



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 AM GMT

PDB ID : 3BMN  
Title : Structure of Pteridine Reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor (Compound AX3)  
Authors : Martini, V.P.; Iulek, J.; Tulloch, L.B.; Hunter, W.N.  
Deposited on : 2007-12-13  
Resolution : 1.98 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.

---

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

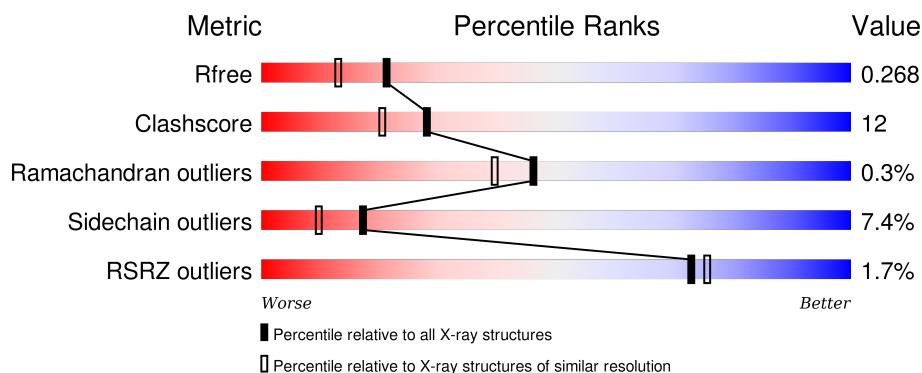
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div> <div></div> <div>66%</div> <div>18%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	288	<div> <div> <div>2%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>
2	C	288	<div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>
2	D	288	<div> <div> <div>2%</div> <div>68%</div> <div>17%</div> <div>•</div> <div>12%</div> </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
3	ACT	D	269	-	-	-	X
6	EDO	D	272	-	-	-	X
6	EDO	D	273	-	-	X	-
7	GOL	A	273[A]	-	-	-	X
7	GOL	A	273[B]	-	-	X	X
7	GOL	C	272[A]	-	-	-	X
7	GOL	C	272[B]	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8465 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
			Total	C	N	O	S			
1	A	251	1907	1205	333	358	11	0	8	0

There are 20 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

- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	1904	1201	334	357	12	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	251	Total	C	N	O	S	0	6	0
			1895	1193	331	358	13			
2	D	253	Total	C	N	O	S	0	7	0
			1921	1210	338	362	11			

There are 60 discrepancies between the modelled and reference sequences:

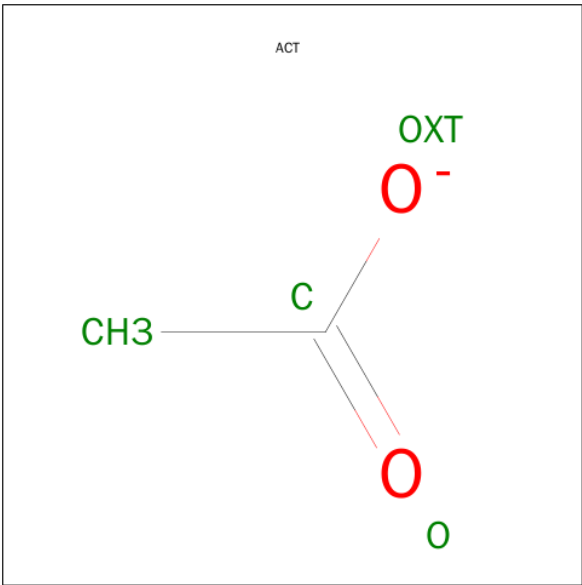
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP O76290
B	-18	GLY	-	EXPRESSION TAG	UNP O76290
B	-17	SER	-	EXPRESSION TAG	UNP O76290
B	-16	SER	-	EXPRESSION TAG	UNP O76290
B	-15	HIS	-	EXPRESSION TAG	UNP O76290
B	-14	HIS	-	EXPRESSION TAG	UNP O76290
B	-13	HIS	-	EXPRESSION TAG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

*Continued on next page...*

*Continued from previous page...*

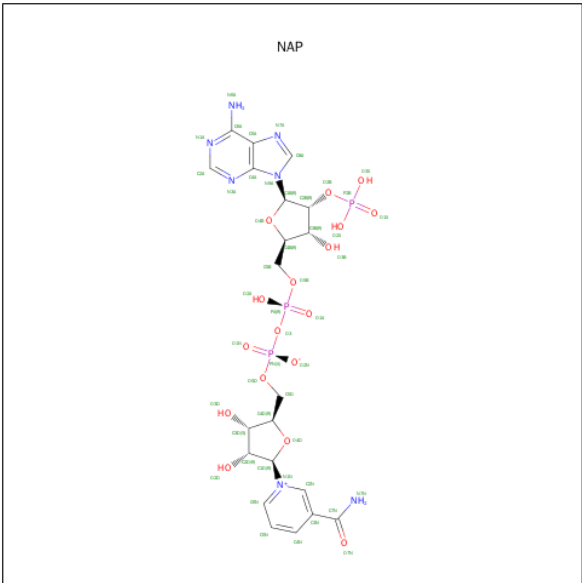
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	EXPRESSION TAG	UNP O76290
C	-4	PRO	-	EXPRESSION TAG	UNP O76290
C	-3	ARG	-	EXPRESSION TAG	UNP O76290
C	-2	GLY	-	EXPRESSION TAG	UNP O76290
C	-1	SER	-	EXPRESSION TAG	UNP O76290
C	0	HIS	-	EXPRESSION TAG	UNP O76290
D	-19	MET	-	EXPRESSION TAG	UNP O76290
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 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	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 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>).



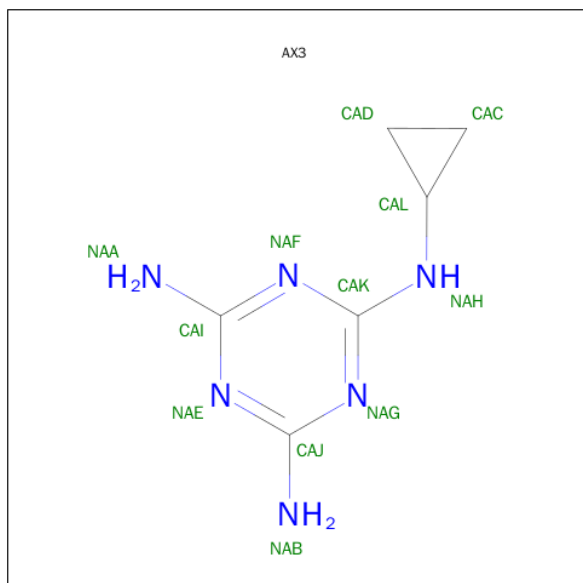
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

