



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:47 AM GMT

PDB ID : 3JQ7  
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 6-phenylpteridine-2,4,7-triamine (DX2)  
Authors : Tulloch, L.B.; Hunter, W.N.  
Deposited on : 2009-09-06  
Resolution : 1.80 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

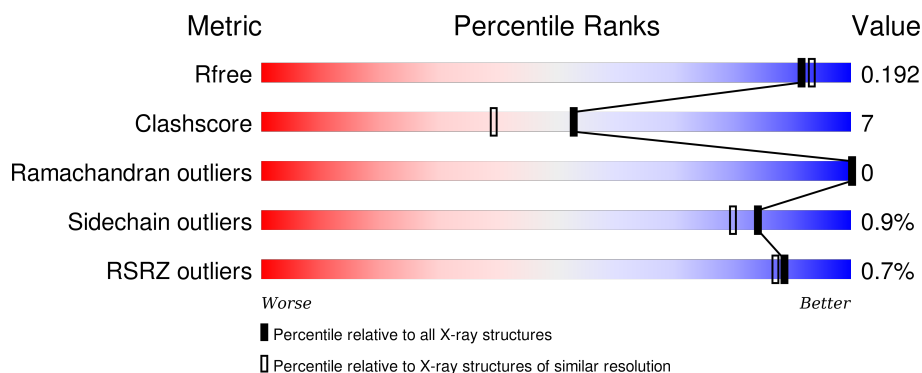
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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
4	DX2	A	271	-	-	-	X
4	DX2	B	271	-	-	X	X
4	DX2	C	270	-	-	-	X
4	DX2	D	270	-	-	X	X
5	ACT	B	270	-	-	-	X
6	DTT	B	272[A]	X	-	X	X
6	DTT	B	272[B]	X	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8353 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	9	0
			1886	1188	329	356	13			
1	C	239	Total	C	N	O	S	0	10	0
			1807	1141	317	339	10			
1	D	249	Total	C	N	O	S	0	10	0
			1879	1182	328	357	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q581W1
A	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-17	SER	-	EXPRESSION TAG	UNP Q581W1
A	-16	SER	-	EXPRESSION TAG	UNP Q581W1
A	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-9	SER	-	EXPRESSION TAG	UNP Q581W1
A	-8	SER	-	EXPRESSION TAG	UNP Q581W1
A	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
A	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
A	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
A	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
A	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-1	SER	-	EXPRESSION TAG	UNP Q581W1
A	0	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-19	MET	-	EXPRESSION TAG	UNP Q581W1
C	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-17	SER	-	EXPRESSION TAG	UNP Q581W1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	EXPRESSION TAG	UNP Q581W1
C	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-9	SER	-	EXPRESSION TAG	UNP Q581W1
C	-8	SER	-	EXPRESSION TAG	UNP Q581W1
C	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
C	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
C	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
C	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
C	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-1	SER	-	EXPRESSION TAG	UNP Q581W1
C	0	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-19	MET	-	EXPRESSION TAG	UNP Q581W1
D	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-17	SER	-	EXPRESSION TAG	UNP Q581W1
D	-16	SER	-	EXPRESSION TAG	UNP Q581W1
D	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-9	SER	-	EXPRESSION TAG	UNP Q581W1
D	-8	SER	-	EXPRESSION TAG	UNP Q581W1
D	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
D	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
D	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
D	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
D	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-1	SER	-	EXPRESSION TAG	UNP Q581W1
D	0	HIS	-	EXPRESSION TAG	UNP Q581W1

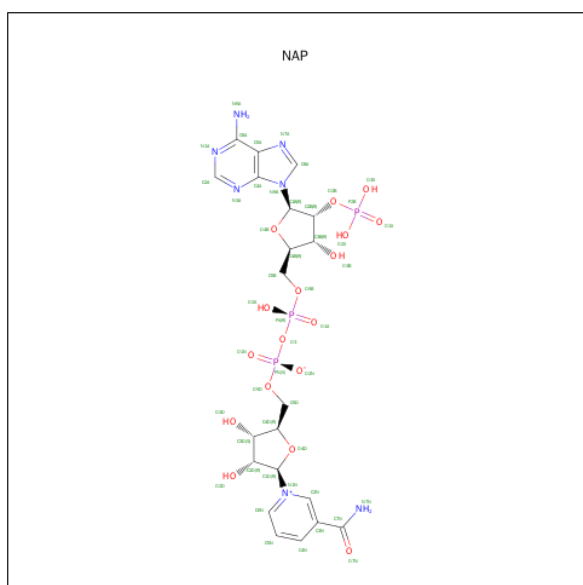
- Molecule 2 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	11	0
			1879	1184	328	355	12			

