



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 AM GMT

PDB ID : 2X9N  
Title : High resolution structure of TbPTR1 in complex with cyromazine  
Authors : Dawson, A.; Tulloch, L.B.; Barrack, K.L.; Hunter, W.N.  
Deposited on : 2010-03-23  
Resolution : 1.15 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

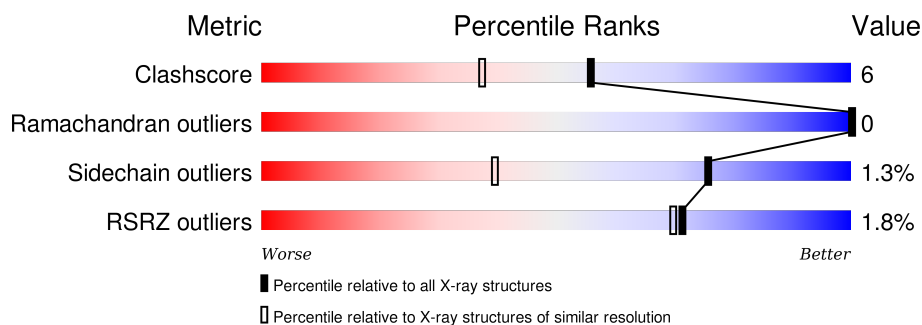
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1593 (1.20-1.08)
Ramachandran outliers	100387	1521 (1.20-1.08)
Sidechain outliers	100360	1518 (1.20-1.08)
RSRZ outliers	91569	1498 (1.20-1.08)

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	B	288	
1	C	288	
1	D	288	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AX3	B	1270[A]	-	-	-	X
3	AX3	B	1270[B]	-	-	X	X
3	AX3	C	1270[A]	-	-	-	X
3	AX3	C	1270[B]	-	-	X	X
3	AX3	D	1270[A]	-	-	-	X
3	AX3	D	1270[B]	-	-	X	X
4	DTD	A	1271[A]	-	-	-	X
4	DTD	A	1271[B]	-	-	-	X
6	D1D	D	1271[A]	-	-	-	X
6	D1D	D	1271[B]	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9198 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PTERIDINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	7	0
			1878	1184	329	353	12			
1	B	248	Total	C	N	O	S	0	9	0
			1890	1197	328	353	12			
1	C	249	Total	C	N	O	S	0	6	0
			1885	1190	329	355	11			
1	D	247	Total	C	N	O	S	0	10	0
			1869	1184	329	344	12			

There are 80 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
B	-19	MET	-	EXPRESSION TAG	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP O76290
D	-15	HIS	-	EXPRESSION TAG	UNP O76290
D	-14	HIS	-	EXPRESSION TAG	UNP O76290
D	-13	HIS	-	EXPRESSION TAG	UNP O76290
D	-12	HIS	-	EXPRESSION TAG	UNP O76290
D	-11	HIS	-	EXPRESSION TAG	UNP O76290
D	-10	HIS	-	EXPRESSION TAG	UNP O76290
D	-9	SER	-	EXPRESSION TAG	UNP O76290
D	-8	SER	-	EXPRESSION TAG	UNP O76290
D	-7	GLY	-	EXPRESSION TAG	UNP O76290
D	-6	LEU	-	EXPRESSION TAG	UNP O76290
D	-5	VAL	-	EXPRESSION TAG	UNP O76290
D	-4	PRO	-	EXPRESSION TAG	UNP O76290
D	-3	ARG	-	EXPRESSION TAG	UNP O76290
D	-2	GLY	-	EXPRESSION TAG	UNP O76290
D	-1	SER	-	EXPRESSION TAG	UNP O76290
D	0	HIS	-	EXPRESSION TAG	UNP O76290

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



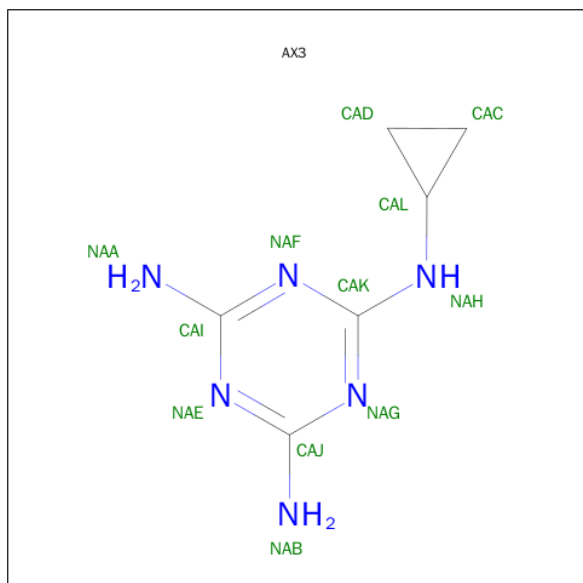
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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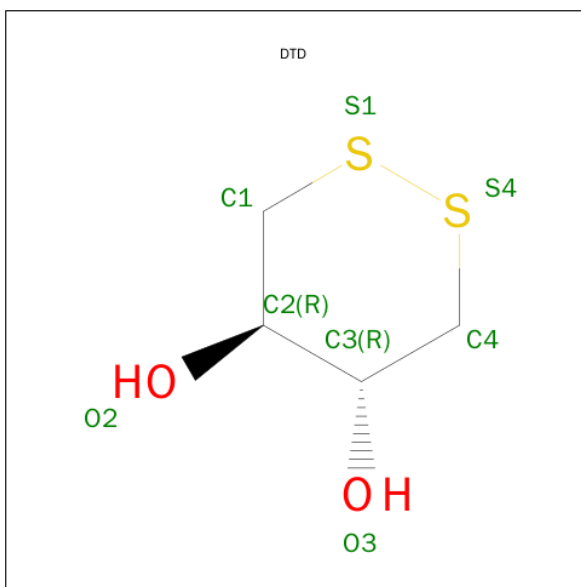
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 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
3	A	1	Total	C	N	0	0
			12	6	6		
3	B	1	Total	C	N	0	1
			16	9	7		
3	C	1	Total	C	N	0	1
			16	9	7		
3	D	1	Total	C	N	0	1
			16	9	7		

- Molecule 4 is DITHIANE DIOL (three-letter code: DTD) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>).