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

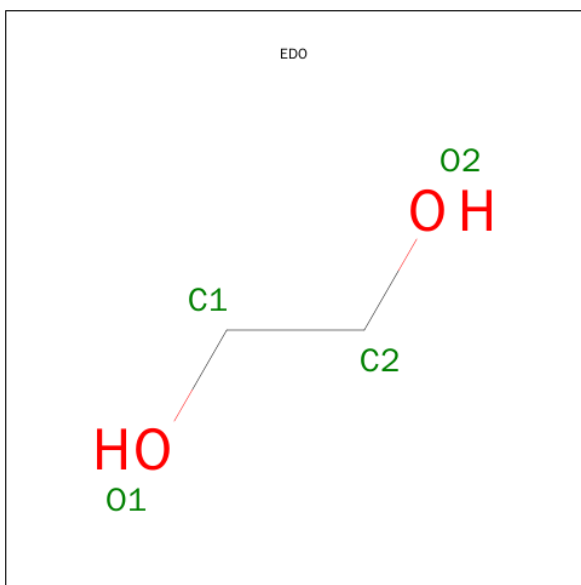
- Molecule 5 is N 2 -CYCLOPROPYL-1,3,5-TRIAZINE-2,4,6-TRIAMINE (three-letter code: AX3) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N		
			12	6	6	0	0
5	B	1	Total	C	N		
			12	6	6	0	0
5	C	1	Total	C	N		
			12	6	6	0	0
5	D	1	Total	C	N		
			12	6	6	0	0

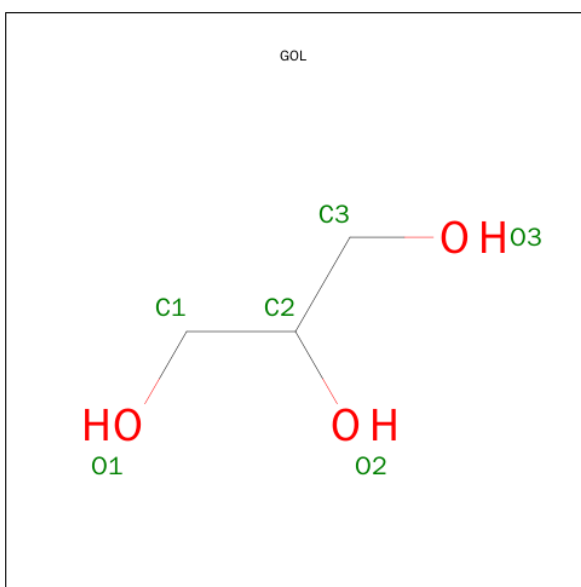
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





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

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



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	1
			8	4	4		
7	B	1	Total	C	O	0	1
			8	4	4		
7	C	1	Total	C	O	0	1
			8	4	4		
7	D	1	Total	C	O	0	0
			6	3	3		

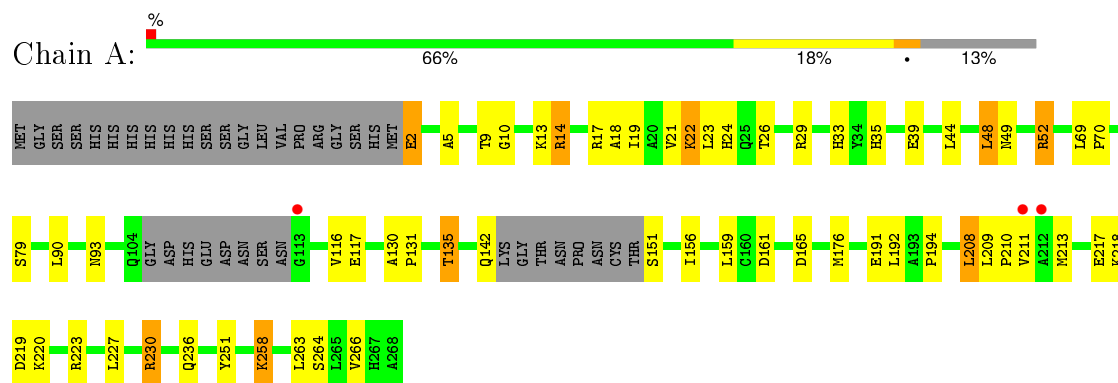
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	108	Total	O	0	0
			108	108		
8	B	153	Total	O	0	0
			153	153		
8	C	144	Total	O	0	0
			144	144		
8	D	135	Total	O	0	0
			135	135		

