



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:59 PM GMT

PDB ID : 3BMQ  
Title : Structure of Pteridine Reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor (Compound AX5)  
Authors : Martini, V.P.; Iulek, J.; Hunter, W.N.  
Deposited on : 2007-12-13  
Resolution : 1.70 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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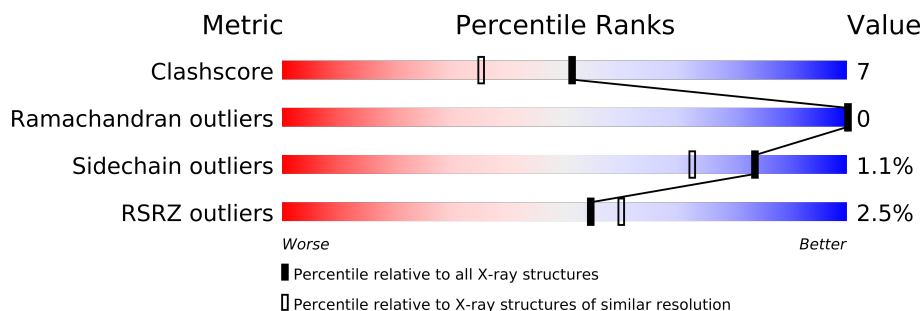
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	288	
1	D	288	
2	B	288	
2	C	288	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	C	269	-	X
6	DTT	A	271[A]	-	X
6	DTT	D	271	-	X
7	GOL	B	272	-	X
7	GOL	C	272	-	X
7	GOL	C	273	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9392 atoms, of which 0 are hydrogen and 0 are deuterium.

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	253	Total	C	N	O	S	0	10	0
			1929	1220	335	362	12			
1	D	253	Total	C	N	O	S	0	14	0
			1961	1240	342	368	11			

There are 40 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	252	Total	C	N	O	S	0	11	0
			1930	1221	337	361	11			
2	C	251	Total	C	N	O	S	0	9	0
			1913	1205	336	361	11			

There are 40 discrepancies between the modelled and reference sequences:

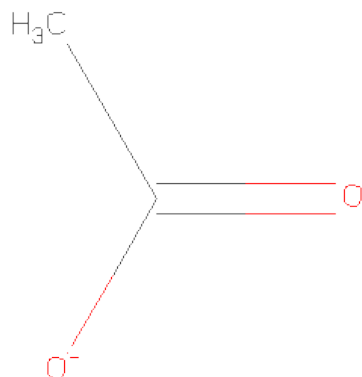
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP O76290
B	-18	GLY	-	EXPRESSION TAG	UNP O76290
B	-17	SER	-	EXPRESSION TAG	UNP O76290
B	-16	SER	-	EXPRESSION TAG	UNP O76290
B	-15	HIS	-	EXPRESSION TAG	UNP O76290
B	-14	HIS	-	EXPRESSION TAG	UNP O76290
B	-13	HIS	-	EXPRESSION TAG	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

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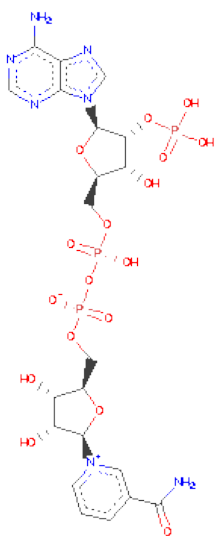
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	PRO	-	EXPRESSION TAG	UNP O76290
B	-3	ARG	-	EXPRESSION TAG	UNP O76290
B	-2	GLY	-	EXPRESSION TAG	UNP O76290
B	-1	SER	-	EXPRESSION TAG	UNP O76290
B	0	HIS	-	EXPRESSION TAG	UNP O76290
C	-19	MET	-	EXPRESSION TAG	UNP O76290
C	-18	GLY	-	EXPRESSION TAG	UNP O76290
C	-17	SER	-	EXPRESSION TAG	UNP O76290
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