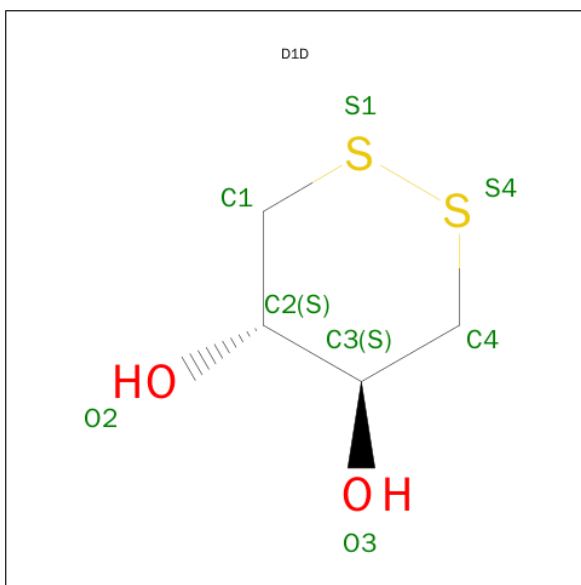
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	1
			9	4	2	3		
4	C	1	Total	C	O	S	0	1
			9	4	2	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

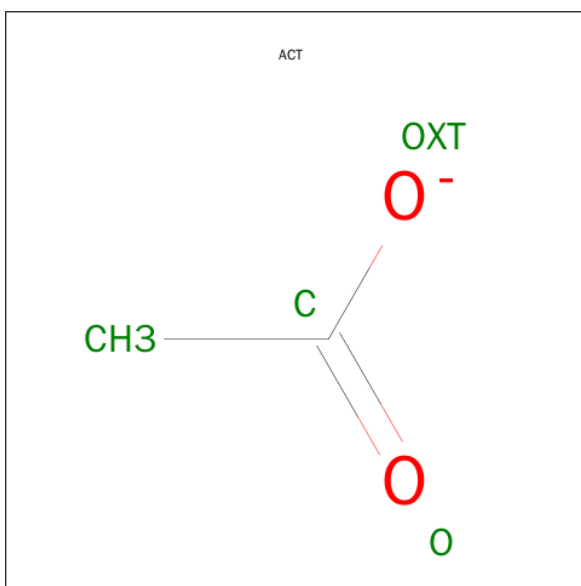
- Molecule 6 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	1
			9	4	2	3		
6	D	1	Total	C	O	S	0	1
			9	4	2	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 8 is water.

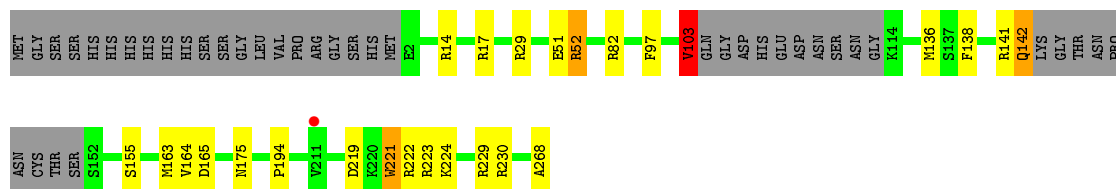
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	382	Total 382	O 382	0	0
8	B	321	Total 321	O 321	0	0
8	C	356	Total 356	O 356	0	0
8	D	323	Total 323	O 323	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

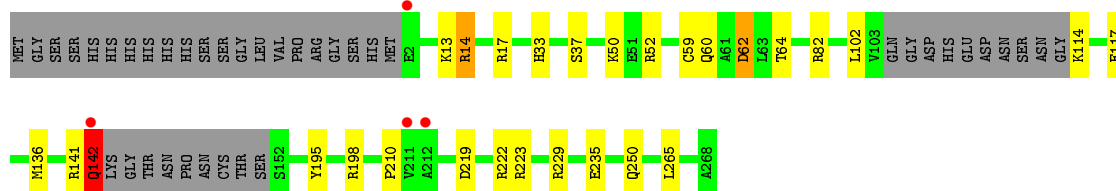
#### • Molecule 1: PTERIDINE REDUCTASE

Chain A: 




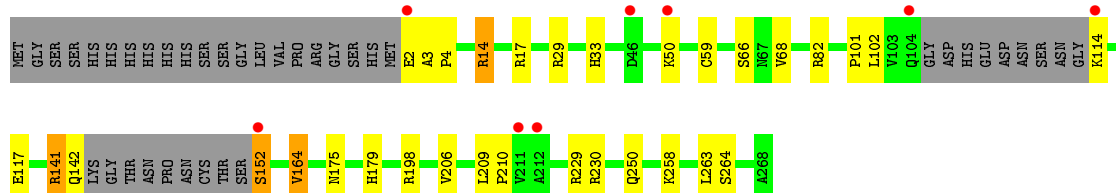
#### • Molecule 1: PTERIDINE REDUCTASE

Chain B: 