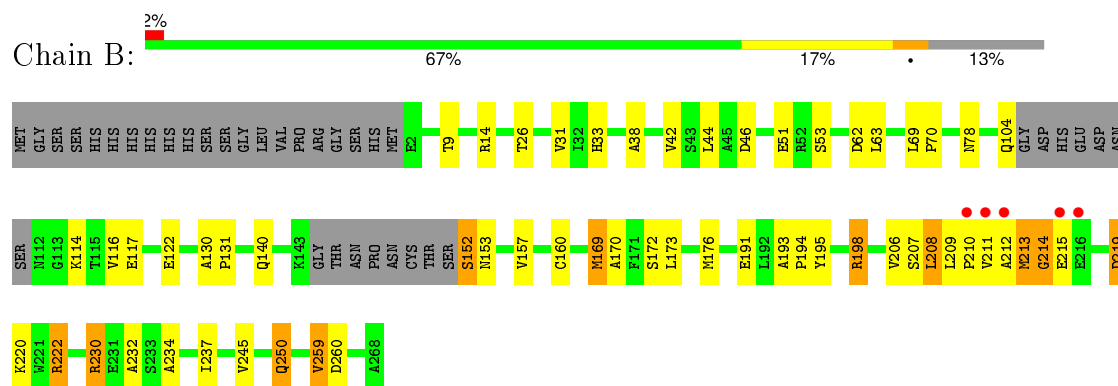
### 3 Residue-property plots

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

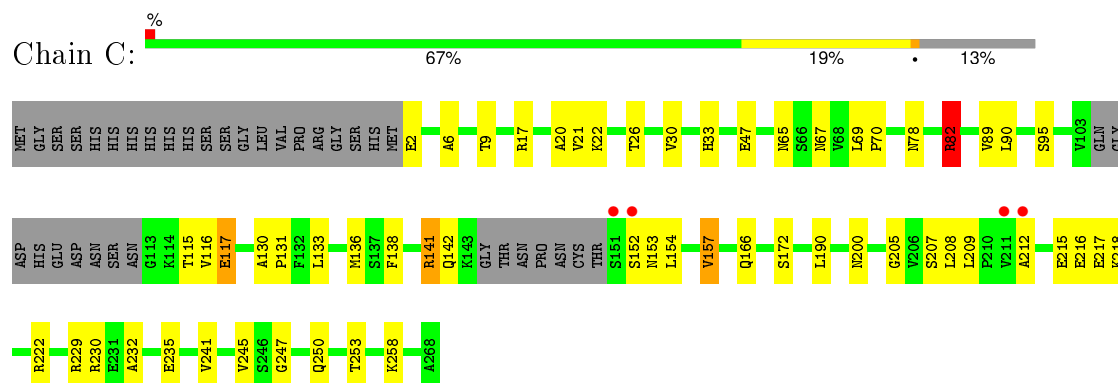
#### • Molecule 1: Pteridine reductase



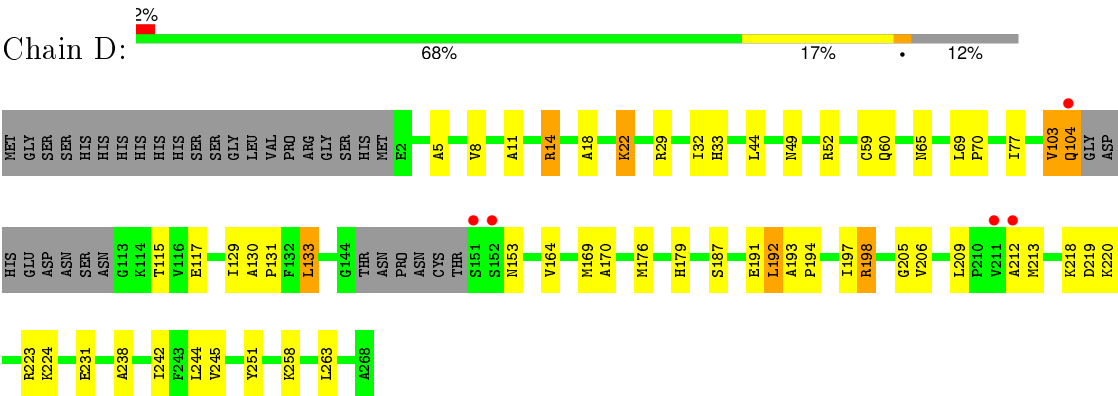
#### • Molecule 2: Pteridine reductase



#### • Molecule 2: 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, $\alpha$ , $\beta$ , $\gamma$	73.84Å 87.50Å 84.23Å 90.00° 116.08° 90.00°	Depositor
Resolution (Å)	75.59 – 1.98 75.65 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.0 (75.59-1.98) 96.0 (75.65-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.267 0.213 , 0.268	Depositor DCC
$R_{free}$ test set	3210 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	1.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 60.7	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 64386 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 26.51 % 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 2.5983e-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: AX3, GOL, EDO, NAP, CSX, ACT

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	0.33	0/1950	0.98	7/2644 (0.3%)
2	B	0.36	0/1946	0.97	6/2639 (0.2%)
2	C	0.34	0/1940	0.93	3/2630 (0.1%)
2	D	0.38	0/1969	0.93	4/2666 (0.2%)
All	All	0.35	0/7805	0.95	20/10579 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CB-CG-OD1	-10.73	108.64	118.30
2	D	198	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	14	ARG	NE-CZ-NH2	-9.71	115.44	120.30
2	D	198	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	52	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	B	46	ASP	CB-CG-OD2	-6.95	112.04	118.30
2	D	14	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	B	260	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	14	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	C	82	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	D	14	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	165	ASP	CB-CG-OD2	5.65	123.39	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	230	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	B	198	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	C	82	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	C	222	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	258	LYS	CB-CA-C	-5.26	99.87	110.40
1	A	230	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	62	ASP	CB-CG-OD1	5.21	122.99	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	212	ALA	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1964	58	0
2	B	1904	0	1950	39	0
2	C	1895	0	1935	37	0
2	D	1921	0	1971	64	0
3	D	4	0	3	0	0
4	A	48	0	25	5	0
4	B	48	0	25	0	0
4	C	48	0	25	2	0
4	D	48	0	25	1	0
5	A	12	0	10	2	0
5	B	12	0	10	2	0
5	C	12	0	10	1	0
5	D	12	0	10	0	0
6	C	4	0	6	0	0
6	D	8	0	12	11	0
7	A	20	0	24	4	0
7	B	8	0	8	0	0
7	C	8	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	6	0	8	0	0
8	A	108	0	0	6	0
8	B	153	0	0	10	0
8	C	144	0	0	10	0
8	D	135	0	0	10	0
All	All	8465	0	8029	187	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 12.