There are 20 discrepancies between the modelled and reference sequences:

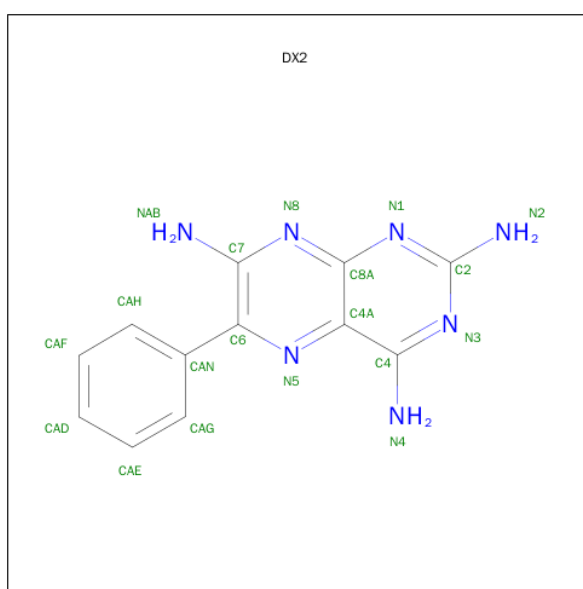
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q581W1
B	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-17	SER	-	EXPRESSION TAG	UNP Q581W1
B	-16	SER	-	EXPRESSION TAG	UNP Q581W1
B	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-9	SER	-	EXPRESSION TAG	UNP Q581W1
B	-8	SER	-	EXPRESSION TAG	UNP Q581W1
B	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
B	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
B	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
B	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
B	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-1	SER	-	EXPRESSION TAG	UNP Q581W1
B	0	HIS	-	EXPRESSION TAG	UNP Q581W1

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 6-PHENYLPTERIDINE-2,4,7-TRIAMINE (three-letter code: DX2) (formula:  $C_{12}H_{11}N_7$ ).



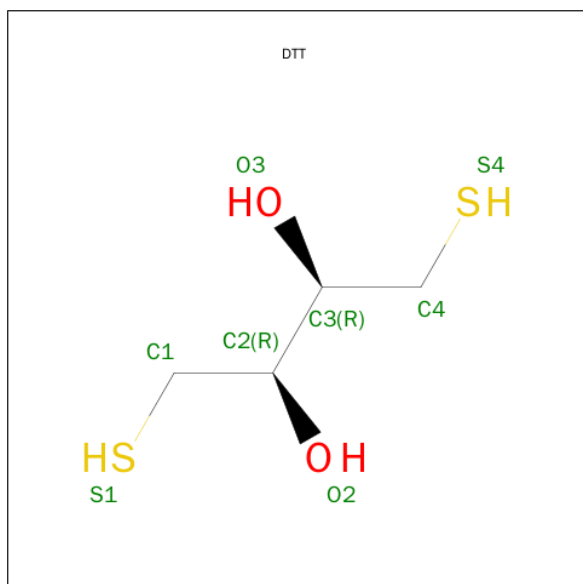
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			19	12	7		
4	B	1	Total	C	N	0	0
			19	12	7		
4	C	1	Total	C	N	0	0
			19	12	7		
4	D	1	Total	C	N	0	0
			19	12	7		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- 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	B	1	Total	C	O	S	0	1
			15	8	4	3		



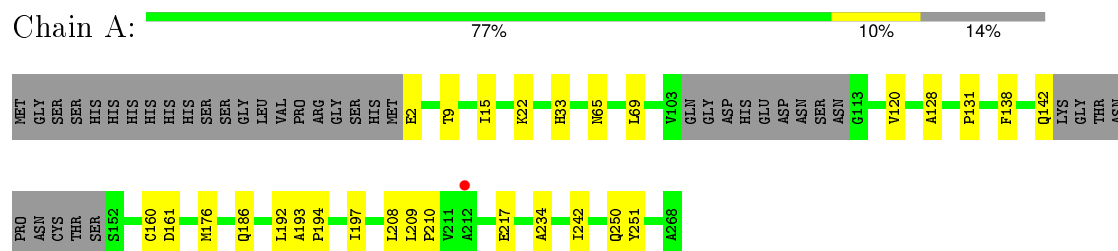
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	167	Total 167	O 167	0	0
7	B	176	Total 176	O 176	0	0
7	C	133	Total 133	O 133	0	0
7	D	135	Total 135	O 135	0	0