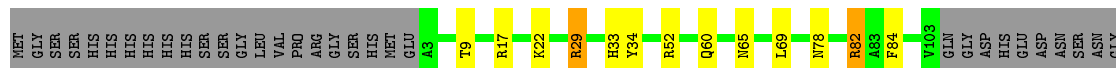
#### • Molecule 1: PTERIDINE REDUCTASE

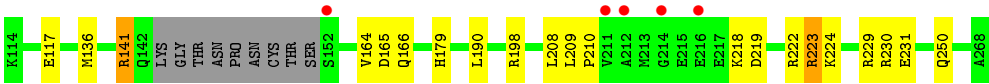
Chain C: 



#### • Molecule 1: PTERIDINE REDUCTASE

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.50 Å 90.00 Å 82.40 Å 90.00° 115.50° 90.00°	Depositor
Resolution (Å)	20.00 – 1.15 19.81 – 1.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-1.15) 95.6 (19.81-1.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.10 Å)	Xtriage
Refinement program	SHELX-97	Depositor
R, $R_{free}$	0.126 , 0.152 0.133 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	7.0	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 74.8	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 385887 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, NA, DTD, D1D, NAP, 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	0.77	1/1943 (0.1%)	1.31	21/2637 (0.8%)
1	B	0.76	0/1967	1.29	19/2669 (0.7%)
1	C	0.80	0/1946	1.37	19/2641 (0.7%)
1	D	0.78	1/1946 (0.1%)	1.52	25/2641 (0.9%)
All	All	0.78	2/7802 (0.0%)	1.37	84/10588 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	GLU	CD-OE1	-5.58	1.19	1.25
1	A	155	SER	CB-OG	-5.08	1.35	1.42