All (187) 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)
2:D:103:VAL:HG13	2:D:104:GLN:N	1.87	0.90
8:B:325:HOH:O	2:D:103:VAL:HG12	1.75	0.87
1:A:131:PRO:O	1:A:135:THR:HG23	1.75	0.85
2:D:77:ILE:HG12	8:D:365:HOH:O	1.75	0.85
1:A:236:GLN:HE21	2:B:250[B]:GLN:HG3	1.43	0.83
8:C:308:HOH:O	2:D:258:LYS:HE3	1.76	0.83
2:D:187:SER:CB	6:D:273:EDO:H22	2.10	0.82
2:B:210:PRO:HD3	5:B:270:AX3:CAD	2.10	0.81
1:A:17:ARG:HG3	1:A:44:LEU:HD22	1.66	0.77
2:D:164:VAL:HG22	2:D:179:HIS:CD2	2.20	0.76
2:B:172:SER:O	2:B:176[B]:MET:HG3	1.85	0.75
1:A:17:ARG:CG	1:A:44:LEU:HD22	2.17	0.75
1:A:263:LEU:O	1:A:266[A]:VAL:HG22	1.86	0.75
2:D:187:SER:CA	6:D:273:EDO:H22	2.21	0.71
2:D:60:GLN:HG3	8:D:319:HOH:O	1.89	0.71
2:D:187:SER:OG	6:D:273:EDO:H22	1.91	0.71
2:D:103:VAL:HG13	2:D:104:GLN:H	1.53	0.70
2:D:104:GLN:OE1	2:D:104:GLN:HA	1.89	0.70
1:A:210:PRO:HG2	1:A:213:MET:HB2	1.74	0.70
2:D:187:SER:HA	6:D:273:EDO:H22	1.74	0.69
1:A:236:GLN:NE2	2:B:250[B]:GLN:HG3	2.07	0.69
2:D:77:ILE:CG1	8:D:365:HOH:O	2.34	0.68
2:B:215:GLU:HB3	8:B:414:HOH:O	1.93	0.67
2:D:22[A]:LYS:NZ	8:D:333:HOH:O	2.27	0.67
2:D:206:VAL:CG1	2:D:209:LEU:HD21	2.27	0.65
2:D:206:VAL:HG23	2:D:263:LEU:HD22	1.79	0.64
2:D:60:GLN:CG	8:D:319:HOH:O	2.44	0.64
2:D:187:SER:CB	6:D:273:EDO:C2	2.76	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:SER:OG	6:D:273:EDO:C2	2.46	0.63
2:D:77:ILE:CD1	8:D:365:HOH:O	2.46	0.63
1:A:19:ILE:O	1:A:23[B]:LEU:HG	2.00	0.62
2:D:77:ILE:N	8:D:365:HOH:O	2.33	0.60
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.83	0.60
1:A:258:LYS:HZ3	7:A:273[B]:GOL:H31	1.68	0.59
1:A:17:ARG:O	1:A:21[A]:VAL:HG13	2.03	0.59
1:A:210:PRO:HB3	5:A:270:AX3:HAC	1.85	0.57
1:A:26:THR:O	1:A:26:THR:HG22	2.04	0.57
1:A:22:LYS:HG2	8:A:364:HOH:O	2.05	0.56
2:D:8:VAL:HG12	2:D:11:ALA:HB2	1.86	0.56
2:C:218:LYS:HD3	8:C:316:HOH:O	2.05	0.56
2:C:82:ARG:CG	2:C:82:ARG:HH11	2.17	0.56
2:D:115:THR:HB	2:D:117[A]:GLU:OE1	2.05	0.56
2:D:103:VAL:CG1	2:D:104:GLN:N	2.59	0.56
1:A:24:HIS:O	1:A:52:ARG:NH2	2.38	0.56
1:A:264:SER:HB2	7:A:273[B]:GOL:H32	1.88	0.56
2:B:38:ALA:O	2:B:42:VAL:HG13	2.06	0.56
2:B:206:VAL:HG23	2:B:209:LEU:HD21	1.87	0.55
2:C:22:LYS:O	2:C:26:THR:HG23	2.06	0.55
2:C:82:ARG:HH11	2:C:82:ARG:HG3	1.71	0.55
2:B:208:LEU:CD2	2:B:234:ALA:HB2	2.37	0.55
2:D:206:VAL:HG12	2:D:209:LEU:HD21	1.88	0.55
2:C:172:SER:HB2	8:C:302:HOH:O	2.07	0.55
1:A:35:HIS:HB3	4:A:269:NAP:O1X	2.07	0.55
2:C:172:SER:CB	8:C:302:HOH:O	2.55	0.54
2:C:22:LYS:NZ	2:C:235:GLU:OE2	2.41	0.54
2:C:232:ALA:HB2	2:D:251:TYR:CD2	2.43	0.54
2:B:153:ASN:ND2	2:B:245:VAL:O	2.41	0.54
2:B:209:LEU:HA	5:B:270:AX3:HAD	1.90	0.54
1:A:14:ARG:HB3	1:A:208:LEU:HD23	1.90	0.54
2:D:77:ILE:HD13	8:D:365:HOH:O	2.06	0.54
2:B:114:LYS:NZ	2:B:122:GLU:OE1	2.41	0.54
1:A:9:THR:HA	1:A:33:HIS:HB3	1.89	0.53
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.44	0.53
2:D:164:VAL:HG12	6:D:272:EDO:H22	1.91	0.52
1:A:17:ARG:HG2	1:A:44:LEU:HD22	1.92	0.52
4:A:269:NAP:O5D	4:A:269:NAP:H2N	2.10	0.52
2:C:212:ALA:HB3	8:C:390:HOH:O	2.08	0.52
1:A:135:THR:HG21	8:A:286:HOH:O	2.09	0.52
2:C:218:LYS:CE	8:C:316:HOH:O	2.58	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:MET:O	2:B:214:GLY:C	2.47	0.52
2:D:153:ASN:ND2	2:D:245:VAL:O	2.43	0.52
2:D:103:VAL:HG22	2:D:104:GLN:H	1.75	0.52
2:D:129:ILE:HG22	2:D:133:LEU:HD22	1.91	0.52
2:B:9:THR:HA	2:B:33:HIS:HB3	1.91	0.52
2:D:213:MET:HG3	2:D:218:LYS:HZ2	1.75	0.51
2:B:219:ASP:HA	2:B:222:ARG:HB2	1.92	0.50
2:B:69:LEU:N	2:B:70:PRO:CD	2.74	0.50
1:A:131:PRO:O	1:A:135:THR:CG2	2.54	0.50
1:A:263:LEU:O	1:A:266[A]:VAL:CG2	2.57	0.50
2:C:232:ALA:HB2	2:D:251:TYR:CE2	2.46	0.50
2:D:219:ASP:O	2:D:223:ARG:HG3	2.10	0.50
4:A:269:NAP:O1A	5:A:270:AX3:HAL	2.10	0.50
2:C:207:SER:O	2:C:208:LEU:C	2.50	0.50
2:B:130:ALA:HB3	2:B:131:PRO:HD3	1.94	0.50
2:C:138:PHE:O	2:C:142:GLN:HG2	2.12	0.50
2:D:198:ARG:NH2	2:D:244:LEU:O	2.36	0.50
2:B:220:LYS:N	8:B:407:HOH:O	2.45	0.50
2:B:219:ASP:CB	8:B:407:HOH:O	2.60	0.49
2:D:191:GLU:OE1	6:D:273:EDO:O1	2.29	0.49
1:A:251:TYR:CD2	2:B:232:ALA:HB2	2.48	0.49
