



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2019 – 06:12 PM EDT

PDB ID : 2X9G  
Title : High resolution structure of TbPTR1 in complex with Pemetrexed  
Authors : Dawson, A.; Barrack, K.L.; Tulloch, L.B.; Hunter, W.N.  
Deposited on : 2010-03-18  
Resolution : 1.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

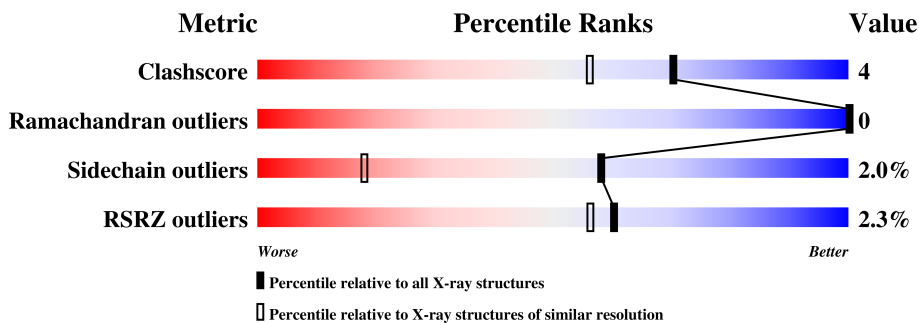
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 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	122126	1373 (1.14-1.06)
Ramachandran outliers	120053	1323 (1.14-1.06)
Sidechain outliers	120020	1321 (1.14-1.06)
RSRZ outliers	108989	1296 (1.14-1.06)

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>80% 7% • 13%</div> </div>
1	B	288	<div> <div>2%</div> <div>79% 6% • 13%</div> </div>
1	C	288	<div> <div>3%</div> <div>76% 10% •• 13%</div> </div>
1	D	288	<div> <div>%</div> <div>74% 10% • 14%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16553 atoms, of which 7199 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	251	Total	C	H	N	O	S	0	9	0
			3670	1202	1766	333	357	12			
1	B	250	Total	C	H	N	O	S	0	8	0
			3654	1193	1761	331	357	12			
1	C	252	Total	C	H	N	O	S	0	8	0
			3656	1195	1751	337	362	11			
1	D	249	Total	C	H	N	O	S	0	12	0
			3685	1206	1773	332	362	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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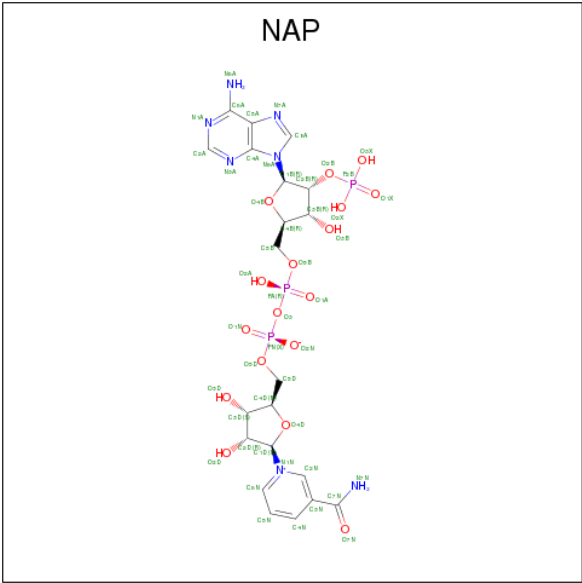
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	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<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



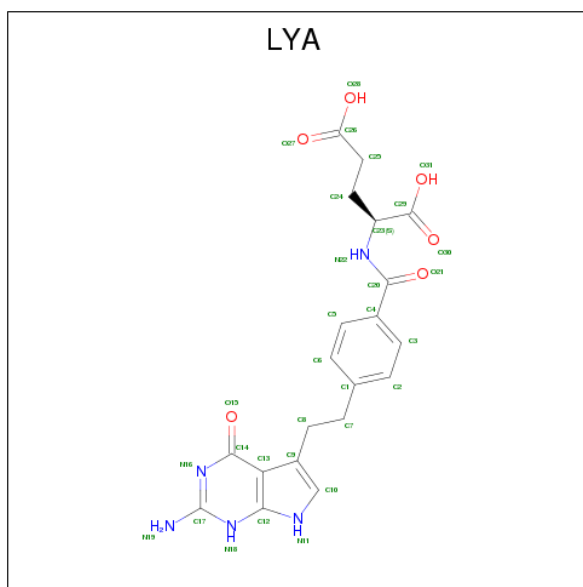
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 66	C 21	H 18	N 7	O 17	P 3	0	0
2	B	1	Total 66	C 21	H 18	N 7	O 17	P 3	0	0