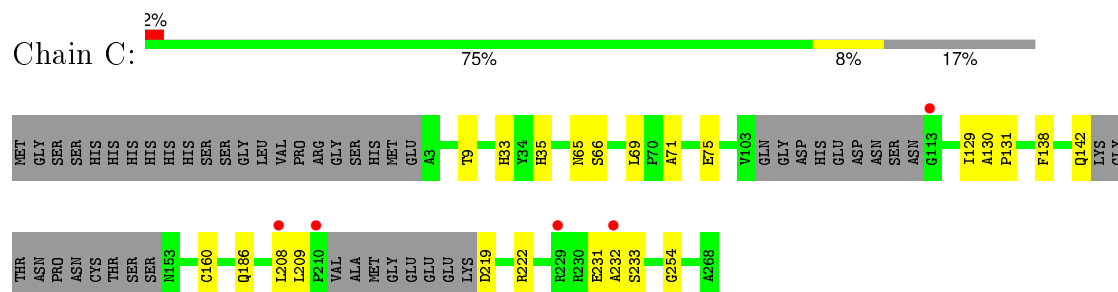
### 3 Residue-property plots

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

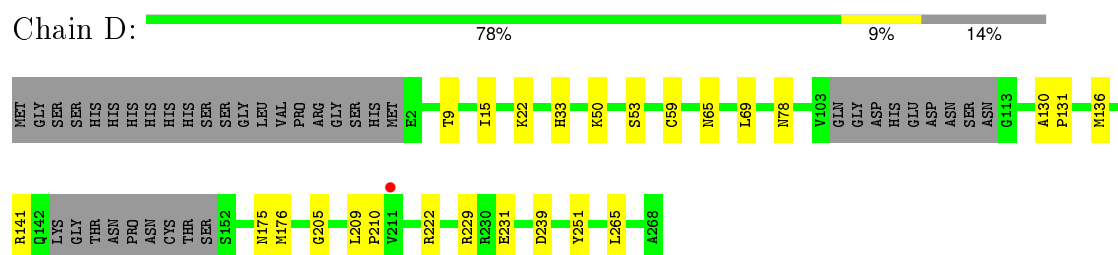
#### • Molecule 1: Pteridine reductase 1



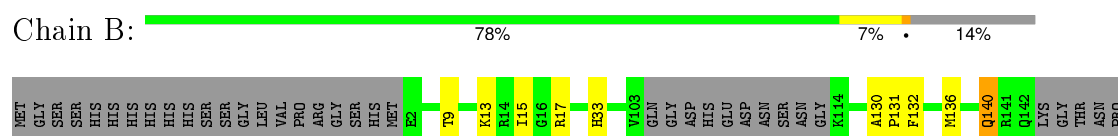
#### • Molecule 1: Pteridine reductase 1



#### • Molecule 1: Pteridine reductase 1



#### • Molecule 2: Pteridine reductase 1



ASN	CYS	THR	SER	SER	N153	D161	C168	N175	Q186	G205	L209	P210	V211	R223	R229	A232	Q236	A268
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.54Å 90.03Å 82.36Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	74.33 – 1.80 74.34 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (74.33-1.80) 99.6 (74.34-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.152 , 0.191 0.153 , 0.192	Depositor DCC
$R_{free}$ test set	4569 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.4	EDS
Estimated twinning fraction	0.007 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	1 of 90588 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 29.61 % 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 1.5051e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, ACT, DTT, DX2, CSX

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	0.66	0/1918	0.65	0/2597
1	C	0.61	0/1835	0.65	0/2488
1	D	0.62	0/1907	0.63	0/2584
2	B	0.68	0/1916	0.68	0/2599
All	All	0.64	0/7576	0.65	0/10268

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1930	22	0
1	C	1807	0	1849	22	0
1	D	1879	0	1912	20	0
2	B	1879	0	1914	25	0
3	A	48	0	25	1	0
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	2	0
4	A	19	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	11	17	0
4	C	19	0	11	6	0
4	D	19	0	11	8	0
5	A	4	0	3	0	0
5	B	4	0	3	0	1
6	B	15	0	18	13	0
7	A	167	0	0	4	0
7	B	176	0	0	2	1
7	C	133	0	0	8	2
7	D	135	0	0	4	0
All	All	8353	0	7773	102	2