2:C:47:GLU:HG2	8:C:413:HOH:O	2.12	0.49
1:A:258:LYS:HD3	7:A:273[B]:GOL:H31	1.94	0.49
2:D:129:ILE:HG22	2:D:133:LEU:CD2	2.43	0.49
2:C:2:GLU:N	8:C:376:HOH:O	2.46	0.48
1:A:93:ASN:OD1	1:A:159[B]:LEU:HD13	2.12	0.48
2:C:115:THR:HB	2:C:117[A]:GLU:OE2	2.13	0.48
2:D:22[A]:LYS:CE	8:D:364:HOH:O	2.62	0.48
1:A:79:SER:HB3	8:A:373:HOH:O	2.13	0.48
1:A:117:GLU:HB2	8:A:282:HOH:O	2.14	0.47
2:B:193:ALA:N	2:B:194:PRO:CD	2.77	0.47
1:A:70:PRO:HG2	2:C:117[A]:GLU:HG3	1.97	0.47
2:C:130:ALA:HB3	2:C:131:PRO:HD3	1.97	0.47
1:A:116:VAL:HG21	2:C:136[A]:MET:HE3	1.97	0.47
1:A:2:GLU:HG3	1:A:29:ARG:NH2	2.30	0.47
2:B:173:LEU:HD23	2:B:176[A]:MET:HE3	1.97	0.46
1:A:219:ASP:O	1:A:223[B]:ARG:HG2	2.16	0.46
2:D:220:LYS:O	2:D:224:LYS:HG3	2.15	0.46
2:B:26:THR:HG22	2:B:26:THR:O	2.15	0.46
2:B:191:GLU:O	2:B:194:PRO:HD2	2.15	0.46
2:B:140:GLN:OE1	8:B:358:HOH:O	2.21	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:VAL:CG2	2:B:209:LEU:HD21	2.45	0.46
1:A:21[B]:VAL:HG13	1:A:22:LYS:HD2	1.98	0.46
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.97	0.46
1:A:135:THR:HB	1:A:156:ILE:HD13	1.98	0.46
2:B:117:GLU:HG3	2:D:70:PRO:HG2	1.97	0.46
2:D:206:VAL:CG2	2:D:263:LEU:HD22	2.46	0.45
1:A:44:LEU:HD12	1:A:48:LEU:HD13	1.99	0.45
2:B:152:SER:N	8:B:364:HOH:O	2.50	0.45
2:C:141:ARG:HD3	8:C:415:HOH:O	2.15	0.45
2:D:49:ASN:HA	2:D:52:ARG:O	2.17	0.45
2:B:195:TYR:CZ	2:D:103:VAL:HG11	2.52	0.44
2:C:209:LEU:HB2	2:C:218:LYS:HE3	1.99	0.44
2:B:207:SER:HB2	2:B:237:ILE:HD11	1.99	0.44
1:A:161:ASP:OD1	1:A:161:ASP:C	2.56	0.44
2:B:215:GLU:OE1	2:B:222:ARG:NH2	2.51	0.44
2:D:33:HIS:HA	2:D:59:CYS:O	2.17	0.44
2:B:212:ALA:O	2:B:214:GLY:N	2.50	0.44
1:A:116:VAL:HG21	2:C:136[A]:MET:CE	2.48	0.44
2:D:5:ALA:HA	2:D:29:ARG:O	2.17	0.44
1:A:159[B]:LEU:HD13	4:A:269:NAP:H4D	1.99	0.44
2:D:18:ALA:HA	2:D:22[A]:LYS:HZ3	1.82	0.43
2:D:192:LEU:HB3	2:D:197:ILE:HB	2.00	0.43
2:D:193:ALA:N	2:D:194:PRO:CD	2.81	0.43
1:A:116:VAL:HG22	8:A:345:HOH:O	2.17	0.43
1:A:227[A]:LEU:HD11	2:B:198:ARG:HG2	1.99	0.43
2:C:241:VAL:O	2:C:245:VAL:HG13	2.18	0.43
2:C:6:ALA:CB	2:C:89:VAL:HG22	2.48	0.43
2:C:153:ASN:ND2	2:C:245:VAL:O	2.51	0.43
2:C:218:LYS:CD	8:C:316:HOH:O	2.65	0.43
2:C:247:GLY:O	2:C:250:GLN:HG2	2.18	0.43
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.18	0.43
2:D:213:MET:O	2:D:218:LYS:NZ	2.37	0.42
1:A:117:GLU:OE2	2:C:67[A]:ASN:ND2	2.47	0.42
2:C:9:THR:HA	2:C:33:HIS:HB3	2.01	0.42
1:A:19:ILE:O	1:A:23[B]:LEU:CG	2.66	0.42
2:D:11:ALA:HB3	2:D:32:ILE:HG23	2.00	0.42
2:C:20:ALA:HB1	2:C:30:VAL:HG21	2.01	0.42
1:A:116:VAL:CG2	8:A:345:HOH:O	2.68	0.42
2:D:205:GLY:O	4:D:270:NAP:H4N	2.19	0.42
2:D:191:GLU:HB2	6:D:273:EDO:O1	2.19	0.42
1:A:14:ARG:NH1	4:A:269:NAP:O1N	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:391:HOH:O	2:D:117[A]:GLU:HG2	2.19	0.42
2:C:157[A]:VAL:HA	2:C:200:ASN:O	2.19	0.42
2:C:17:ARG:O	2:C:21:VAL:HG23	2.20	0.42
1:A:191:GLU:O	1:A:194:PRO:HD2	2.19	0.42
1:A:209:LEU:HB2	1:A:218:LYS:HE2	2.02	0.42
2:B:173:LEU:HD23	2:B:176[A]:MET:CE	2.48	0.42
2:C:200:ASN:OD1	2:C:253:THR:HA	2.20	0.42
4:C:269:NAP:H2D	5:C:270:AX3:NAE	2.34	0.42
2:D:65:ASN:HA	2:D:69:LEU:HD22	2.02	0.42
2:D:238:ALA:O	2:D:242:ILE:HG12	2.20	0.42
1:A:18:ALA:HA	1:A:21[B]:VAL:HG12	2.01	0.42
2:B:219:ASP:HB2	8:B:407:HOH:O	2.17	0.42
2:B:169:MET:O	2:B:170:ALA:HB3	2.19	0.42
1:A:264:SER:CB	7:A:273[B]:GOL:H32	2.48	0.41
2:B:207:SER:O	2:B:208:LEU:C	2.57	0.41
1:A:5:ALA:HA	1:A:29:ARG:O	2.19	0.41
2:D:169:MET:O	2:D:170:ALA:HB3	2.20	0.41
2:D:18:ALA:O	2:D:22[A]:LYS:HD3	2.20	0.41
2:D:22[A]:LYS:NZ	8:D:364:HOH:O	2.33	0.41
2:C:69:LEU:O	2:C:70:PRO:C	2.56	0.41
2:C:205:GLY:O	4:C:269:NAP:H4N	2.21	0.41
2:D:187:SER:HB3	6:D:273:EDO:C2	2.50	0.41
2:D:187:SER:HB3	6:D:273:EDO:H21	2.02	0.40
2:D:14:ARG:NH2	2:D:209:LEU:O	2.54	0.40
2:B:160:CYS:HB3	8:B:307:HOH:O	2.22	0.40
1:A:258:LYS:HE3	8:B:276:HOH:O	2.21	0.40
1:A:9:THR:O	1:A:10:GLY:C	2.59	0.40
2:D:130:ALA:HB3	2:D:131:PRO:HD3	2.03	0.40
1:A:49:ASN:HA	1:A:52:ARG:O	2.22	0.40
1:A:117:GLU:CD	2:C:67[A]:ASN:HD22	2.23	0.40
1:A:130:ALA:HB3	1:A:131:PRO:CD	2.51	0.40