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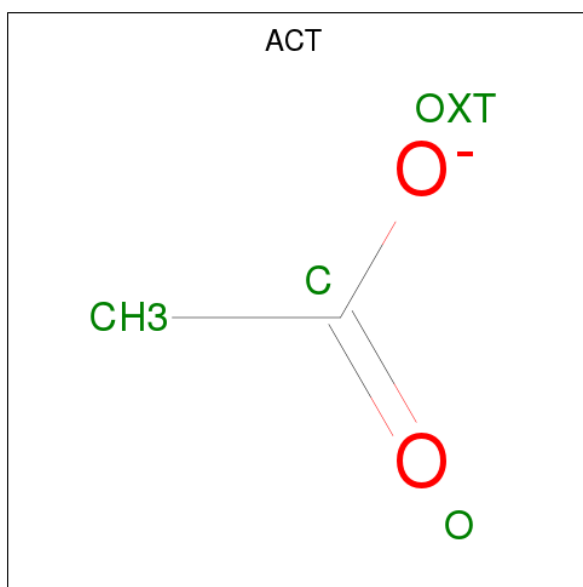
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	
			66	21	18	7	17	3	
2	D	1	Total	C	H	N	O	P	
			66	21	18	7	17	3	

- Molecule 3 is 2-{4-[2-(2-AMINO-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDIN-5-YL)-ETHYL]-BENZOYLAMINO}-PENTANEDIOIC ACID (three-letter code: LYA) (formula: C<sub>20</sub>H<sub>21</sub>N<sub>5</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		
			62	26	19	6	11	0	1
3	B	1	Total	C	H	N	O		
			62	26	19	6	11	0	1
3	C	1	Total	C	H	N	O		
			62	26	19	6	11	0	1
3	D	1	Total	C	H	N	O		
			62	26	19	6	11	0	1

- Molecule 4 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
4	B	1	Total	C	O	0	0
			4	2	2		

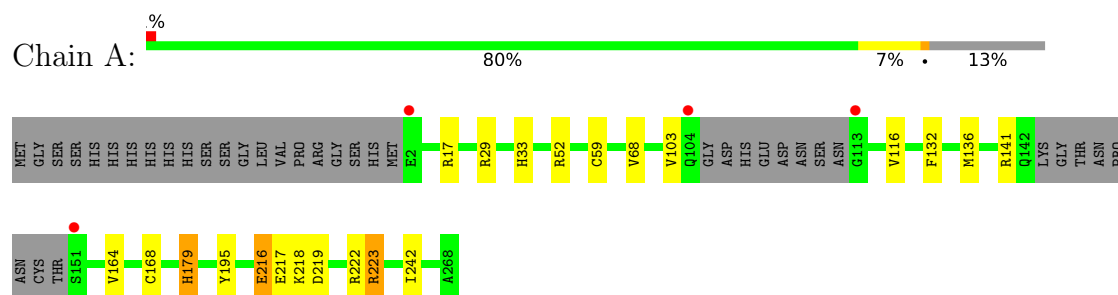
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	344	Total	O	0	0
			344	344		
5	B	380	Total	O	0	0
			380	380		
5	C	333	Total	O	0	0
			333	333		
5	D	315	Total	O	0	0
			315	315		

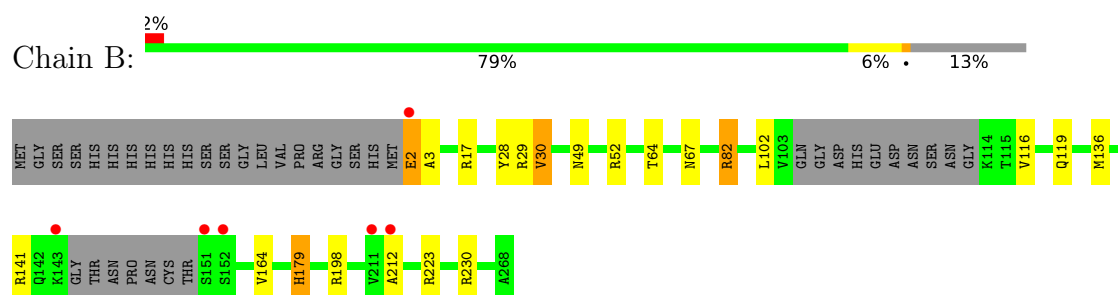
### 3 Residue-property plots [i](#)