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



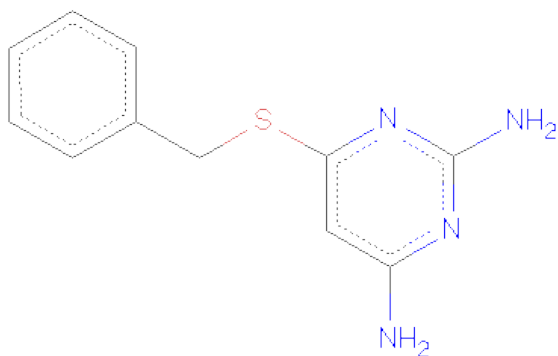
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



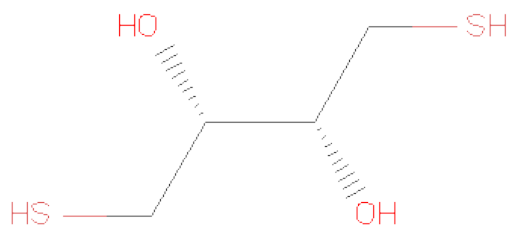
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 6-(BENZYL-SULFANYL)PYRIMIDINE-2,4-DIAMINE (three-letter code: AX5) (formula:  $C_{11}H_{12}N_4S$ ).



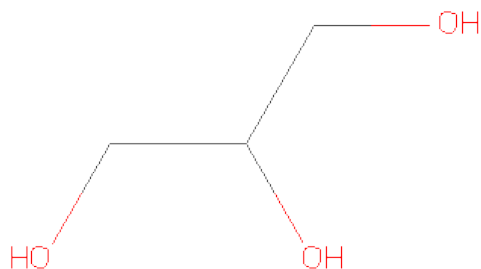
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			16	11	4	1		
5	B	1	Total	C	N	S	0	0
			16	11	4	1		
5	C	1	Total	C	N	S	0	0
			16	11	4	1		
5	D	1	Total	C	N	S	0	0
			16	11	4	1		

- Molecule 6 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	350	Total	O	0	0
			350	350		
8	B	382	Total	O	0	0
			382	382		
8	C	319	Total	O	0	0
			319	319		
8	D	310	Total	O	0	2
			310	310		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.72Å 91.16Å 82.83Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	74.54 – 1.70 13.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	85.5 (74.54-1.70) 85.3 (13.28-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.68 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.131 , 0.178 0.143 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.5	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	133 of 93475 reflections (0.142%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AX5, 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	0.89	3/1972 (0.2%)	0.79	2/2670 (0.1%)
1	D	0.84	0/2022	0.83	3/2736 (0.1%)
2	B	0.86	0/1989	0.83	4/2694 (0.1%)
2	C	0.84	0/1967	0.81	3/2665 (0.1%)
All	All	0.86	3/7950 (0.0%)	0.82	12/10765 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	CB-CG	5.82	1.63	1.52
1	A	117	GLU	CG-CD	5.23	1.59	1.51
1	A	182	VAL	CB-CG2	5.00	1.63	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	198	ARG	NE-CZ-NH2	-6.90	116.85	120.30
2	C	14	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	62	ASP	CB-CG-OD1	6.27	123.94	118.30
2	B	198	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	82	ARG	NE-CZ-NH1	5.99	123.30	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1994	29	0
1	D	1961	0	2033	33	0
2	B	1930	0	1999	25	0
2	C	1913	0	1962	29	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
4	A	48	0	25	1	0
4	B	48	0	25	1	0
4	C	48	0	25	1	0
4	D	48	0	25	1	0
5	A	16	0	12	0	0
5	B	16	0	12	0	0
5	C	16	0	12	0	0
5	D	16	0	12	1	0
6	A	8	0	4	0	0
6	D	8	0	10	7	0
7	B	6	0	8	6	0
7	C	12	0	16	10	0
8	A	350	0	0	15	3
8	B	382	0	0	16	3
8	C	319	0	0	10	1
8	D	310	0	0	12	1
All	All	9392	0	8180	119	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:620:HOH:O	1:D:265:LEU:HD23	1.22	1.29
1:A:142:GLN:NE2	8:A:603:HOH:O	1.74	1.16
2:C:140[B]:GLN:NE2	8:C:473:HOH:O	1.88	1.06
1:D:164:VAL:CG2	8:D:893:HOH:O	2.05	1.03
1:D:164:VAL:HG22	8:D:893:HOH:O	1.58	1.01