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	252/288 (88%)	241 (96%)	11 (4%)	0	100	100
2	B	251/288 (87%)	235 (94%)	14 (6%)	2 (1%)	24	14
2	C	251/288 (87%)	240 (96%)	11 (4%)	0	100	100
2	D	254/288 (88%)	242 (95%)	11 (4%)	1 (0%)	39	31
All	All	1008/1152 (88%)	958 (95%)	47 (5%)	3 (0%)	46	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	213	MET
2	B	214	GLY
2	D	103	VAL

### 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	206/230 (90%)	191 (93%)	15 (7%)	17	10
2	B	205/231 (89%)	182 (89%)	23 (11%)	7	3
2	C	205/231 (89%)	184 (90%)	21 (10%)	9	4
2	D	207/231 (90%)	200 (97%)	7 (3%)	44	39
All	All	823/923 (89%)	757 (92%)	66 (8%)	17	8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	13	LYS
1	A	22	LYS
1	A	39	GLU
1	A	48	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	69	LEU
1	A	90	LEU
1	A	135	THR
1	A	151	SER
1	A	192	LEU
1	A	208	LEU
1	A	211	VAL
1	A	217	GLU
1	A	220	LYS
1	A	230	ARG
2	B	14	ARG
2	B	31[A]	VAL
2	B	31[B]	VAL
2	B	44	LEU
2	B	51	GLU
2	B	53	SER
2	B	63[A]	LEU
2	B	63[B]	LEU
2	B	78	ASN
2	B	104	GLN
2	B	116	VAL
2	B	152	SER
2	B	157	VAL
2	B	169	MET
2	B	208	LEU
2	B	211	VAL
2	B	219	ASP
2	B	222	ARG
2	B	230	ARG
2	B	250[A]	GLN
2	B	250[B]	GLN
2	B	259[A]	VAL
2	B	259[B]	VAL
2	C	78	ASN
2	C	82	ARG
2	C	90	LEU
2	C	95	SER
2	C	116	VAL
2	C	117[A]	GLU
2	C	117[B]	GLU
2	C	133	LEU
2	C	141	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	152	SER
2	C	154	LEU
2	C	157[A]	VAL
2	C	157[B]	VAL
2	C	166	GLN
2	C	190	LEU
2	C	215	GLU
2	C	216	GLU
2	C	217	GLU
2	C	229	ARG
2	C	230	ARG
2	C	258	LYS
2	D	22[A]	LYS
2	D	22[B]	LYS
2	D	44	LEU
2	D	104	GLN
2	D	133	LEU
2	D	192	LEU
2	D	231	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	65	ASN
2	B	104	GLN
2	B	112	ASN
2	B	140	GLN
2	C	250	GLN
2	D	54	ASN
2	D	65	ASN

### 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$
1	CSX	A	168	1	3,6,7	0.53	0	3,6,8	1.58	1 (33%)

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	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	168	CSX	CB-CA-C	-2.37	104.96	111.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

21 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	-	42,52,52	1.53	3 (7%)	54,80,80	2.94	19 (35%)
5	AX3	A	270	-	13,13,13	1.04	2 (15%)	16,18,18	2.80	7 (43%)
7	GOL	A	271	-	5,5,5	0.36	0	5,5,5	0.60	0
7	GOL	A	272	-	5,5,5	0.31	0	5,5,5	0.50	0
7	GOL	A	273[A]	-	5,5,5	0.34	0	5,5,5	2.49	2 (40%)
7	GOL	A	273[B]	-	5,5,5	0.35	0	5,5,5	2.61	2 (40%)
4	NAP	B	269	-	42,52,52	1.52	3 (7%)	54,80,80	2.78	15 (27%)
5	AX3	B	270	-	13,13,13	1.03	2 (15%)	16,18,18	2.94	9 (56%)
7	GOL	B	271[A]	-	5,5,5	0.27	0	5,5,5	0.90	0
7	GOL	B	271[B]	-	5,5,5	0.27	0	5,5,5	0.85	0
4	NAP	C	269	-	42,52,52	1.51	3 (7%)	54,80,80	2.62	15 (27%)
5	AX3	C	270	-	13,13,13	0.95	1 (7%)	16,18,18	3.32	8 (50%)
6	EDO	C	271	-	3,3,3	0.49	0	2,2,2	0.26	0
7	GOL	C	272[A]	-	5,5,5	0.29	0	5,5,5	0.52	0
7	GOL	C	272[B]	-	5,5,5	0.27	0	5,5,5	0.82	0
3	ACT	D	269	-	1,3,3	1.10	0	0,3,3	0.00	-
4	NAP	D	270	-	42,52,52	1.47	3 (7%)	54,80,80	2.66	14 (25%)
5	AX3	D	271	-	13,13,13	1.04	2 (15%)	16,18,18	3.02	7 (43%)
6	EDO	D	272	-	3,3,3	0.51	0	2,2,2	0.45	0
6	EDO	D	273	-	3,3,3	0.41	0	2,2,2	0.75	0
7	GOL	D	274	-	5,5,5	0.35	0	5,5,5	0.71	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
4	NAP	A	269	-	-	0/27/67/67	0/5/5/5
5	AX3	A	270	-	-	0/4/6/6	0/1/2/2
7	GOL	A	271	-	-	0/4/4/4	0/0/0/0
7	GOL	A	272	-	-	0/4/4/4	0/0/0/0
7	GOL	A	273[A]	-	-	0/4/4/4	0/0/0/0
7	GOL	A	273[B]	-	-	0/4/4/4	0/0/0/0
4	NAP	B	269	-	-	0/27/67/67	0/5/5/5
5	AX3	B	270	-	-	0/4/6/6	0/1/2/2
7	GOL	B	271[A]	-	-	0/4/4/4	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	271[B]	-	-	0/4/4/4	0/0/0/0
4	NAP	C	269	-	-	0/27/67/67	0/5/5/5
5	AX3	C	270	-	-	0/4/6/6	0/1/2/2
6	EDO	C	271	-	-	0/1/1/1	0/0/0/0
7	GOL	C	272[A]	-	-	0/4/4/4	0/0/0/0
7	GOL	C	272[B]	-	-	0/4/4/4	0/0/0/0
3	ACT	D	269	-	-	0/0/0/0	0/0/0/0
4	NAP	D	270	-	-	0/27/67/67	0/5/5/5
5	AX3	D	271	-	-	0/4/6/6	0/1/2/2
6	EDO	D	272	-	-	0/1/1/1	0/0/0/0
6	EDO	D	273	-	-	0/1/1/1	0/0/0/0
7	GOL	D	274	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	270	AX3	CAD-CAL	2.01	1.53	1.48
5	B	270	AX3	CAD-CAL	2.04	1.53	1.48
5	B	270	AX3	CAC-CAL	2.05	1.53	1.48
5	C	270	AX3	CAC-CAL	2.17	1.53	1.48
4	D	270	NAP	C2A-N1A	2.17	1.38	1.33
4	C	269	NAP	C2A-N1A	2.25	1.38	1.33
5	D	271	AX3	CAC-CAL	2.28	1.53	1.48
5	A	270	AX3	CAC-CAL	2.43	1.54	1.48
4	A	269	NAP	C2A-N1A	2.44	1.38	1.33
5	D	271	AX3	CAD-CAL	2.45	1.54	1.48
4	B	269	NAP	C2A-N1A	2.54	1.38	1.33
4	A	269	NAP	C2A-N3A	3.17	1.37	1.32
4	C	269	NAP	C2A-N3A	3.39	1.38	1.32
4	B	269	NAP	C2A-N3A	3.47	1.38	1.32
4	D	270	NAP	C2A-N3A	3.53	1.38	1.32
4	D	270	NAP	O7N-C7N	7.48	1.40	1.24
4	B	269	NAP	O7N-C7N	7.61	1.40	1.24
4	C	269	NAP	O7N-C7N	7.67	1.40	1.24
4	A	269	NAP	O7N-C7N	7.82	1.40	1.24