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

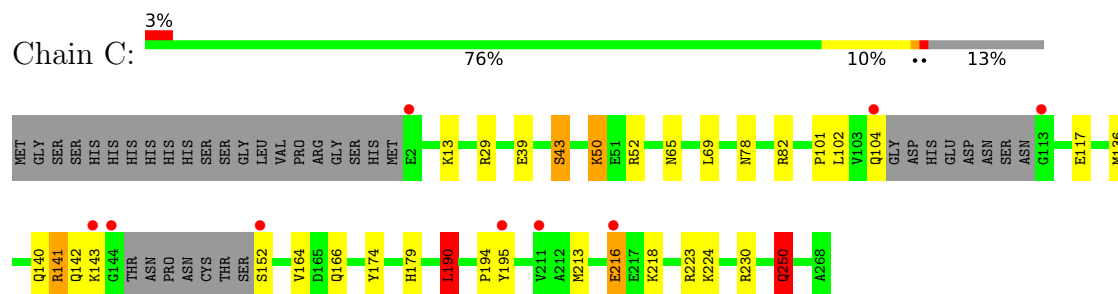
#### ● Molecule 1: PTERIDINE REDUCTASE



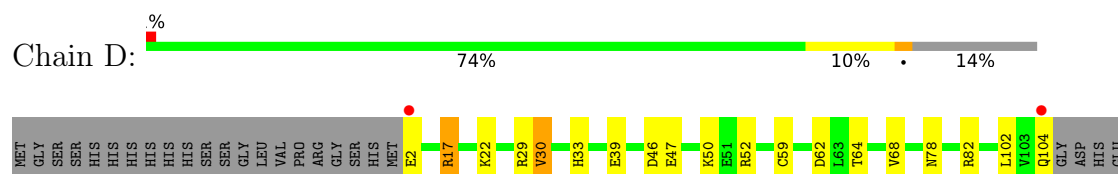
#### ● Molecule 1: PTERIDINE REDUCTASE

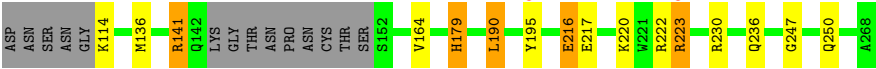


#### ● Molecule 1: PTERIDINE REDUCTASE



#### ● Molecule 1: PTERIDINE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.72Å 90.57Å 82.58Å 90.00° 115.61° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 19.99 – 1.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-1.10) 93.1 (19.99-1.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.121 , 0.147 0.130 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.2	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.67 % 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 8.2712e-03.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAP, LYA, 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	0.67	0/1971	1.18	16/2675 (0.6%)
1	B	0.73	3/1958 (0.2%)	1.25	18/2656 (0.7%)
1	C	0.83	2/1966 (0.1%)	1.26	23/2664 (0.9%)
1	D	0.78	3/2002 (0.1%)	1.32	26/2718 (1.0%)
All	All	0.76	8/7897 (0.1%)	1.25	83/10713 (0.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43[B]	SER	CA-CB	15.06	1.75	1.52
1	C	43[A]	SER	CA-CB	15.06	1.75	1.52
1	D	30[B]	VAL	CA-CB	8.51	1.72	1.54
1	D	30[A]	VAL	CA-CB	8.51	1.72	1.54
1	D	30[C]	VAL	CA-CB	8.51	1.72	1.54
1	B	30[B]	VAL	CA-CB	5.91	1.67	1.54
1	B	30[A]	VAL	CA-CB	5.91	1.67	1.54
1	B	30[C]	VAL	CA-CB	5.91	1.67	1.54