All (4) 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	Distance(Å)	Clash(Å)
8:C:375:HOH:O	8:D:587:HOH:O[2_556]	1.91	0.29
8:A:401:HOH:O	8:B:703:HOH:O[2_545]	2.09	0.11
8:A:612:HOH:O	8:B:364:HOH:O[2_545]	2.11	0.09
8:A:597:HOH:O	8:B:568:HOH:O[2_545]	2.16	0.04

## 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	254/288 (88%)	245 (96%)	9 (4%)	0	100	100
1	D	260/288 (90%)	251 (96%)	9 (4%)	0	100	100
2	B	256/288 (89%)	248 (97%)	8 (3%)	0	100	100
2	C	254/288 (88%)	246 (97%)	8 (3%)	0	100	100
All	All	1024/1152 (89%)	990 (97%)	34 (3%)	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	208/230 (90%)	206 (99%)	2 (1%)	85	76
1	D	213/230 (93%)	211 (99%)	2 (1%)	87	79
2	B	211/231 (91%)	207 (98%)	4 (2%)	69	50
2	C	207/231 (90%)	204 (99%)	3 (1%)	78	62
All	All	839/922 (91%)	828 (99%)	11 (1%)	84	66

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104[B]	GLN
2	B	143	LYS
2	C	250	GLN
2	B	104[A]	GLN
2	C	67	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	D	65	ASN
2	C	67	ASN
1	A	179	HIS
2	B	142	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSX	A	168[A]	-	1,2,7	0.81	0	0,1,8	0.00	-
1	CSX	A	168[B]	-	0,3,7	0.00	-	0,2,8	0.00	-
1	CSX	D	168	1	4,6,7	9.13	1 (25%)	3,6,8	2.23	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	A	168[A]	-	-	0/0/0/7	0/0/0/0
1	CSX	A	168[B]	-	-	0/0/1/7	0/0/0/0
1	CSX	D	168	1	-	0/2/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	CSX	O-C	18.12	1.23	1.11

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	CSX	C-CA-N	-3.13	110.70	113.83
1	D	168	CSX	CB-CA-N	2.06	113.71	110.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAP	A	269	-	52,52,52	1.40	6 (11%)	80,80,80	2.18	15 (18%)
5	AX5	A	270	-	17,17,17	1.68	3 (17%)	22,22,22	2.01	7 (31%)
6	DTT	A	271[A]	-	0,1,7	0.00	-	0,0,8	0.00	-
3	ACT	B	269	-	1,3,3	1.44	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	B	270	-	52,52,52	1.19	6 (11%)	80,80,80	2.27	16 (20%)
5	AX5	B	271	-	17,17,17	1.02	2 (11%)	22,22,22	2.36	4 (18%)
7	GOL	B	272	-	5,5,5	0.38	0	5,5,5	1.10	1 (20%)
3	ACT	C	269	-	1,3,3	3.02	1 (100%)	0,3,3	0.00	-
4	NAP	C	270	-	52,52,52	1.33	5 (9%)	80,80,80	1.92	11 (13%)
5	AX5	C	271	-	17,17,17	1.82	3 (17%)	22,22,22	2.49	9 (40%)
7	GOL	C	272	-	5,5,5	0.39	0	5,5,5	0.68	0
7	GOL	C	273	-	5,5,5	0.56	0	5,5,5	0.67	0
4	NAP	D	269	-	52,52,52	1.20	4 (7%)	80,80,80	2.13	14 (17%)
5	AX5	D	270	-	17,17,17	1.60	3 (17%)	22,22,22	2.42	8 (36%)
6	DTT	D	271	-	7,7,7	1.00	0	8,8,8	2.99	4 (50%)