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 (102) 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:B:168:CYS:SG	6:B:272[B]:DTT:S4	2.50	1.03
4:B:271:DX2:HAG	4:B:271:DX2:HNAB	1.26	1.01
4:C:270:DX2:HAH	4:C:270:DX2:HNAB	1.30	0.95
4:B:271:DX2:HAF	6:B:272[A]:DTT:H41	1.53	0.91
1:D:210:PRO:HD3	4:D:270:DX2:HAG	1.55	0.88
4:D:270:DX2:HAG	4:D:270:DX2:HNAB	1.41	0.85
6:B:272[A]:DTT:H12	6:B:272[A]:DTT:S4	2.16	0.85
1:D:59:CSX:OD	7:D:385:HOH:O	1.98	0.82
2:B:209:LEU:HD23	4:B:271:DX2:CAE	2.10	0.81
1:A:209:LEU:HD23	4:A:271:DX2:CAF	2.11	0.80
4:B:271:DX2:CAF	6:B:272[A]:DTT:H41	2.13	0.78
1:A:209:LEU:HD23	4:A:271:DX2:HAF	1.65	0.77
1:D:222:ARG:HD3	1:D:231:GLU:OE2	1.86	0.76
2:B:209:LEU:CD2	4:B:271:DX2:HAE	2.16	0.76
1:D:22:LYS:HE3	1:D:239:ASP:OD1	1.87	0.75
2:B:210:PRO:HD3	4:B:271:DX2:HAG	1.68	0.73
1:A:250:GLN:HG2	7:A:287:HOH:O	1.88	0.73
1:C:66:SER:HB3	7:C:344:HOH:O	1.87	0.73
2:B:209:LEU:CD2	4:B:271:DX2:CAE	2.66	0.73
2:B:136:MET:O	2:B:140:GLN:HG2	1.88	0.72
2:B:209:LEU:HD22	4:B:271:DX2:HAE	1.75	0.67
4:B:271:DX2:HAH	6:B:272[B]:DTT:H2	1.77	0.67
1:D:175[B]:ASN:ND2	7:D:347:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ARG:HA	2:B:229:ARG:HG3	1.81	0.61
2:B:161:ASP:OD2	6:B:272[A]:DTT:O2	2.17	0.61
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.84	0.60
4:C:270:DX2:HAE	7:C:398:HOH:O	2.02	0.58
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.84	0.58
1:A:9:THR:HA	1:A:33:HIS:HB3	1.85	0.57
1:C:209:LEU:CD1	4:C:270:DX2:HAF	2.35	0.57
1:C:232:ALA:C	7:C:316:HOH:O	2.41	0.57
2:B:205:GLY:O	6:B:272[A]:DTT:H42	2.05	0.56
1:A:120:VAL:HG11	1:C:129[A]:ILE:HD13	1.88	0.55
1:D:210:PRO:HD3	4:D:270:DX2:CAG	2.31	0.55
4:C:270:DX2:CAH	4:C:270:DX2:HNAB	2.12	0.54
4:B:271:DX2:HAG	4:B:271:DX2:NAB	2.05	0.54
1:A:209:LEU:HA	4:A:271:DX2:HAH	1.91	0.53
1:D:209:LEU:HD23	4:D:270:DX2:CAE	2.39	0.52
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.44	0.52
2:B:132:PHE:CZ	2:B:136:MET:CE	2.93	0.52
4:B:271:DX2:CAH	6:B:272[A]:DTT:H41	2.41	0.51
2:B:210:PRO:HD3	4:B:271:DX2:CAG	2.40	0.50
1:A:138:PHE:O	1:A:142:GLN:HG2	2.12	0.50
1:C:71:ALA:O	1:C:75:GLU:HG2	2.12	0.50
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.94	0.49
1:C:160:CYS:HB3	7:C:285:HOH:O	2.10	0.49
4:B:271:DX2:CAG	4:B:271:DX2:HNAB	2.09	0.49
1:C:209:LEU:HD13	4:C:270:DX2:HAF	1.93	0.49
1:C:138:PHE:O	1:C:142:GLN:HG2	2.13	0.49
1:A:160[B]:CYS:SG	1:A:161:ASP:N	2.86	0.49
4:C:270:DX2:NAB	4:C:270:DX2:HAH	2.09	0.49
2:B:9:THR:HA	2:B:33:HIS:HB3	1.95	0.48
1:D:205:GLY:O	3:D:269:NAP:H4N	2.12	0.48
1:C:231:GLU:HG2	7:C:316:HOH:O	2.14	0.48
1:C:219:ASP:HA	1:C:222:ARG:HD2	1.95	0.48
1:C:9:THR:HA	1:C:33:HIS:HB3	1.95	0.48
4:D:270:DX2:HAF	7:D:346:HOH:O	2.13	0.48
2:B:15:ILE:HB	3:B:269:NAP:H51N	1.97	0.47
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.98	0.46
2:B:175[A]:ASN:ND2	7:B:587:HOH:O	1.96	0.46
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.96	0.46
1:A:210:PRO:HD3	4:A:271:DX2:CAH	2.46	0.46
2:B:132:PHE:CZ	2:B:136:MET:HE3	2.51	0.46
1:C:35:HIS:HB2	3:C:269:NAP:C2A	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:271:DX2:HAH	6:B:272[B]:DTT:C2	2.44	0.46
1:C:233:SER:N	7:C:316:HOH:O	2.48	0.46
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.50	0.46
1:A:15:ILE:HB	3:A:269:NAP:H51N	1.98	0.46
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.98	0.45
1:D:210:PRO:HG3	4:D:270:DX2:NAB	2.32	0.45
2:B:229:ARG:NH2	7:B:491:HOH:O	2.50	0.44
4:B:271:DX2:HAF	6:B:272[A]:DTT:C4	2.36	0.44
1:A:250:GLN:CD	2:B:236:GLN:HE21	2.20	0.44
1:D:210:PRO:CD	4:D:270:DX2:HAG	2.38	0.44
1:A:120:VAL:CG1	1:C:129[A]:ILE:HD13	2.47	0.44
1:C:208:LEU:HD21	7:C:300:HOH:O	2.17	0.44
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.53	0.44
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.49	0.43
4:D:270:DX2:HAG	4:D:270:DX2:NAB	2.18	0.43
1:A:128:ALA:C	1:A:131:PRO:HD2	2.38	0.43
4:B:271:DX2:HAF	6:B:272[B]:DTT:H41	2.00	0.43
4:B:271:DX2:CAH	6:B:272[B]:DTT:H2	2.47	0.43
1:A:2:GLU:N	7:A:420:HOH:O	2.51	0.43
1:A:192:LEU:HB3	1:A:197:ILE:HB	2.01	0.43
7:A:431:HOH:O	1:C:186:GLN:HB2	2.19	0.42
1:C:130:ALA:HB3	1:C:131:PRO:HD3	2.02	0.42
2:B:186:GLN:HB2	7:D:395:HOH:O	2.20	0.42
1:A:208:LEU:HD11	1:A:234:ALA:HB2	2.00	0.42
1:D:15:ILE:HB	3:D:269:NAP:H51N	2.02	0.42
1:C:129[A]:ILE:CD1	7:C:286:HOH:O	2.68	0.41
1:D:9:THR:HA	1:D:33:HIS:HB3	2.03	0.41
1:C:254:GLY:HA3	1:D:265:LEU:HD11	2.02	0.41
2:B:13[A]:LYS:HA	2:B:17:ARG:HB2	2.03	0.41
1:A:186:GLN:NE2	7:A:375:HOH:O	2.24	0.41
2:B:130:ALA:HB3	2:B:131:PRO:HD3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:270:ACT:OXT	7:C:372:HOH:O[1_454]	1.85	0.35
7:B:536:HOH:O	7:C:372:HOH:O[1_454]	1.96	0.24