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ARG	CD-NE-CZ	19.22	150.51	123.60
1	C	141	ARG	NE-CZ-NH1	16.09	128.34	120.30
1	B	141	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	B	82	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	C	141	ARG	CD-NE-CZ	12.74	141.43	123.60
1	D	82	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	D	223	ARG	NE-CZ-NH1	-11.86	114.37	120.30
1	B	17	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	D	222	ARG	NE-CZ-NH2	-10.49	115.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	B	82	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	C	29	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	B	223	ARG	NE-CZ-NH1	-9.31	115.65	120.30
1	C	141	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	223	ARG	NE-CZ-NH2	8.89	124.75	120.30
1	D	17	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	C	52	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	D	52	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	D	223	ARG	CD-NE-CZ	-8.11	112.25	123.60
1	B	82	ARG	CD-NE-CZ	8.07	134.91	123.60
1	A	141	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	141	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	B	29	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	141	ARG	CD-NE-CZ	7.61	134.25	123.60
1	C	216	GLU	CA-CB-CG	7.47	129.84	113.40
1	C	195	TYR	CB-CG-CD1	7.39	125.43	121.00
1	D	82	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	222	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	52	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	D	82	ARG	CD-NE-CZ	7.04	133.46	123.60
1	C	250[A]	GLN	CA-CB-CG	6.98	128.76	113.40
1	C	250[B]	GLN	CA-CB-CG	6.98	128.76	113.40
1	B	230	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	223	ARG	CG-CD-NE	6.75	125.97	111.80
1	C	117[A]	GLU	CA-CB-CG	6.72	128.18	113.40
1	C	117[B]	GLU	CA-CB-CG	6.72	128.18	113.40
1	B	2	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	C	39	GLU	OE1-CD-OE2	-6.52	115.47	123.30
1	D	216[A]	GLU	N-CA-CB	6.32	121.98	110.60
1	D	216[B]	GLU	N-CA-CB	6.32	121.98	110.60
1	C	136	MET	CA-CB-CG	6.25	123.92	113.30
1	C	195	TYR	CG-CD1-CE1	6.20	126.26	121.30
1	D	230	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	29	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	D	195	TYR	CG-CD2-CE2	6.15	126.22	121.30
1	B	141	ARG	CD-NE-CZ	5.97	131.96	123.60
1	D	222	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	A	132	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	A	223	ARG	CD-NE-CZ	-5.87	115.39	123.60
1	C	82[A]	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	82[B]	ARG	NE-CZ-NH1	5.81	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	TYR	CB-CG-CD1	5.72	124.43	121.00
1	B	230	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	198	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	28	TYR	CB-CG-CD1	5.66	124.39	121.00
1	A	216[A]	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	A	216[B]	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	B	29	ARG	NH1-CZ-NH2	5.59	125.54	119.40
1	B	17	ARG	NH1-CZ-NH2	5.55	125.50	119.40
1	A	141	ARG	CG-CD-NE	5.53	123.42	111.80
1	C	223	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	195	TYR	CD1-CG-CD2	-5.46	111.90	117.90
1	D	141	ARG	CG-CD-NE	5.42	123.17	111.80
1	D	46	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	52	ARG	CD-NE-CZ	5.29	131.00	123.60
1	C	50	LYS	CA-CB-CG	5.28	125.01	113.40
1	A	132	PHE	CB-CG-CD1	5.25	124.48	120.80
1	C	190	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	190	LEU	CB-CG-CD1	-5.23	102.12	111.00
1	D	216[A]	GLU	CB-CG-CD	5.22	128.29	114.20
1	D	216[B]	GLU	CB-CG-CD	5.22	128.29	114.20
1	A	52	ARG	N-CA-CB	5.17	119.91	110.60
1	D	195	TYR	CB-CG-CD2	5.15	124.09	121.00
1	B	223	ARG	CG-CD-NE	5.12	122.56	111.80
1	C	224	LYS	CG-CD-CE	5.12	127.27	111.90
1	C	230	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	216[A]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	D	216[B]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	195	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	A	29	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	A	17	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	68	VAL	CA-CB-CG2	5.05	118.48	110.90
1	D	223	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1904	1766	1932	12	0
1	B	1893	1761	1925	13	0
1	C	1905	1751	1923	15	0
1	D	1912	1773	1937	27	0
2	A	48	18	25	0	0
2	B	48	18	25	0	0
2	C	48	18	25	0	0
2	D	48	18	25	1	0
3	A	43	19	12	1	0
3	B	43	19	12	0	0
3	C	43	19	12	0	0
3	D	43	19	12	1	0
4	B	4	0	3	0	0
5	A	344	0	0	4	0
5	B	380	0	0	6	0
5	C	333	0	0	4	0
5	D	315	0	0	14	0
All	All	9354	7199	7868	62	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 4.