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	269	NAP	N3A-C2A-N1A	-12.28	119.49	128.89
4	D	270	NAP	N3A-C2A-N1A	-11.93	119.76	128.89
4	B	269	NAP	N3A-C2A-N1A	-11.76	119.89	128.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	269	NAP	N3A-C2A-N1A	-9.81	121.38	128.89
4	C	269	NAP	O7N-C7N-C3N	-8.35	110.47	119.59
4	D	270	NAP	O7N-C7N-C3N	-7.95	110.91	119.59
4	B	269	NAP	O7N-C7N-C3N	-6.69	112.28	119.59
4	A	269	NAP	C3N-C2N-N1N	-6.55	112.81	120.36
4	A	269	NAP	O7N-C7N-C3N	-6.21	112.81	119.59
5	B	270	AX3	CAK-NAH-CAL	-5.89	116.96	123.51
5	D	271	AX3	NAF-CAK-NAG	-5.23	118.18	126.22
4	C	269	NAP	O3-PN-O5D	-5.06	89.52	102.94
5	A	270	AX3	NAF-CAK-NAG	-5.01	118.52	126.22
5	C	270	AX3	NAF-CAK-NAG	-5.01	118.52	126.22
4	D	270	NAP	C3N-C2N-N1N	-4.72	114.92	120.36
5	B	270	AX3	NAE-CAJ-NAG	-4.52	118.13	125.53
7	A	273[A]	GOL	O2-C2-C3	-4.35	88.71	108.65
5	A	270	AX3	CAK-NAH-CAL	-4.30	118.72	123.51
7	A	273[B]	GOL	C3-C2-C1	-4.21	94.59	111.12
4	A	269	NAP	C6N-C5N-C4N	-3.92	113.52	119.44
5	C	270	AX3	NAE-CAI-NAF	-3.69	119.49	125.53
4	A	269	NAP	C4B-O4B-C1B	-3.57	105.80	109.72
7	A	273[B]	GOL	O2-C2-C3	-3.50	92.61	108.65
4	D	270	NAP	C4B-O4B-C1B	-3.37	106.02	109.72
4	D	270	NAP	C6N-C5N-C4N	-3.29	114.47	119.44
4	B	269	NAP	O3-PN-O5D	-3.25	94.32	102.94
5	D	271	AX3	NAE-CAI-NAF	-3.24	120.23	125.53
4	B	269	NAP	O3-PA-O5B	-3.22	94.39	102.94
4	B	269	NAP	PN-O3-PA	-2.99	124.34	132.73
4	C	269	NAP	O3-PA-O5B	-2.98	95.04	102.94
4	A	269	NAP	O3-PA-O5B	-2.89	95.27	102.94
4	D	270	NAP	C4A-C5A-N7A	-2.81	106.89	109.48
4	C	269	NAP	C1B-N9A-C4A	-2.72	122.84	126.94
4	D	270	NAP	C1B-N9A-C4A	-2.71	122.85	126.94
5	B	270	AX3	NAE-CAI-NAF	-2.68	121.15	125.53
7	A	273[A]	GOL	C3-C2-C1	-2.66	100.71	111.12
5	A	270	AX3	NAE-CAJ-NAG	-2.56	121.34	125.53
4	A	269	NAP	C4A-C5A-N7A	-2.53	107.15	109.48
5	B	270	AX3	NAF-CAK-NAG	-2.48	122.41	126.22
4	B	269	NAP	O3X-P2B-O1X	-2.47	102.64	110.58
5	C	270	AX3	NAE-CAJ-NAG	-2.38	121.63	125.53
4	B	269	NAP	C1B-N9A-C4A	-2.33	123.43	126.94
4	C	269	NAP	C4A-C5A-N7A	-2.24	107.42	109.48
4	A	269	NAP	C2D-C3D-C4D	-2.24	98.01	102.61
4	A	269	NAP	O4B-C1B-C2B	-2.19	102.64	106.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	269	NAP	O5D-PN-O1N	-2.13	101.34	109.62
4	A	269	NAP	O3X-P2B-O1X	-2.07	103.90	110.58
5	D	271	AX3	NAE-CAJ-NAG	-2.01	122.24	125.53
4	B	269	NAP	O7N-C7N-N7N	-2.00	119.78	122.59
4	C	269	NAP	O2A-PA-O5B	2.05	118.82	108.46
4	A	269	NAP	O2N-PN-O1N	2.08	123.78	112.53
4	A	269	NAP	O4D-C1D-N1N	2.08	110.42	108.13
4	D	270	NAP	O7N-C7N-N7N	2.09	125.54	122.59
4	C	269	NAP	O4D-C1D-N1N	2.11	110.45	108.13
4	D	270	NAP	O2N-PN-O1N	2.12	124.01	112.53
4	A	269	NAP	O4D-C4D-C3D	2.17	109.51	105.15
4	C	269	NAP	C2A-N1A-C6A	2.18	122.66	118.77
4	A	269	NAP	C2A-N1A-C6A	2.19	122.68	118.77
4	C	269	NAP	P2B-O2B-C2B	2.19	126.82	121.56
4	B	269	NAP	O2N-PN-O1N	2.20	124.43	112.53
4	C	269	NAP	O4D-C4D-C5D	2.20	117.21	109.32
4	C	269	NAP	O2X-P2B-O1X	2.34	118.10	110.58
5	C	270	AX3	NAA-CAI-NAE	2.39	121.16	117.20
5	B	270	AX3	CAI-NAF-CAK	2.46	117.16	113.57
4	D	270	NAP	C2N-C3N-C4N	2.51	121.08	118.29
4	D	270	NAP	C5N-C4N-C3N	2.57	123.57	120.33
4	B	269	NAP	O2N-PN-O3	2.66	117.17	105.09
4	A	269	NAP	O7N-C7N-N7N	2.68	126.36	122.59
4	A	269	NAP	C3N-C7N-N7N	2.75	120.82	117.82
4	D	270	NAP	C4D-O4D-C1D	2.80	112.80	109.72
4	B	269	NAP	O3X-P2B-O2X	2.84	118.20	107.38
4	A	269	NAP	C5N-C6N-N1N	2.85	125.40	120.47
5	A	270	AX3	NAB-CAJ-NAE	2.93	122.05	117.20
4	C	269	NAP	O2N-PN-O1N	3.00	128.78	112.53
5	B	270	AX3	NAB-CAJ-NAG	3.20	122.50	117.20
4	B	269	NAP	O2D-C2D-C3D	3.21	122.26	111.83
5	B	270	AX3	CAJ-NAE-CAI	3.63	121.34	114.80
5	D	271	AX3	NAB-CAJ-NAE	3.72	123.35	117.20
5	A	270	AX3	CAI-NAF-CAK	3.78	119.08	113.57
5	B	270	AX3	NAH-CAK-NAG	3.83	122.54	116.95
5	C	270	AX3	NAB-CAJ-NAE	4.09	123.97	117.20
5	B	270	AX3	CAJ-NAG-CAK	4.28	119.82	113.57
5	A	270	AX3	NAH-CAK-NAF	4.32	123.27	116.95
5	D	271	AX3	CAJ-NAG-CAK	4.42	120.02	113.57
5	C	270	AX3	CAJ-NAG-CAK	4.53	120.17	113.57
5	A	270	AX3	CAJ-NAG-CAK	5.20	121.16	113.57
4	D	270	NAP	C3N-C7N-N7N	5.24	123.56	117.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	271	AX3	NAH-CAK-NAF	5.31	124.71	116.95
4	B	269	NAP	O4B-C1B-N9A	5.36	119.31	108.10
5	D	271	AX3	CAI-NAF-CAK	5.56	121.68	113.57
5	C	270	AX3	CAI-NAF-CAK	5.67	121.83	113.57
4	D	270	NAP	O4B-C1B-N9A	5.90	120.44	108.10
4	C	269	NAP	O4B-C1B-N9A	5.99	120.64	108.10
4	A	269	NAP	O4B-C1B-N9A	6.50	121.71	108.10
5	C	270	AX3	NAH-CAK-NAF	6.55	126.52	116.95
4	C	269	NAP	C3N-C7N-N7N	6.91	125.38	117.82
4	A	269	NAP	C2N-C3N-C4N	7.09	126.19	118.29
4	B	269	NAP	C3N-C7N-N7N	9.25	127.94	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	269	NAP	5	0
5	A	270	AX3	2	0
7	A	273[B]	GOL	4	0
5	B	270	AX3	2	0
4	C	269	NAP	2	0
5	C	270	AX3	1	0
4	D	270	NAP	1	0
6	D	272	EDO	1	0
6	D	273	EDO	10	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	250/288 (86%)	0.12	3 (1%) 81 83	12, 25, 44, 52	0
2	B	252/288 (87%)	0.21	5 (1%) 68 71	15, 24, 47, 64	1 (0%)
2	C	251/288 (87%)	0.11	4 (1%) 74 77	14, 24, 43, 57	0
2	D	253/288 (87%)	0.13	5 (1%) 68 71	14, 24, 41, 56	0
All	All	1006/1152 (87%)	0.14	17 (1%) 73 75	12, 24, 44, 64	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	212	ALA	5.3
2	D	104	GLN	4.6
2	D	211	VAL	4.6
2	B	211	VAL	4.4
2	C	211	VAL	4.1
2	D	151	SER	3.3
1	A	212	ALA	3.1
2	C	151	SER	2.9
2	B	210	PRO	2.6
1	A	113	GLY	2.5
2	B	216	GLU	2.4
1	A	211	VAL	2.3
2	B	215	GLU	2.3
2	B	212	ALA	2.2
2	C	212	ALA	2.1
2	D	152	SER	2.1
2	C	152	SER	2.0