## 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	248/288 (86%)	237 (96%)	11 (4%)	0	100	100
1	C	235/288 (82%)	229 (97%)	6 (3%)	0	100	100
1	D	247/288 (86%)	237 (96%)	10 (4%)	0	100	100
2	B	246/288 (85%)	237 (96%)	9 (4%)	0	100	100
All	All	976/1152 (85%)	940 (96%)	36 (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	202/229 (88%)	201 (100%)	1 (0%)	92	91
1	C	193/229 (84%)	193 (100%)	0	100	100
1	D	201/229 (88%)	198 (98%)	3 (2%)	72	62
2	B	202/230 (88%)	199 (98%)	3 (2%)	72	62
All	All	798/917 (87%)	791 (99%)	7 (1%)	84	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
2	B	140	GLN

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Mol	Chain	Res	Type
2	B	211	VAL
2	B	229	ARG
1	D	53	SER
1	D	136	MET
1	D	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	166	GLN
2	B	54	ASN
2	B	65	ASN
2	B	78	ASN
2	B	140	GLN
2	B	166	GLN
2	B	236	GLN
1	D	67[A]	ASN
1	D	140	GLN
1	D	166	GLN
1	D	186	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	1	3,6,7	0.71	0	3,6,8	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSX	A	59	1	3,6,7	0.60	0	3,6,8	1.07	0
2	CSX	B	59	2	3,6,7	0.49	0	3,6,8	1.28	1 (33%)
1	CSX	C	168	1	3,6,7	0.51	0	3,6,8	1.27	0
1	CSX	C	59	1	3,6,7	0.62	0	3,6,8	1.19	0
1	CSX	D	168	1	3,6,7	0.61	0	3,6,8	1.89	1 (33%)
1	CSX	D	59	1	3,6,7	0.57	0	3,6,8	1.19	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
1	CSX	A	168	1	-	0/1/5/7	0/0/0/0
1	CSX	A	59	1	-	0/1/5/7	0/0/0/0
2	CSX	B	59	2	-	0/1/5/7	0/0/0/0
1	CSX	C	168	1	-	0/1/5/7	0/0/0/0
1	CSX	C	59	1	-	0/1/5/7	0/0/0/0
1	CSX	D	168	1	-	0/1/5/7	0/0/0/0
1	CSX	D	59	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	CSX	CB-CA-C	-2.46	104.73	111.46
2	B	59	CSX	O-C-CA	-2.18	119.80	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	59	CSX	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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
3	NAP	A	269	-	42,52,52	1.63	3 (7%)	54,80,80	2.13	6 (11%)
5	ACT	A	270	-	1,3,3	0.95	0	0,3,3	0.00	-
4	DX2	A	271	-	19,21,21	2.49	6 (31%)	23,30,30	4.56	10 (43%)
3	NAP	B	269	-	42,52,52	1.49	3 (7%)	54,80,80	2.21	10 (18%)
5	ACT	B	270	-	1,3,3	1.50	0	0,3,3	0.00	-
4	DX2	B	271	-	19,21,21	1.86	4 (21%)	23,30,30	2.09	8 (34%)
6	DTT	B	272[A]	-	7,7,7	0.50	0	4,8,8	0.95	0
6	DTT	B	272[B]	-	7,7,7	0.48	0	4,8,8	0.92	0
3	NAP	C	269	-	42,52,52	1.53	3 (7%)	54,80,80	1.99	7 (12%)
4	DX2	C	270	-	19,21,21	2.20	4 (21%)	23,30,30	1.90	5 (21%)
3	NAP	D	269	-	42,52,52	1.58	4 (9%)	54,80,80	2.31	7 (12%)
4	DX2	D	270	-	19,21,21	2.00	3 (15%)	23,30,30	2.09	6 (26%)