All (62) 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:C:250[A]:GLN:HE21	1:D:236:GLN:HE21	1.30	0.80
1:B:212:ALA:HB3	5:B:2287:HOH:O	1.86	0.76
1:A:136[B]:MET:HG3	1:C:102:LEU:O	1.86	0.75
1:C:13:LYS:HE3	5:C:2005:HOH:O	1.91	0.70
1:D:220:LYS:O	1:D:223:ARG:HG3	1.92	0.69
1:D:216[B]:GLU:HG2	1:D:217:GLU:OE2	1.94	0.67
1:D:64[B]:THR:HG21	5:D:2122:HOH:O	1.95	0.67
1:A:217:GLU:HG2	5:A:2273:HOH:O	1.95	0.66
1:D:62:ASP:OD1	1:D:64[B]:THR:HG23	1.97	0.63
1:D:190:LEU:HD23	5:D:2224:HOH:O	1.98	0.63
1:D:64[A]:THR:HG21	5:D:2121:HOH:O	2.02	0.59
1:B:164:VAL:HG22	1:B:179[B]:HIS:CD2	2.38	0.59
1:A:116[B]:VAL:HG23	5:A:2197:HOH:O	2.04	0.58
1:B:2:GLU:HG3	5:B:2003:HOH:O	2.04	0.58
1:D:164:VAL:HG22	1:D:179[B]:HIS:CD2	2.39	0.57
1:A:164:VAL:HG22	1:A:179[B]:HIS:CD2	2.40	0.56
1:B:64[A]:THR:HG21	5:B:2154:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ARG:HB3	5:D:2147:HOH:O	2.07	0.55
1:D:50:LYS:HG3	5:D:2078:HOH:O	2.08	0.54
1:C:250[A]:GLN:NE2	1:D:236:GLN:HE21	2.00	0.54
1:A:103:VAL:CG1	1:C:143:LYS:HD3	2.38	0.53
1:C:190:LEU:HD21	5:C:2144:HOH:O	2.07	0.53
1:D:39:GLU:HG3	5:D:2064:HOH:O	2.09	0.53
1:C:101:PRO:HD2	5:C:2187:HOH:O	2.08	0.53
1:C:141:ARG:HG2	5:C:2206:HOH:O	2.07	0.52
1:D:250:GLN:HG2	5:D:2200:HOH:O	2.10	0.51
1:C:140:GLN:O	1:C:143:LYS:HB3	2.11	0.50
1:A:68[C]:VAL:HG13	5:A:2131:HOH:O	2.12	0.50
1:D:64[B]:THR:HG23	2:D:1269:NAP:H62A	1.77	0.50
1:B:82:ARG:HB2	5:B:2184:HOH:O	2.13	0.49
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.48	0.48
1:D:141:ARG:HG2	5:D:2190:HOH:O	2.13	0.48
1:B:2:GLU:HG2	1:B:3:ALA:N	2.29	0.47
1:A:216[A]:GLU:OE1	1:A:223:ARG:NH2	2.47	0.47
1:B:82:ARG:NH1	5:B:2186:HOH:O	2.48	0.46
1:D:17:ARG:NH2	1:D:47[B]:GLU:OE1	2.49	0.46
1:D:78[A]:ASN:OD1	1:D:141:ARG:NH1	2.48	0.46
1:A:33:HIS:HA	1:A:59:CYS:O	2.16	0.46
1:C:78[B]:ASN:OD1	1:C:141:ARG:NH2	2.49	0.46
1:D:114:LYS:NZ	5:D:2178:HOH:O	2.48	0.46
1:D:250:GLN:NE2	5:D:2287:HOH:O	2.50	0.45
1:C:194:PRO:HG3	5:D:2257:HOH:O	2.17	0.45
1:D:247:GLY:O	1:D:250:GLN:HG3	2.17	0.45
1:B:49:ASN:ND2	5:B:2110:HOH:O	2.49	0.45
1:A:218:LYS:NZ	5:A:2275:HOH:O	2.49	0.43
1:A:223:ARG:HD2	1:A:223:ARG:HH11	1.61	0.43
1:B:116:VAL:HA	1:B:119:GLN:HE21	1.82	0.43
1:B:136[B]:MET:HG3	1:D:102:LEU:O	2.19	0.43
1:A:168:CYS:HB3	3:A:1270[B]:LYA:C26	2.50	0.42
1:B:102:LEU:O	1:D:136[B]:MET:HG3	2.20	0.41
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.03	0.41
3:D:1270[A]:LYA:O28	3:D:1270[A]:LYA:H23	2.21	0.41
1:D:190:LEU:HB3	5:D:2224:HOH:O	2.21	0.41
1:D:33:HIS:HA	1:D:59:CYS:O	2.21	0.40
1:C:213:MET:O	1:C:218:LYS:HE3	2.21	0.40
1:A:219:ASP:O	1:A:223:ARG:HG3	2.21	0.40
1:D:50:LYS:HE3	5:D:2080:HOH:O	2.21	0.40
1:D:47[B]:GLU:HG3	5:D:2068:HOH:O	2.21	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	255/288 (88%)	246 (96%)	9 (4%)	0	100	100
1	B	253/288 (88%)	244 (96%)	9 (4%)	0	100	100
1	C	254/288 (88%)	245 (96%)	9 (4%)	0	100	100
1	D	258/288 (90%)	250 (97%)	8 (3%)	0	100	100
All	All	1020/1152 (88%)	985 (97%)	35 (3%)	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	207/231 (90%)	204 (99%)	3 (1%)	69	32
1	B	208/231 (90%)	205 (99%)	3 (1%)	69	32
1	C	207/231 (90%)	198 (96%)	9 (4%)	32	3
1	D	213/231 (92%)	208 (98%)	5 (2%)	53	14
All	All	835/924 (90%)	815 (98%)	20 (2%)	58	13