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82[A]	ARG	NE-CZ-NH2	-26.21	107.19	120.30
1	D	82[B]	ARG	NE-CZ-NH2	-26.21	107.19	120.30
1	C	29	ARG	NE-CZ-NH2	-16.75	111.93	120.30
1	B	142	GLN	CA-CB-CG	15.02	146.45	113.40
1	D	82[A]	ARG	NH1-CZ-NH2	13.76	134.54	119.40
1	D	82[B]	ARG	NH1-CZ-NH2	13.76	134.54	119.40
1	C	141	ARG	CD-NE-CZ	13.14	141.99	123.60
1	C	82	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	29	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	52[A]	ARG	NE-CZ-NH1	-11.47	114.56	120.30
1	A	52[B]	ARG	NE-CZ-NH1	-11.47	114.56	120.30
1	D	165	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	A	82	ARG	CD-NE-CZ	10.36	138.11	123.60
1	D	82[A]	ARG	CD-NE-CZ	-10.28	109.21	123.60
1	D	82[B]	ARG	CD-NE-CZ	-10.28	109.21	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	C	141	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	A	141	ARG	CD-NE-CZ	9.80	137.32	123.60
1	C	230	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	B	17	ARG	NE-CZ-NH1	-9.51	115.55	120.30
1	D	141	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	D	230	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	B	198	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	D	29	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	C	229	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	117	GLU	OE1-CD-OE2	8.57	133.59	123.30
1	A	142	GLN	CB-CG-CD	8.52	133.75	111.60
1	B	82	ARG	CD-NE-CZ	8.14	135.00	123.60
1	A	230	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	D	229	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	D	52	ARG	CD-NE-CZ	7.80	134.51	123.60
1	D	17	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	29	ARG	CD-NE-CZ	-7.75	112.75	123.60
1	B	223	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	17	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	14	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	222	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	14	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	117[A]	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	117[B]	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	114	LYS	CA-C-O	-6.82	105.79	120.10
1	D	34	TYR	CB-CG-CD1	6.79	125.07	121.00
1	C	82	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	103	VAL	N-CA-CB	-6.72	96.71	111.50
1	B	82	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	82	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	141	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	223	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	198	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	29	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	223	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	229	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	C	114	LYS	CA-C-N	6.29	131.03	117.20
1	D	34	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	B	141	ARG	CG-CD-NE	6.16	124.74	111.80
1	D	223	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	GLN	CB-CG-CD	6.12	127.52	111.60
1	A	14	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	219	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	52	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	D	52	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	229	ARG	NH1-CZ-NH2	5.76	125.73	119.40
1	C	230	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	62	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	29	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	221	TRP	CE3-CZ3-CH2	-5.69	114.94	121.20
1	C	114	LYS	N-CA-CB	5.69	120.84	110.60
1	A	222	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	141	ARG	CD-NE-CZ	5.61	131.45	123.60
1	D	222	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	17	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	D	141	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	17	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	198	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	250	GLN	CB-CG-CD	5.35	125.50	111.60
1	D	231	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	D	219	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	97	PHE	CB-CG-CD1	5.23	124.46	120.80
1	C	17	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	198	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	219	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	141	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	165	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1878	0	1908	15	0
1	B	1890	0	1938	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1885	0	1919	28	0
1	D	1869	0	1914	23	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	12	0	10	1	0
3	B	16	0	9	11	0
3	C	16	0	12	10	0
3	D	16	0	11	15	0
4	A	9	0	4	1	0
4	C	9	0	4	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	B	9	0	4	1	0
6	D	9	0	4	4	0
7	C	4	0	3	0	0