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	NAP	A	269	-	-	0/27/67/67	0/5/5/5
5	ACT	A	270	-	-	0/0/0/0	0/0/0/0
4	DX2	A	271	-	-	0/4/4/4	0/3/3/3
3	NAP	B	269	-	-	0/27/67/67	0/5/5/5
5	ACT	B	270	-	-	0/0/0/0	0/0/0/0
4	DX2	B	271	-	-	0/4/4/4	0/3/3/3
6	DTT	B	272[A]	-	1/1/2/2	0/8/8/8	0/0/0/0
6	DTT	B	272[B]	-	1/1/2/2	0/8/8/8	0/0/0/0
3	NAP	C	269	-	-	0/27/67/67	0/5/5/5
4	DX2	C	270	-	-	0/4/4/4	0/3/3/3
3	NAP	D	269	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DX2	D	270	-	-	0/4/4/4	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	270	DX2	CAN-C6	-7.93	1.40	1.49
4	D	270	DX2	CAN-C6	-7.63	1.40	1.49
4	A	271	DX2	CAN-C6	-7.41	1.40	1.49
4	B	271	DX2	CAN-C6	-6.40	1.42	1.49
4	C	270	DX2	C6-C7	-3.28	1.41	1.45
4	A	271	DX2	C6-C7	-2.82	1.41	1.45
4	B	271	DX2	C6-C7	-2.44	1.42	1.45
4	D	270	DX2	C6-N5	2.02	1.35	1.32
4	C	270	DX2	C6-N5	2.12	1.35	1.32
4	B	271	DX2	C6-N5	2.36	1.35	1.32
3	D	269	NAP	C2A-N1A	2.39	1.38	1.33
4	D	270	DX2	C7-N8	2.40	1.36	1.32
4	C	270	DX2	C7-N8	2.51	1.36	1.32
3	D	269	NAP	O4D-C1D	2.53	1.44	1.41
3	C	269	NAP	C2A-N1A	2.55	1.38	1.33
4	B	271	DX2	C7-N8	2.55	1.36	1.32
3	A	269	NAP	C2A-N1A	2.85	1.39	1.33
3	B	269	NAP	C2A-N1A	2.87	1.39	1.33
4	A	271	DX2	C6-N5	2.90	1.36	1.32
4	A	271	DX2	CAF-CAH	3.02	1.45	1.38
3	C	269	NAP	C2A-N3A	3.53	1.38	1.32
4	A	271	DX2	C7-N8	3.63	1.38	1.32
3	A	269	NAP	C2A-N3A	3.76	1.38	1.32
4	A	271	DX2	CAH-CAN	3.89	1.47	1.39
3	D	269	NAP	C2A-N3A	3.92	1.39	1.32
3	B	269	NAP	C2A-N3A	4.10	1.39	1.32
3	B	269	NAP	O7N-C7N	6.25	1.37	1.24
3	D	269	NAP	O7N-C7N	7.30	1.39	1.24
3	C	269	NAP	O7N-C7N	7.61	1.40	1.24
3	A	269	NAP	O7N-C7N	7.68	1.40	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	269	NAP	N3A-C2A-N1A	-12.97	118.97	128.89
3	C	269	NAP	N3A-C2A-N1A	-11.68	119.95	128.89
3	B	269	NAP	N3A-C2A-N1A	-11.14	120.37	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	269	NAP	N3A-C2A-N1A	-11.14	120.37	128.89
4	A	271	DX2	CAH-CAN-CAG	-9.41	99.75	117.55
4	A	271	DX2	CAD-CAF-CAH	-8.45	107.81	120.19
3	B	269	NAP	O7N-C7N-C3N	-5.41	113.68	119.59
3	A	269	NAP	O7N-C7N-C3N	-4.84	114.30	119.59
4	C	270	DX2	N1-C2-N3	-4.39	120.76	127.44
4	A	271	DX2	N1-C2-N3	-4.33	120.86	127.44
4	B	271	DX2	N1-C2-N3	-4.17	121.10	127.44
4	D	270	DX2	N1-C2-N3	-4.16	121.11	127.44