## 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. 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
1	CSX	A	168	7/8	0.88	0.12	-	21,24,34,35	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(Å <sup>2</sup> )	Q<0.9
7	GOL	A	273[B]	6/6	0.78	0.29	22.27	25,34,41,44	2
7	GOL	A	273[A]	6/6	0.78	0.29	17.98	25,39,41,44	2
6	EDO	D	272	4/4	0.91	0.20	5.52	24,40,43,47	0
3	ACT	D	269	4/4	0.91	0.16	3.03	35,36,37,38	0
6	EDO	C	271	4/4	0.80	0.13	1.94	39,39,40,42	0
7	GOL	C	272[B]	6/6	0.85	0.15	1.73	28,32,33,34	2
7	GOL	C	272[A]	6/6	0.85	0.15	1.73	24,30,33,34	2
6	EDO	D	273	4/4	0.96	0.12	1.64	21,23,23,27	0
7	GOL	A	272	6/6	0.69	0.18	1.15	32,42,45,47	0
5	AX3	D	271	12/12	0.93	0.13	0.67	15,20,37,38	0
5	AX3	C	270	12/12	0.94	0.12	0.05	13,23,34,37	0
7	GOL	B	271[B]	6/6	0.85	0.14	0.00	22,26,31,33	2
7	GOL	B	271[A]	6/6	0.85	0.14	0.00	12,26,31,33	2
5	AX3	B	270	12/12	0.92	0.13	-0.01	25,32,39,39	0
7	GOL	D	274	6/6	0.91	0.12	-0.44	20,31,36,37	0
4	NAP	C	269	48/48	0.96	0.10	-0.65	8,21,25,31	0
4	NAP	D	270	48/48	0.96	0.10	-0.67	2,23,27,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAP	B	269	48/48	0.95	0.10	-0.76	7,21,27,30	0
7	GOL	A	271	6/6	0.84	0.12	-0.90	34,42,44,44	0
4	NAP	A	269	48/48	0.96	0.09	-1.28	4,23,31,33	0
5	AX3	A	270	12/12	0.92	0.09	-1.63	10,22,31,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.