8	A	382	0	0	7	0
8	B	321	0	0	8	0
8	C	356	0	0	13	0
8	D	323	0	0	8	0
All	All	9198	0	7840	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:O	3:D:1270[B]:AX3:HAD	1.70	0.92
3:D:1270[B]:AX3:CAC	6:D:1271[B]:D1D:H4C2	2.10	0.81
1:C:210:PRO:HB3	3:C:1270[A]:AX3:HADA	1.63	0.79
1:C:152:SER:HB3	8:C:2196:HOH:O	1.83	0.79
1:A:175:ASN:HB2	8:A:2279:HOH:O	1.84	0.77
1:C:175:ASN:HB2	8:C:2267:HOH:O	1.85	0.75
1:C:14:ARG:NH2	3:C:1270[B]:AX3:HAC	2.02	0.74
1:A:194:PRO:HG3	8:C:2304:HOH:O	1.89	0.73
1:B:62:ASP:OD1	1:B:64[B]:THR:HG23	1.88	0.73
1:B:50:LYS:HG3	8:B:2084:HOH:O	1.88	0.71
1:B:210:PRO:CA	3:B:1270[B]:AX3:HADA	2.20	0.71
1:C:3:ALA:HA	8:C:2055:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:N	3:C:1270[B]:AX3:HACA	2.08	0.69
2:B:1269:NAP:N7N	3:B:1270[B]:AX3:HACA	2.07	0.69
1:D:210:PRO:HG3	3:D:1270[B]:AX3:HAC	1.74	0.68
1:A:51:GLU:OE1	1:A:52[B]:ARG:HG3	1.95	0.67
3:B:1270[A]:AX3:HAD	8:B:2249:HOH:O	1.96	0.66
3:B:1270[B]:AX3:HAL	6:B:1271[B]:D1D:H1C2	1.78	0.66
1:A:163:MET:HG3	8:A:2382:HOH:O	1.95	0.66
3:D:1270[B]:AX3:HACA	6:D:1271[B]:D1D:S4	2.36	0.65
1:D:164:VAL:HG22	1:D:179:HIS:CE1	2.32	0.65
8:A:2238:HOH:O	1:B:136[B]:MET:HE1	1.98	0.64
1:C:210:PRO:CA	3:C:1270[B]:AX3:HACA	2.28	0.64
1:C:258[B]:LYS:HE2	1:C:264:SER:OG	1.97	0.64
3:D:1270[B]:AX3:HACA	6:D:1271[B]:D1D:H4C2	1.78	0.63
2:B:1269:NAP:C7N	3:B:1270[B]:AX3:HACA	2.29	0.62
3:C:1270[A]:AX3:HAD	8:C:2206:HOH:O	1.98	0.62
1:A:224:LYS:NZ	8:A:2321:HOH:O	2.33	0.61
1:B:142:GLN:HG3	8:B:2173:HOH:O	2.02	0.60
1:B:210:PRO:N	3:B:1270[B]:AX3:HADA	2.17	0.59
1:B:210:PRO:HD3	3:B:1270[B]:AX3:HAC	1.84	0.59
1:D:179:HIS:HD2	8:D:2242:HOH:O	1.86	0.58
1:B:142:GLN:HB2	8:B:2213:HOH:O	2.02	0.58
1:A:52[B]:ARG:HD2	8:A:2125:HOH:O	2.04	0.57
1:A:164:VAL:HA	8:A:2281:HOH:O	2.04	0.57
3:D:1270[A]:AX3:HACA	8:D:2188:HOH:O	2.04	0.56
1:C:210:PRO:CB	3:C:1270[A]:AX3:HADA	2.34	0.56
1:C:102:LEU:O	1:D:136[A]:MET:HG3	2.05	0.56
3:A:1270:AX3:HACA	4:A:1271[B]:DTD:S1	2.47	0.54
1:C:210:PRO:HD3	3:C:1270[B]:AX3:HAD	1.89	0.54
1:D:164:VAL:HG22	1:D:179:HIS:ND1	2.21	0.54
1:A:136[B]:MET:HE1	8:B:2185:HOH:O	2.08	0.54
1:B:210:PRO:HA	3:B:1270[B]:AX3:HADA	1.89	0.54
2:D:1269:NAP:PA	3:D:1270[A]:AX3:HADA	2.48	0.54
1:D:210:PRO:N	3:D:1270[B]:AX3:HADA	2.23	0.54
1:C:101:PRO:HG3	8:C:2210:HOH:O	2.08	0.53
1:C:14:ARG:HH22	3:C:1270[B]:AX3:HAC	1.73	0.53
1:B:210:PRO:HG3	3:B:1270[B]:AX3:CAL	2.40	0.51
1:B:13:LYS:HE2	1:B:37:SER:OG	2.10	0.51
1:C:179:HIS:HD2	8:D:2242:HOH:O	1.94	0.50
1:D:78:ASN:O	1:D:82[B]:ARG:HG2	2.13	0.49
1:C:210:PRO:HG3	3:C:1270[B]:AX3:CAL	2.43	0.49
1:C:4:PRO:HD2	8:C:2055:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PRO:CA	3:D:1270[B]:AX3:HADA	2.44	0.48
1:A:103:VAL:HG11	1:B:195:TYR:CE2	2.49	0.48
1:C:66:SER:OG	1:C:68[C]:VAL:HG22	2.13	0.48
3:D:1270[B]:AX3:HAC	6:D:1271[B]:D1D:H4C1	1.95	0.48
1:C:258[B]:LYS:HD3	8:C:2340:HOH:O	2.13	0.47
1:D:210:PRO:HG3	3:D:1270[B]:AX3:CAC	2.41	0.47
1:C:3:ALA:CB	8:C:2055:HOH:O	2.63	0.47
1:B:14:ARG:NH2	3:B:1270[B]:AX3:CAD	2.78	0.46
1:C:258[B]:LYS:HE2	1:C:264:SER:HG	1.81	0.46
1:C:142:GLN:NE2	8:C:2241:HOH:O	2.48	0.46
1:B:114:LYS:N	8:B:2188:HOH:O	2.49	0.46
1:C:206[A]:VAL:HG23	1:C:263:LEU:HD22	1.98	0.46
3:B:1270[A]:AX3:HACA	8:B:2180:HOH:O	2.15	0.45
1:D:82[B]:ARG:NH2	8:D:2171:HOH:O	2.48	0.45
1:B:33:HIS:HA	1:B:59:CYS:O	2.17	0.45
1:D:223:ARG:NH1	8:D:2267:HOH:O	2.49	0.45
1:D:250:GLN:NE2	8:D:2299:HOH:O	2.49	0.45
1:D:29:ARG:HD2	1:D:84:PHE:CD1	2.53	0.44
1:C:152:SER:N	8:C:2246:HOH:O	2.49	0.44
1:D:209:LEU:HD13	1:D:218:LYS:HB3	1.99	0.44
1:C:3:ALA:CA	8:C:2055:HOH:O	2.59	0.44
1:A:268:ALA:OXT	1:D:224:LYS:HE2	2.18	0.43
1:A:136[B]:MET:HG3	1:B:102:LEU:O	2.18	0.43
1:D:82[A]:ARG:HH21	1:D:82[A]:ARG:HD3	1.09	0.42
1:D:22[A]:LYS:HG2	8:D:2054:HOH:O	2.19	0.42
1:A:103:VAL:HG11	1:B:195:TYR:CZ	2.54	0.42
1:B:265:LEU:HB2	1:D:190[B]:LEU:HD21	2.02	0.42
2:C:1269:NAP:C7N	3:C:1270[B]:AX3:HADA	2.50	0.42
1:D:136[A]:MET:HG2	8:D:2211:HOH:O	2.18	0.42
1:C:206[C]:VAL:CG2	1:C:209:LEU:HD21	2.49	0.42
1:C:33:HIS:HA	1:C:59:CYS:O	2.20	0.42
1:A:229:ARG:NH2	8:A:2324:HOH:O	2.53	0.42
1:B:235:GLU:HG2	8:B:2012:HOH:O	2.20	0.41
1:C:164:VAL:O	1:C:179:HIS:HE1	2.04	0.41
1:D:65:ASN:HA	1:D:69:LEU:HD22	2.02	0.41
2:D:1269:NAP:O2A	3:D:1270[A]:AX3:HADA	2.21	0.40
1:A:138:PHE:O	1:A:142:GLN:HG2	2.22	0.40
1:C:141:ARG:HG2	8:C:2230:HOH:O	2.21	0.40
1:D:9:THR:HA	1:D:33:HIS:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	B	254/288 (88%)	245 (96%)	9 (4%)	0	100	100
1	C	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	D	253/288 (88%)	244 (96%)	9 (4%)	0	100	100
All	All	1009/1152 (88%)	973 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	205/231 (89%)	204 (100%)	1 (0%)	92	73
1	B	209/231 (90%)	207 (99%)	2 (1%)	82	52
1	C	206/231 (89%)	202 (98%)	4 (2%)	65	24
1	D	205/231 (89%)	202 (98%)	3 (2%)	72	34
All	All	825/924 (89%)	815 (99%)	10 (1%)	76	43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	60	GLN