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179[A]	HIS
1	A	179[B]	HIS
1	A	242	ILE
1	B	67	ASN
1	B	179[A]	HIS
1	B	179[B]	HIS
1	C	50	LYS
1	C	104	GLN
1	C	142	GLN
1	C	152	SER
1	C	166	GLN
1	C	190	LEU
1	C	216	GLU
1	C	250[A]	GLN
1	C	250[B]	GLN
1	D	2	GLU
1	D	22	LYS
1	D	104	GLN
1	D	179[A]	HIS
1	D	179[B]	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	119	GLN
1	D	67	ASN
1	D	104	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

13 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
2	NAP	A	1269	-	43,52,52	0.91	1 (2%)	53,80,80	1.21	3 (5%)
3	LYA	A	1270[A]	-	26,33,33	0.91	1 (3%)	29,46,46	2.73	8 (27%)
3	LYA	A	1270[B]	-	26,33,33	1.03	2 (7%)	29,46,46	2.65	6 (20%)
2	NAP	B	1269	-	43,52,52	0.95	1 (2%)	53,80,80	1.41	7 (13%)
3	LYA	B	1270[A]	-	26,33,33	0.91	1 (3%)	29,46,46	2.59	5 (17%)
3	LYA	B	1270[B]	-	26,33,33	1.02	2 (7%)	29,46,46	2.68	7 (24%)
4	ACT	B	1271	-	1,3,3	5.04	1 (100%)	0,3,3	0.00	-
2	NAP	C	1269	-	43,52,52	0.75	1 (2%)	53,80,80	1.19	2 (3%)
3	LYA	C	1270[A]	-	26,33,33	0.87	0	29,46,46	2.38	6 (20%)
3	LYA	C	1270[B]	-	26,33,33	0.96	1 (3%)	29,46,46	2.71	10 (34%)
2	NAP	D	1269	-	43,52,52	0.96	1 (2%)	53,80,80	1.13	4 (7%)
3	LYA	D	1270[A]	-	26,33,33	1.22	3 (11%)	29,46,46	2.97	11 (37%)
3	LYA	D	1270[B]	-	26,33,33	1.23	2 (7%)	29,46,46	2.88	10 (34%)

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	LYA	A	1270[A]	-	-	0/16/22/22	0/3/3/3
3	LYA	A	1270[B]	-	-	0/16/22/22	0/3/3/3
2	NAP	B	1269	-	-	0/27/67/67	0/5/5/5
3	LYA	B	1270[A]	-	-	0/16/22/22	0/3/3/3
3	LYA	B	1270[B]	-	-	0/16/22/22	0/3/3/3
4	ACT	B	1271	-	-	0/0/0/0	0/0/0/0
2	NAP	C	1269	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LYA	C	1270[A]	-	-	0/16/22/22	0/3/3/3
3	LYA	C	1270[B]	-	-	0/16/22/22	0/3/3/3
2	NAP	D	1269	-	-	0/27/67/67	0/5/5/5
3	LYA	D	1270[A]	-	-	0/16/22/22	0/3/3/3
3	LYA	D	1270[B]	-	-	0/16/22/22	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270[A]	LYA	C24-C23	-2.82	1.49	1.53
3	D	1270[A]	LYA	C23-N22	-2.27	1.43	1.46
2	B	1269	NAP	C4A-N3A	-2.19	1.32	1.35
3	B	1270[B]	LYA	C4-C20	2.01	1.54	1.50
2	C	1269	NAP	P2B-O2B	2.02	1.63	1.59
3	A	1270[B]	LYA	C4-C20	2.02	1.54	1.50
3	C	1270[B]	LYA	C23-N22	2.12	1.49	1.46
2	A	1269	NAP	P2B-O2B	2.42	1.63	1.59
2	D	1269	NAP	P2B-O2B	2.94	1.64	1.59
3	A	1270[A]	LYA	C14-N16	3.18	1.38	1.33
3	A	1270[B]	LYA	C14-N16	3.18	1.38	1.33
3	D	1270[B]	LYA	C23-N22	3.23	1.50	1.46
3	B	1270[B]	LYA	C14-N16	3.37	1.38	1.33
3	B	1270[A]	LYA	C14-N16	3.37	1.38	1.33
3	D	1270[A]	LYA	C14-N16	3.96	1.39	1.33
3	D	1270[B]	LYA	C14-N16	3.96	1.39	1.33
4	B	1271	ACT	CH3-C	5.04	1.55	1.48