4	A	271	DX2	C7-C6-N5	-3.73	117.37	120.46
3	D	269	NAP	C1B-N9A-C4A	-3.68	121.39	126.94
4	B	271	DX2	C7-C6-N5	-3.15	117.85	120.46
3	A	269	NAP	C4B-O4B-C1B	-3.08	106.33	109.72
4	D	270	DX2	C7-C6-N5	-3.00	117.97	120.46
3	C	269	NAP	C1B-N9A-C4A	-2.92	122.54	126.94
3	B	269	NAP	C3N-C2N-N1N	-2.69	117.26	120.36
4	C	270	DX2	C7-C6-N5	-2.68	118.23	120.46
3	A	269	NAP	C1B-N9A-C4A	-2.65	122.94	126.94
3	D	269	NAP	C4B-O4B-C1B	-2.49	106.98	109.72
3	B	269	NAP	O4B-C4B-C3B	-2.29	100.53	105.15
3	C	269	NAP	C4B-O4B-C1B	-2.25	107.25	109.72
4	B	271	DX2	C4A-C8A-N1	-2.19	118.57	122.11
3	C	269	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
3	B	269	NAP	C1B-N9A-C4A	-2.06	123.83	126.94
3	B	269	NAP	O4D-C1D-N1N	2.04	110.37	108.13
4	B	271	DX2	CAN-C6-C7	2.04	124.90	122.31
4	B	271	DX2	CAG-CAN-C6	2.08	123.84	120.60
3	D	269	NAP	P2B-O2B-C2B	2.23	126.92	121.56
4	B	271	DX2	N8-C8A-N1	2.44	121.13	115.79
4	D	270	DX2	N8-C8A-N1	2.49	121.23	115.79
4	C	270	DX2	N8-C8A-N1	2.62	121.51	115.79
3	B	269	NAP	C2A-N1A-C6A	2.70	123.60	118.77
4	A	271	DX2	N8-C8A-N1	2.71	121.72	115.79
3	C	269	NAP	O4B-C1B-N9A	2.80	113.96	108.10
3	B	269	NAP	C2N-C3N-C4N	2.81	121.42	118.29
4	B	271	DX2	CAF-CAH-CAN	2.90	124.39	120.56
4	C	270	DX2	CAN-C6-C7	2.98	126.09	122.31
3	C	269	NAP	O4D-C1D-N1N	3.22	111.67	108.13
3	C	269	NAP	C3N-C7N-N7N	3.42	121.56	117.82
3	A	269	NAP	O4B-C1B-N9A	3.49	115.40	108.10
4	D	270	DX2	CAN-C6-C7	3.58	126.85	122.31
3	B	269	NAP	O4B-C1B-N9A	3.64	115.72	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	270	DX2	C6-N5-C4A	3.88	121.05	118.15
4	D	270	DX2	C6-C7-NAB	3.96	124.08	121.14
4	D	270	DX2	C6-N5-C4A	4.09	121.21	118.15
3	D	269	NAP	O4B-C1B-N9A	4.19	116.87	108.10
3	D	269	NAP	C3N-C7N-N7N	4.53	122.77	117.82
3	D	269	NAP	O4D-C1D-N1N	4.54	113.12	108.13
4	A	271	DX2	CAD-CAE-CAG	4.56	126.86	120.19
4	A	271	DX2	CAN-C6-C7	4.58	128.12	122.31
4	A	271	DX2	C6-N5-C4A	4.66	121.63	118.15
3	B	269	NAP	C3N-C7N-N7N	4.98	123.27	117.82
4	B	271	DX2	C6-N5-C4A	5.52	122.28	118.15
3	A	269	NAP	C3N-C7N-N7N	5.58	123.92	117.82
4	A	271	DX2	CAH-CAN-C6	8.25	133.47	120.60
4	A	271	DX2	CAF-CAH-CAN	10.77	134.81	120.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	272[B]	DTT	C3
6	B	272[A]	DTT	C3