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Mol	Chain	Res	Type
1	B	142	GLN
1	C	2	GLU
1	C	50	LYS
1	C	152	SER
1	C	164	VAL
1	D	60	GLN
1	D	141	ARG
1	D	166	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	104	GLN
1	C	175	ASN
1	C	179	HIS
1	C	250	GLN
1	D	179	HIS
1	D	250	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAP	A	1269	-	42,52,52	0.95	1 (2%)	54,80,80	1.41	7 (12%)
3	AX3	A	1270	-	13,13,13	1.27	2 (15%)	16,18,18	1.85	6 (37%)
4	DTD	A	1271[A]	-	6,8,8	0.69	0	6,10,10	2.47	2 (33%)
4	DTD	A	1271[B]	-	6,8,8	0.67	0	6,10,10	2.47	2 (33%)
2	NAP	B	1269	-	42,52,52	0.93	1 (2%)	54,80,80	1.35	6 (11%)
3	AX3	B	1270[A]	-	13,13,13	1.44	1 (7%)	16,18,18	2.46	5 (31%)
3	AX3	B	1270[B]	-	13,13,13	3.01	3 (23%)	16,18,18	5.67	7 (43%)
6	D1D	B	1271[A]	-	6,8,8	0.46	0	6,10,10	1.94	2 (33%)
6	D1D	B	1271[B]	-	6,8,8	0.40	0	6,10,10	1.94	2 (33%)
2	NAP	C	1269	-	42,52,52	0.85	1 (2%)	54,80,80	1.09	2 (3%)
3	AX3	C	1270[A]	-	13,13,13	1.41	2 (15%)	16,18,18	5.18	8 (50%)
3	AX3	C	1270[B]	-	13,13,13	2.15	4 (30%)	16,18,18	3.10	9 (56%)
4	DTD	C	1271[A]	-	6,8,8	1.32	1 (16%)	6,10,10	3.52	4 (66%)
4	DTD	C	1271[B]	-	6,8,8	1.34	1 (16%)	6,10,10	3.52	4 (66%)
7	ACT	C	1272	-	1,3,3	3.51	1 (100%)	0,3,3	0.00	-
2	NAP	D	1269	-	42,52,52	0.80	0	54,80,80	1.35	7 (12%)
3	AX3	D	1270[A]	-	13,13,13	1.30	1 (7%)	16,18,18	3.79	8 (50%)
3	AX3	D	1270[B]	-	13,13,13	1.33	1 (7%)	16,18,18	9.22	8 (50%)
6	D1D	D	1271[A]	-	6,8,8	0.88	0	6,10,10	2.89	3 (50%)
6	D1D	D	1271[B]	-	6,8,8	0.86	0	6,10,10	2.89	3 (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
2	NAP	A	1269	-	-	0/27/67/67	0/5/5/5
3	AX3	A	1270	-	-	0/4/6/6	0/1/2/2
4	DTD	A	1271[A]	-	-	0/0/11/11	0/0/1/1
4	DTD	A	1271[B]	-	-	0/0/11/11	0/0/1/1
2	NAP	B	1269	-	-	0/27/67/67	0/5/5/5
3	AX3	B	1270[A]	-	-	0/4/6/6	0/1/2/2
3	AX3	B	1270[B]	-	-	0/4/6/6	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D1D	B	1271[A]	-	-	0/0/11/11	0/0/1/1
6	D1D	B	1271[B]	-	-	0/0/11/11	0/0/1/1
2	NAP	C	1269	-	-	0/27/67/67	0/5/5/5
3	AX3	C	1270[A]	-	-	0/4/6/6	0/1/2/2
3	AX3	C	1270[B]	-	-	0/4/6/6	0/1/2/2
4	DTD	C	1271[A]	-	-	0/0/11/11	0/0/1/1
4	DTD	C	1271[B]	-	-	0/0/11/11	0/0/1/1
7	ACT	C	1272	-	-	0/0/0/0	0/0/0/0
2	NAP	D	1269	-	-	0/27/67/67	0/5/5/5
3	AX3	D	1270[A]	-	-	0/4/6/6	0/1/2/2
3	AX3	D	1270[B]	-	-	0/4/6/6	0/1/2/2
6	D1D	D	1271[A]	-	-	0/0/11/11	0/0/1/1
6	D1D	D	1271[B]	-	-	0/0/11/11	0/0/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1270[B]	AX3	CAK-NAH	-9.31	1.23	1.34
3	C	1270[B]	AX3	CAK-NAH	-5.76	1.27	1.34
3	B	1270[B]	AX3	CAI-NAA	-4.18	1.25	1.34
3	B	1270[A]	AX3	CAI-NAA	-4.18	1.25	1.34
4	C	1271[A]	DTD	C3-C2	-2.81	1.47	1.52
4	C	1271[B]	DTD	C3-C2	-2.81	1.47	1.52
3	D	1270[A]	AX3	CAI-NAA	-2.59	1.28	1.34
3	D	1270[B]	AX3	CAI-NAA	-2.59	1.28	1.34
3	C	1270[B]	AX3	CAJ-NAB	-2.10	1.29	1.34
3	C	1270[A]	AX3	CAJ-NAB	-2.10	1.29	1.34
2	B	1269	NAP	C2A-N1A	-2.05	1.30	1.33
3	A	1270	AX3	CAC-CAL	2.02	1.53	1.48
3	C	1270[B]	AX3	CAL-NAH	2.05	1.52	1.46
2	C	1269	NAP	C4N-C3N	2.08	1.42	1.39
3	B	1270[B]	AX3	CAC-CAL	2.29	1.54	1.48
3	A	1270	AX3	CAD-CAL	2.44	1.54	1.48
3	C	1270[A]	AX3	CAK-NAH	2.49	1.37	1.34
3	C	1270[B]	AX3	CAD-CAL	2.60	1.54	1.48
2	A	1269	NAP	O4B-C1B	2.91	1.44	1.41
7	C	1272	ACT	CH3-C	3.51	1.53	1.48