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1270[A]	LYA	C13-C14-N16	-10.16	115.00	124.08
3	A	1270[B]	LYA	C13-C14-N16	-10.16	115.00	124.08
3	B	1270[B]	LYA	C13-C14-N16	-10.12	115.04	124.08
3	B	1270[A]	LYA	C13-C14-N16	-10.12	115.04	124.08
3	D	1270[A]	LYA	C13-C14-N16	-9.45	115.64	124.08
3	D	1270[B]	LYA	C13-C14-N16	-9.45	115.64	124.08
3	C	1270[B]	LYA	C13-C14-N16	-8.79	116.22	124.08
3	C	1270[A]	LYA	C13-C14-N16	-8.79	116.22	124.08
3	C	1270[B]	LYA	C24-C23-C29	-5.85	103.76	112.18
2	C	1269	NAP	C4B-O4B-C1B	-5.70	103.89	109.83
2	B	1269	NAP	C4B-O4B-C1B	-5.60	103.99	109.83
2	A	1269	NAP	C4B-O4B-C1B	-5.07	104.54	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270[B]	LYA	C24-C23-C29	-4.49	105.72	112.18
3	D	1270[A]	LYA	N18-C17-N16	-3.95	121.91	127.25
3	D	1270[B]	LYA	N18-C17-N16	-3.95	121.91	127.25
3	B	1270[B]	LYA	N18-C17-N16	-3.94	121.92	127.25
3	B	1270[A]	LYA	N18-C17-N16	-3.94	121.92	127.25
3	D	1270[B]	LYA	C23-N22-C20	-3.76	117.34	122.31
3	A	1270[A]	LYA	N18-C17-N16	-3.75	122.18	127.25
3	A	1270[B]	LYA	N18-C17-N16	-3.75	122.18	127.25
3	C	1270[B]	LYA	C23-N22-C20	-3.64	117.50	122.31
3	D	1270[B]	LYA	C24-C23-N22	-3.62	104.90	110.19
3	A	1270[A]	LYA	C23-N22-C20	-3.55	117.62	122.31
2	D	1269	NAP	C4B-O4B-C1B	-3.29	106.40	109.83
3	C	1270[B]	LYA	N18-C17-N16	-3.29	122.80	127.25
3	C	1270[A]	LYA	N18-C17-N16	-3.29	122.80	127.25
3	D	1270[B]	LYA	C29-C23-N22	-3.22	105.41	112.39
3	D	1270[A]	LYA	C9-C13-C12	-3.06	105.32	110.30
3	D	1270[B]	LYA	C9-C13-C12	-3.06	105.32	110.30
3	A	1270[A]	LYA	C29-C23-N22	-3.02	105.85	112.39
3	B	1270[B]	LYA	C24-C23-C29	-3.00	107.86	112.18
3	C	1270[B]	LYA	C24-C23-N22	-2.89	105.96	110.19
3	A	1270[B]	LYA	C24-C23-C29	-2.79	108.16	112.18
2	A	1269	NAP	C4A-C5A-N7A	-2.68	106.61	109.40
3	C	1270[B]	LYA	C25-C24-C23	-2.60	107.70	113.01
3	B	1270[A]	LYA	C29-C23-N22	-2.40	107.18	112.39
3	B	1270[B]	LYA	O21-C20-N22	-2.35	118.18	122.46
3	D	1270[A]	LYA	O21-C20-C4	-2.35	116.75	120.94
2	B	1269	NAP	O7N-C7N-C3N	-2.29	116.85	119.62
3	C	1270[B]	LYA	C29-C23-N22	-2.20	107.62	112.39
2	B	1269	NAP	C1B-N9A-C4A	-2.17	122.89	126.64
2	A	1269	NAP	C1B-N9A-C4A	-2.14	122.94	126.64
3	C	1270[B]	LYA	C9-C13-C12	-2.07	106.92	110.30
3	C	1270[A]	LYA	C9-C13-C12	-2.07	106.92	110.30
3	A	1270[A]	LYA	C24-C23-C29	-2.07	109.20	112.18
2	B	1269	NAP	C5A-C6A-N1A	-2.04	115.51	120.31
2	B	1269	NAP	PN-O3-PA	-2.02	126.14	132.57
2	D	1269	NAP	C3N-C7N-N7N	2.05	120.08	117.75
2	D	1269	NAP	C5A-C6A-N6A	2.07	123.64	120.38
3	D	1270[A]	LYA	C23-N22-C20	2.15	125.15	122.31
2	D	1269	NAP	O3B-C3B-C2B	2.22	117.43	111.15
3	C	1270[B]	LYA	C14-C13-C12	2.22	116.28	115.04
3	C	1270[A]	LYA	C14-C13-C12	2.22	116.28	115.04
3	A	1270[A]	LYA	C14-C13-C12	2.56	116.47	115.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1270[B]	LYA	C14-C13-C12	2.56	116.47	115.04
3	A	1270[B]	LYA	C4-C20-N22	2.67	122.13	117.03
3	A	1270[A]	LYA	O21-C20-N22	2.74	127.47	122.46
3	B	1270[B]	LYA	C14-C13-C12	2.75	116.57	115.04
3	B	1270[A]	LYA	C14-C13-C12	2.75	116.57	115.04
3	D	1270[A]	LYA	C25-C24-C23	2.80	118.72	113.01
3	B	1270[B]	LYA	C4-C20-N22	2.82	122.40	117.03
2	C	1269	NAP	C5A-C6A-N6A	2.88	124.90	120.38
3	D	1270[A]	LYA	C7-C8-C9	2.89	117.27	112.43
3	D	1270[B]	LYA	C7-C8-C9	2.89	117.27	112.43
3	D	1270[A]	LYA	C14-C13-C12	3.05	116.74	115.04
3	D	1270[B]	LYA	C14-C13-C12	3.05	116.74	115.04
2	B	1269	NAP	C5A-C6A-N6A	3.13	125.30	120.38
2	B	1269	NAP	C3N-C7N-N7N	3.19	121.38	117.75
3	C	1270[A]	LYA	C29-C23-N22	3.64	120.29	112.39
3	D	1270[A]	LYA	C24-C23-N22	4.95	117.44	110.19
3	D	1270[A]	LYA	C14-N16-C17	5.24	123.53	116.06
3	D	1270[B]	LYA	C14-N16-C17	5.24	123.53	116.06
3	C	1270[B]	LYA	C14-N16-C17	5.45	123.82	116.06
3	C	1270[A]	LYA	C14-N16-C17	5.45	123.82	116.06
3	D	1270[A]	LYA	C29-C23-N22	5.45	124.22	112.39
3	A	1270[A]	LYA	C14-N16-C17	6.34	125.09	116.06
3	A	1270[B]	LYA	C14-N16-C17	6.34	125.09	116.06
3	B	1270[B]	LYA	C14-N16-C17	6.34	125.09	116.06
3	B	1270[A]	LYA	C14-N16-C17	6.34	125.09	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1270[B]	LYA	1	0
2	D	1269	NAP	1	0
3	D	1270[A]	LYA	1	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