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	269	NAP	1	0
4	A	271	DX2	4	0
3	B	269	NAP	1	0
5	B	270	ACT	0	1
4	B	271	DX2	17	0
6	B	272[A]	DTT	7	0
6	B	272[B]	DTT	6	0
3	C	269	NAP	1	0
4	C	270	DX2	6	0
3	D	269	NAP	2	0
4	D	270	DX2	8	0

## 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	247/288 (85%)	-0.49	1 (0%) 93 91	19, 24, 40, 56	4 (1%)
1	C	237/288 (82%)	-0.37	5 (2%) 67 62	18, 25, 45, 63	1 (0%)
1	D	247/288 (85%)	-0.40	1 (0%) 93 91	19, 25, 41, 68	1 (0%)
2	B	246/288 (85%)	-0.57	0 100 100	18, 24, 37, 44	0
All	All	977/1152 (84%)	-0.46	7 (0%) 89 87	18, 24, 40, 68	6 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	6.6
1	C	232	ALA	3.1
1	C	210	PRO	2.8
1	D	211	VAL	2.7
1	C	229	ARG	2.6
1	C	208	LEU	2.4
1	A	212	ALA	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	C	59	7/8	0.96	0.08	-	22,24,31,33	0
1	CSX	A	59	7/8	0.95	0.07	-	25,25,28,34	0
2	CSX	B	59	7/8	0.96	0.08	-	19,22,30,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSX	D	59	7/8	0.96	0.07	-	25,27,30,37	0
1	CSX	C	168	7/8	0.95	0.08	-	23,26,39,42	1
1	CSX	A	168	7/8	0.95	0.07	-	28,31,54,56	0
1	CSX	D	168	7/8	0.95	0.09	-	26,29,41,58	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
6	DTT	B	272[A]	8/8	0.86	0.22	20.22	39,48,52,59	7
6	DTT	B	272[B]	8/8	0.86	0.22	20.10	40,49,57,59	7
4	DX2	B	271	19/19	0.92	0.15	9.51	22,28,35,38	0
5	ACT	B	270	4/4	0.97	0.14	6.82	25,27,29,29	0
4	DX2	A	271	19/19	0.88	0.23	5.15	26,31,37,37	0
4	DX2	D	270	19/19	0.88	0.24	3.26	29,36,41,41	0
4	DX2	C	270	19/19	0.68	0.27	2.44	79,81,81,81	0
3	NAP	C	269	48/48	0.94	0.13	1.05	20,32,37,41	48
5	ACT	A	270	4/4	0.99	0.13	0.71	28,29,29,30	0
3	NAP	D	269	48/48	0.97	0.09	0.39	17,25,30,33	0
3	NAP	B	269	48/48	0.98	0.07	0.21	20,24,27,29	0
3	NAP	A	269	48/48	0.98	0.07	-0.72	19,24,29,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.