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270[B]	AX3	CAK-NAH-CAL	-33.68	86.03	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1270[B]	AX3	CAK-NAH-CAL	-20.22	101.01	123.51
3	C	1270[A]	AX3	CAK-NAH-CAL	-19.03	102.33	123.51
3	C	1270[B]	AX3	CAK-NAH-CAL	-10.06	112.32	123.51
3	D	1270[A]	AX3	NAA-CAI-NAF	-6.55	106.35	117.20
3	D	1270[B]	AX3	NAA-CAI-NAF	-6.55	106.35	117.20
6	D	1271[B]	D1D	O3-C3-C4	-5.58	100.37	110.05
6	D	1271[A]	D1D	O3-C3-C4	-5.58	100.37	110.05
2	A	1269	NAP	C4B-O4B-C1B	-5.25	103.95	109.72
4	A	1271[B]	DTD	O3-C3-C4	-5.25	100.94	110.05
4	A	1271[A]	DTD	O3-C3-C4	-5.25	100.94	110.05
3	B	1270[B]	AX3	NAA-CAI-NAF	-4.98	108.96	117.20
3	B	1270[A]	AX3	NAA-CAI-NAF	-4.98	108.96	117.20
2	C	1269	NAP	C4B-O4B-C1B	-4.62	104.65	109.72
2	D	1269	NAP	C4B-O4B-C1B	-4.46	104.82	109.72
3	C	1270[A]	AX3	NAH-CAK-NAF	-4.24	110.76	116.95
3	D	1270[A]	AX3	NAE-CAI-NAF	-3.69	119.48	125.53
3	D	1270[B]	AX3	NAE-CAI-NAF	-3.69	119.48	125.53
3	D	1270[A]	AX3	NAE-CAJ-NAG	-3.52	119.77	125.53
3	D	1270[B]	AX3	NAE-CAJ-NAG	-3.52	119.77	125.53
2	B	1269	NAP	C1B-N9A-C4A	-3.37	121.86	126.94
2	B	1269	NAP	C4B-O4B-C1B	-3.35	106.04	109.72
2	B	1269	NAP	C5N-C4N-C3N	-3.27	116.23	120.33
2	B	1269	NAP	O7N-C7N-C3N	-3.23	116.06	119.59
6	D	1271[B]	D1D	O2-C2-C1	-3.18	104.53	110.05
6	D	1271[A]	D1D	O2-C2-C1	-3.18	104.53	110.05
3	A	1270	AX3	NAE-CAI-NAF	-3.14	120.39	125.53
3	B	1270[B]	AX3	NAH-CAK-NAF	-3.12	112.40	116.95
6	B	1271[A]	D1D	O2-C2-C1	-3.00	104.85	110.05
6	B	1271[B]	D1D	O2-C2-C1	-3.00	104.85	110.05
3	B	1270[A]	AX3	NAH-CAK-NAG	-2.86	112.77	116.95
2	A	1269	NAP	C1B-N9A-C4A	-2.86	122.63	126.94
2	D	1269	NAP	C4A-C5A-N7A	-2.81	106.89	109.48
2	D	1269	NAP	C1B-N9A-C4A	-2.70	122.86	126.94
2	A	1269	NAP	C5N-C4N-C3N	-2.66	117.00	120.33
4	A	1271[B]	DTD	O3-C3-C2	-2.55	104.54	110.27
4	A	1271[A]	DTD	O3-C3-C2	-2.55	104.54	110.27
3	C	1270[B]	AX3	CAD-CAL-CAC	-2.52	57.82	60.44
2	D	1269	NAP	O7N-C7N-C3N	-2.49	116.86	119.59
3	A	1270	AX3	NAF-CAK-NAG	-2.33	122.63	126.22
3	A	1270	AX3	CAK-NAH-CAL	-2.16	121.10	123.51
3	C	1270[B]	AX3	NAE-CAI-NAF	-2.14	122.02	125.53
3	C	1270[A]	AX3	NAE-CAI-NAF	-2.14	122.02	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1269	NAP	PN-O3-PA	-2.04	126.99	132.73
3	C	1270[B]	AX3	NAH-CAK-NAF	-2.04	113.97	116.95
2	D	1269	NAP	N6A-C6A-N1A	-2.04	114.83	119.20
3	C	1270[B]	AX3	NAE-CAJ-NAG	-2.03	122.21	125.53
3	C	1270[A]	AX3	NAE-CAJ-NAG	-2.03	122.21	125.53
2	A	1269	NAP	N3A-C2A-N1A	-2.01	127.36	128.89
2	C	1269	NAP	N3A-C2A-N1A	-2.00	127.36	128.89
2	A	1269	NAP	C2N-C3N-C4N	2.04	120.56	118.29
2	B	1269	NAP	O3B-C3B-C2B	2.06	117.11	111.16
3	A	1270	AX3	NAA-CAI-NAE	2.10	120.68	117.20
3	C	1270[B]	AX3	CAD-CAC-CAL	2.27	62.13	59.78
4	C	1271[A]	DTD	O2-C2-C3	2.36	115.56	110.27
4	C	1271[B]	DTD	O2-C2-C3	2.36	115.56	110.27
6	D	1271[B]	D1D	C1-C2-C3	2.39	117.45	112.51
6	D	1271[A]	D1D	C1-C2-C3	2.39	117.45	112.51
3	A	1270	AX3	NAH-CAK-NAG	2.40	120.46	116.95
2	A	1269	NAP	O3B-C3B-C2B	2.44	118.21	111.16
3	C	1270[B]	AX3	NAA-CAI-NAE	2.52	121.38	117.20
3	C	1270[A]	AX3	NAA-CAI-NAE	2.52	121.38	117.20
3	B	1270[B]	AX3	CAC-CAD-CAL	2.54	62.40	59.78
2	D	1269	NAP	C3N-C7N-N7N	2.55	120.60	117.82
6	B	1271[A]	D1D	C1-C2-C3	2.61	117.91	112.51
6	B	1271[B]	D1D	C1-C2-C3	2.61	117.91	112.51
3	C	1270[B]	AX3	CAJ-NAE-CAI	2.62	119.52	114.80
3	C	1270[A]	AX3	CAJ-NAE-CAI	2.62	119.52	114.80
2	A	1269	NAP	C6N-C5N-C4N	2.64	123.43	119.44