### 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	251/288 (87%)	-0.53	4 (1%) 72 68	6, 11, 26, 56	0
1	B	250/288 (86%)	-0.60	6 (2%) 59 54	6, 9, 24, 56	0
1	C	252/288 (87%)	-0.43	9 (3%) 42 38	6, 10, 28, 67	0
1	D	249/288 (86%)	-0.55	4 (1%) 72 68	6, 10, 25, 53	0
All	All	1002/1152 (86%)	-0.53	23 (2%) 60 56	6, 10, 26, 67	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	GLY	8.8
1	C	113	GLY	8.1
1	A	151	SER	6.8
1	A	113	GLY	6.4
1	C	143	LYS	5.8
1	D	104	GLN	5.6
1	C	104	GLN	5.2
1	C	2	GLU	5.2
1	A	104	GLN	5.0
1	B	151	SER	4.3
1	B	143	LYS	3.5
1	B	211	VAL	3.3
1	A	2	GLU	3.1
1	B	2	GLU	2.9
1	D	2	GLU	2.7
1	C	211	VAL	2.7
1	C	195	TYR	2.6
1	D	195	TYR	2.6
1	B	152	SER	2.4
1	B	212	ALA	2.3
1	C	152	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	223	ARG	2.2
1	C	216	GLU	2.0

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

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

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	LYA	D	1270[A]	31/31	0.94	0.12	8,16,32,37	17
3	LYA	D	1270[B]	31/31	0.94	0.12	8,16,24,32	17
3	LYA	C	1270[B]	31/31	0.96	0.10	7,15,24,31	17
3	LYA	C	1270[A]	31/31	0.96	0.10	7,17,32,35	17
3	LYA	A	1270[A]	31/31	0.96	0.11	8,16,26,34	17
3	LYA	A	1270[B]	31/31	0.96	0.11	8,16,23,31	17
3	LYA	B	1270[B]	31/31	0.98	0.07	6,13,19,23	17
3	LYA	B	1270[A]	31/31	0.98	0.07	6,13,19,21	17
4	ACT	B	1271	4/4	0.99	0.04	12,13,13,14	0
2	NAP	A	1269	48/48	0.99	0.04	6,8,11,14	0
2	NAP	B	1269	48/48	1.00	0.03	5,7,9,10	0
2	NAP	C	1269	48/48	1.00	0.04	5,7,9,10	0
2	NAP	D	1269	48/48	1.00	0.03	6,8,10,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.