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	NAP	A	269	-	-	0/35/67/67	0/3/5/5
5	AX5	A	270	-	-	0/5/5/5	0/2/2/2
6	DTT	A	271[A]	-	-	0/0/0/8	0/0/0/0
3	ACT	B	269	-	-	0/0/0/0	0/0/0/0
4	NAP	B	270	-	-	0/35/67/67	0/3/5/5
5	AX5	B	271	-	-	0/5/5/5	0/2/2/2
7	GOL	B	272	-	-	0/4/4/4	0/0/0/0
3	ACT	C	269	-	-	0/0/0/0	0/0/0/0
4	NAP	C	270	-	-	0/35/67/67	0/3/5/5
5	AX5	C	271	-	-	0/5/5/5	0/2/2/2
7	GOL	C	272	-	-	0/4/4/4	0/0/0/0
7	GOL	C	273	-	-	0/4/4/4	0/0/0/0
4	NAP	D	269	-	-	0/35/67/67	0/3/5/5
5	AX5	D	270	-	-	0/5/5/5	0/2/2/2
6	DTT	D	271	-	1/1/2/2	0/8/8/8	0/0/0/0

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	270	NAP	O7N-C7N	6.15	1.38	1.24
5	C	271	AX5	C4-N3	6.02	1.39	1.34
4	A	269	NAP	O7N-C7N	5.79	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	270	AX5	C4-N3	5.17	1.38	1.34
4	D	269	NAP	O7N-C7N	4.42	1.34	1.24

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	269	NAP	N3A-C2A-N1A	-13.12	117.74	128.71
4	B	270	NAP	N3A-C2A-N1A	-11.90	118.76	128.71
4	D	269	NAP	N3A-C2A-N1A	-10.07	120.29	128.71
4	C	270	NAP	N3A-C2A-N1A	-9.22	121.00	128.71
5	B	271	AX5	C2-N3-C4	8.83	121.69	115.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	271	DTT	C2

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	253/288 (87%)	-0.52	5 (1%) 62 67	6, 9, 20, 37	0
1	D	253/288 (87%)	-0.43	8 (3%) 45 50	6, 9, 21, 41	0
2	B	252/288 (87%)	-0.58	6 (2%) 56 61	6, 8, 19, 44	0
2	C	251/288 (87%)	-0.51	7 (2%) 50 56	5, 9, 21, 32	0
All	All	1009/1152 (87%)	-0.51	26 (2%) 54 58	5, 9, 20, 44	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	144	GLY	8.1
2	C	105	GLY	7.8
2	B	112	ASN	6.6
1	D	151	SER	6.2
1	D	113	GLY	6.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSX	A	168[B]	4/8	0.07	0.07	11,12,13,18	4
1	CSX	A	168[A]	3/8	0.07	-0.28	13,13,14,19	3
1	CSX	D	168	7/8	0.07	-0.49	11,15,29,29	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	DTT	A	271[A]	2/8	0.19	17.23	48,48,48,48	0
7	GOL	C	272	6/6	0.21	12.00	39,41,42,44	0
7	GOL	B	272	6/6	0.15	8.90	28,28,31,32	0
7	GOL	C	273	6/6	0.09	6.20	25,30,32,34	0
6	DTT	D	271	8/8	0.12	4.36	23,36,38,47	0
3	ACT	C	269	4/4	0.08	2.32	13,16,19,20	0
5	AX5	B	271	16/16	0.06	0.59	6,10,20,20	0
5	AX5	A	270	16/16	0.06	0.16	5,10,19,21	0
5	AX5	C	271	16/16	0.07	0.12	7,12,24,25	0
5	AX5	D	270	16/16	0.06	-0.36	8,12,25,27	0
3	ACT	B	269	4/4	0.06	-0.65	10,10,11,12	0
4	NAP	D	269	48/48	0.04	-1.10	4,7,10,13	0
4	NAP	C	270	48/48	0.04	-1.22	4,7,9,11	0
4	NAP	A	269	48/48	0.04	-1.29	2,6,9,12	0
4	NAP	B	270	48/48	0.04	-1.34	2,6,8,8	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.