4	C	1271[A]	DTD	C1-C2-C3	2.82	118.34	112.51
4	C	1271[B]	DTD	C1-C2-C3	2.82	118.34	112.51
3	B	1270[B]	AX3	NAB-CAJ-NAE	2.88	121.97	117.20
3	B	1270[A]	AX3	NAB-CAJ-NAE	2.88	121.97	117.20
2	B	1269	NAP	C6N-C5N-C4N	2.93	123.88	119.44
3	C	1270[B]	AX3	NAB-CAJ-NAE	3.11	122.35	117.20
3	C	1270[A]	AX3	NAB-CAJ-NAE	3.11	122.35	117.20
3	D	1270[A]	AX3	CAK-NAH-CAL	3.18	127.05	123.51
3	B	1270[B]	AX3	NAF-CAK-NAG	3.20	131.14	126.22
3	B	1270[A]	AX3	NAF-CAK-NAG	3.20	131.14	126.22
3	D	1270[A]	AX3	CAI-NAF-CAK	3.28	118.36	113.57
3	D	1270[B]	AX3	CAI-NAF-CAK	3.28	118.36	113.57
3	D	1270[A]	AX3	NAB-CAJ-NAE	3.36	122.76	117.20
3	D	1270[B]	AX3	NAB-CAJ-NAE	3.36	122.76	117.20
3	C	1270[A]	AX3	NAH-CAK-NAG	3.64	122.27	116.95
3	D	1270[A]	AX3	CAJ-NAE-CAI	3.89	121.81	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270[B]	AX3	CAJ-NAE-CAI	3.89	121.81	114.80
3	A	1270	AX3	CAI-NAF-CAK	4.20	119.69	113.57
4	C	1271[A]	DTD	O3-C3-C2	5.05	121.61	110.27
4	C	1271[B]	DTD	O3-C3-C2	5.05	121.61	110.27
3	B	1270[B]	AX3	NAA-CAI-NAE	5.42	126.17	117.20
3	B	1270[A]	AX3	NAA-CAI-NAE	5.42	126.17	117.20
4	C	1271[A]	DTD	C4-C3-C2	5.64	124.18	112.51
4	C	1271[B]	DTD	C4-C3-C2	5.64	124.18	112.51
3	D	1270[A]	AX3	NAA-CAI-NAE	10.25	134.16	117.20
3	D	1270[B]	AX3	NAA-CAI-NAE	10.25	134.16	117.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1270	AX3	1	0
4	A	1271[B]	DTD	1	0
2	B	1269	NAP	2	0
3	B	1270[A]	AX3	2	0
3	B	1270[B]	AX3	9	0
6	B	1271[B]	D1D	1	0
2	C	1269	NAP	1	0
3	C	1270[A]	AX3	3	0
3	C	1270[B]	AX3	7	0
2	D	1269	NAP	2	0
3	D	1270[A]	AX3	3	0
3	D	1270[B]	AX3	12	0
6	D	1271[B]	D1D	4	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	248/288 (86%)	-0.13	1 (0%)	93 91	5, 10, 21, 40	0
1	B	248/288 (86%)	0.02	4 (1%)	74 73	5, 10, 26, 42	2 (0%)
1	C	249/288 (86%)	-0.04	8 (3%)	51 49	5, 10, 27, 41	0
1	D	247/288 (85%)	0.04	5 (2%)	68 66	6, 10, 26, 39	0
All	All	992/1152 (86%)	-0.03	18 (1%)	71 70	5, 10, 26, 42	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	5.7
1	D	212	ALA	5.3
1	B	211	VAL	5.2
1	B	212	ALA	3.9
1	D	214	GLY	3.7
1	B	2	GLU	3.3
1	C	211	VAL	2.7
1	C	152	SER	2.6
1	B	142	GLN	2.5
1	C	114	LYS	2.5
1	C	2	GLU	2.4
1	C	212	ALA	2.3
1	D	152	SER	2.3
1	C	104	GLN	2.2
1	C	50	LYS	2.2
1	A	211	VAL	2.2
1	D	216	GLU	2.1
1	C	46	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	D1D	D	1271[B]	8/8	0.86	0.35	11.31	19,23,25,26	8
6	D1D	D	1271[A]	8/8	0.86	0.35	8.56	19,22,23,25	8
3	AX3	C	1270[B]	12/12	0.94	0.14	8.42	17,20,22,22	4
3	AX3	C	1270[A]	12/12	0.94	0.14	8.42	17,19,22,23	4
3	AX3	D	1270[B]	12/12	0.93	0.18	4.18	16,22,30,31	4
3	AX3	B	1270[B]	12/12	0.92	0.18	3.35	14,20,22,23	4
4	DTD	A	1271[B]	8/8	0.95	0.09	3.09	13,25,31,39	1
4	DTD	A	1271[A]	8/8	0.95	0.09	3.09	13,25,31,39	1
3	AX3	B	1270[A]	12/12	0.92	0.18	1.25	14,19,21,22	4
3	AX3	D	1270[A]	12/12	0.93	0.18	1.01	16,21,24,24	4
4	DTD	C	1271[B]	8/8	0.94	0.10	0.73	28,31,33,36	1
6	D1D	B	1271[B]	8/8	0.93	0.10	0.59	26,32,34,38	1
6	D1D	B	1271[A]	8/8	0.93	0.10	0.59	28,32,34,38	1
4	DTD	C	1271[A]	8/8	0.94	0.10	-0.13	26,31,33,36	1
3	AX3	A	1270	12/12	0.99	0.06	-0.59	6,7,16,17	0
2	NAP	C	1269	48/48	0.99	0.04	-0.86	5,8,11,13	0
2	NAP	A	1269	48/48	0.99	0.05	-0.95	5,7,9,11	0
2	NAP	D	1269	48/48	0.99	0.05	-1.05	7,8,11,12	0
7	ACT	C	1272	4/4	0.99	0.05	-1.15	11,11,12,14	0
2	NAP	B	1269	48/48	0.99	0.04	-1.28	6,8,11,15	0
5	NA	A	1272	1/1	0.95	0.09	-	31,31,31,31	0
5	NA	D	1272	1/1	0.98	0.14	-	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.