	D1D	3	0
5	B	270	NAP	2	0
7	B	272	DTT	3	0
8	B	273[B]	D1D	7	0
9	B	274[C]	GOL	5	0
9	B	275	GOL	1	0
5	C	271	NAP	1	0
6	C	272[A]	AX4	7	0
8	C	274[B]	D1D	2	0
5	D	270	NAP	1	0
6	D	271[A]	AX4	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	273[B]	D1D	2	0

## 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, 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%)	-0.10	10 (3%) 43 40	7, 10, 24, 54	0
1	C	252/288 (87%)	-0.08	10 (3%) 42 39	8, 11, 27, 45	0
1	D	251/288 (87%)	-0.11	9 (3%) 46 43	9, 11, 25, 53	0
2	B	248/288 (86%)	-0.27	6 (2%) 62 60	7, 9, 18, 48	0
All	All	1006/1152 (87%)	-0.14	35 (3%) 48 44	7, 11, 24, 54	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	THR	8.7
1	D	113	GLY	7.9
1	D	144	GLY	7.9
1	C	151	SER	7.6
1	A	113	GLY	7.6
1	C	113	GLY	7.3
1	A	144	GLY	6.8
2	B	113	GLY	6.6
1	C	104	GLN	6.4
1	C	212	ALA	6.4
2	B	1	MET	6.3
1	A	151	SER	5.8
1	A	104	GLN	5.4
1	C	152	SER	5.4
1	A	145	THR	4.9
1	D	143	LYS	4.7
1	D	212	ALA	4.7
1	D	2	GLU	4.6
2	B	2	GLU	4.5
1	C	2	GLU	4.4
2	B	211	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	211	VAL	3.8
1	C	143	LYS	3.8
1	A	143	LYS	3.6
1	C	216	GLU	3.2
1	D	152	SER	3.1
1	D	195[A]	TYR	3.0
1	D	211	VAL	3.0
1	A	212	ALA	2.8
2	B	212	ALA	2.6
1	A	2[A]	GLU	2.5
1	A	195	TYR	2.5
1	C	195	TYR	2.2
1	D	216	GLU	2.2
2	B	103	VAL	2.2

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSX	B	168	7/8	0.93	0.10	-	11,13,26,28	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	DTT	B	272	8/8	0.93	0.21	10.86	25,45,53,57	0
3	ACT	A	270	4/4	0.91	0.24	9.98	24,24,25,27	0
3	ACT	A	271	4/4	0.77	0.15	9.71	21,26,28,29	0
3	ACT	D	269	4/4	0.93	0.19	8.57	23,23,23,26	0
3	ACT	C	269	4/4	0.95	0.18	6.79	21,21,22,24	0
8	D1D	D	273[B]	8/8	0.90	0.18	4.39	26,28,30,31	8
3	ACT	B	269	4/4	0.83	0.20	4.15	23,23,24,26	0
8	D1D	A	276[B]	8/8	0.94	0.15	3.50	27,31,34,34	8
8	D1D	C	274[B]	8/8	0.94	0.14	3.26	17,21,25,27	8
7	DTT	A	275	8/8	0.96	0.17	3.05	29,46,52,59	0
9	GOL	B	275	6/6	0.78	0.16	2.42	25,29,30,34	0
9	GOL	B	274[C]	6/6	0.93	0.11	2.10	15,23,28,31	6
7	DTT	C	273	8/8	0.95	0.15	1.89	27,42,49,56	0
8	D1D	B	273[B]	8/8	0.96	0.11	1.38	16,18,20,21	8
6	AX4	A	274[A]	16/16	0.96	0.10	1.34	7,10,11,14	7
7	DTT	D	272	8/8	0.96	0.12	1.10	27,46,52,58	0
6	AX4	D	271[A]	16/16	0.97	0.10	0.64	10,13,15,15	7
3	ACT	C	270	4/4	0.97	0.09	-0.11	15,17,18,18	0
6	AX4	C	272[A]	16/16	0.97	0.08	-0.11	9,13,17,18	7
9	GOL	A	277	6/6	0.94	0.08	-0.14	15,18,19,23	0
6	AX4	B	271[A]	16/16	0.97	0.07	-0.14	7,10,15,18	7
5	NAP	D	270	48/48	0.98	0.06	-0.80	8,10,12,13	0
3	ACT	A	269	4/4	0.98	0.06	-0.82	11,12,12,16	0
5	NAP	A	273	48/48	0.98	0.06	-0.86	6,9,10,13	0
5	NAP	B	270	48/48	0.99	0.05	-1.37	5,8,10,11	0
5	NAP	C	271	48/48	0.98	0.05	-1.69	7,10,11,12	0
4	NA	A	272	1/1	0.98	0.04	-3.33	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.