



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:59 PM GMT

PDB ID : 1MXF  
Title : Crystal Structure of Inhibitor Complex of Putative Pteridine Reductase 2 (PTR2) from Trypanosoma cruzi  
Authors : Schormann, N.; Pal, B.; Senkovich, O.; Carson, M.; Howard, A.; Smith, C.; Delucas, L.; Chattopadhyay, D.  
Deposited on : 2002-10-02  
Resolution : 2.30 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

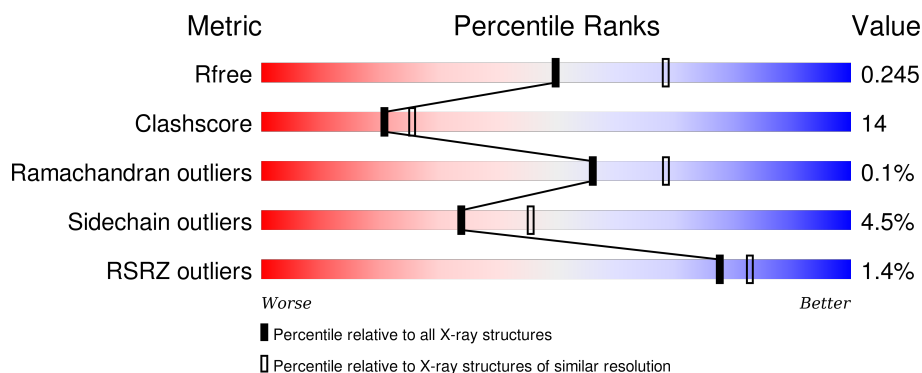
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	276	<div> <div>2%</div> <div>60%</div> <div>27%</div> <div>11%</div> </div>
1	B	276	<div> <div>%</div> <div>64%</div> <div>23%</div> <div>11%</div> </div>
1	C	276	<div> <div>%</div> <div>64%</div> <div>22%</div> <div>11%</div> </div>
1	D	276	<div> <div>%</div> <div>68%</div> <div>20%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTX	B	2278	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8018 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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	0	0	0
			1837	1158	335	333	8	3			
1	B	247	Total	C	N	O	S	Se	0	0	0
			1837	1158	335	333	8	3			
1	C	247	Total	C	N	O	S	Se	0	0	0
			1837	1158	335	333	8	3			
1	D	247	Total	C	N	O	S	Se	0	0	0
			1837	1158	335	333	8	3			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



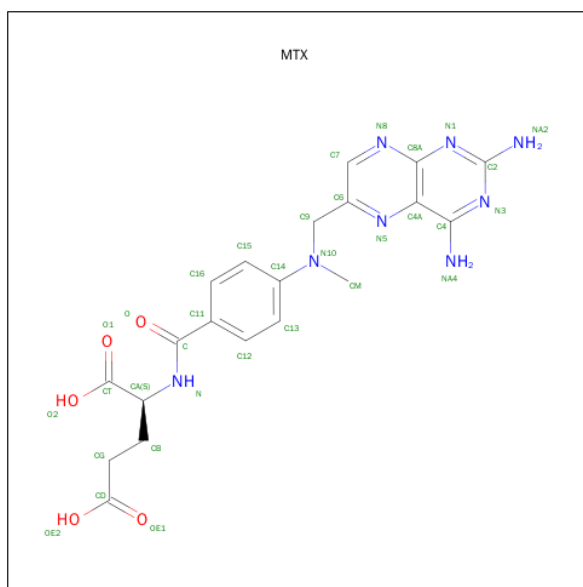
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			33	20	8	5		
3	B	1	Total	C	N	O		
			33	20	8	5		
3	C	1	Total	C	N	O		
			33	20	8	5		
3	D	1	Total	C	N	O		
			33	20	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O		
			79	79		
4	B	64	Total	O		
			64	64		
4	C	98	Total	O		
			98	98		

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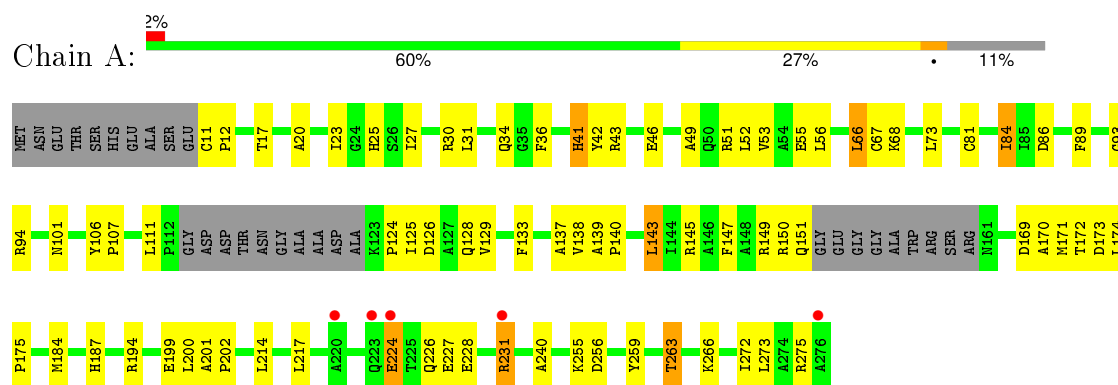
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	105	Total	O	0	0
			105	105		

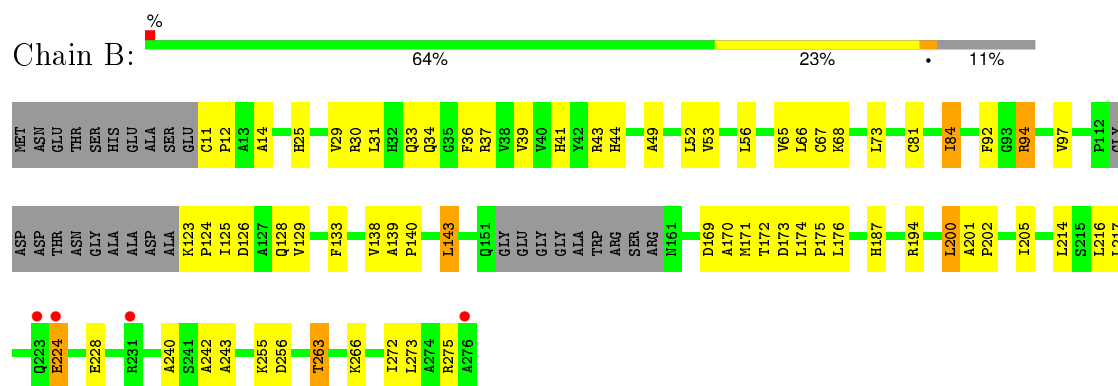
### 3 Residue-property plots

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.

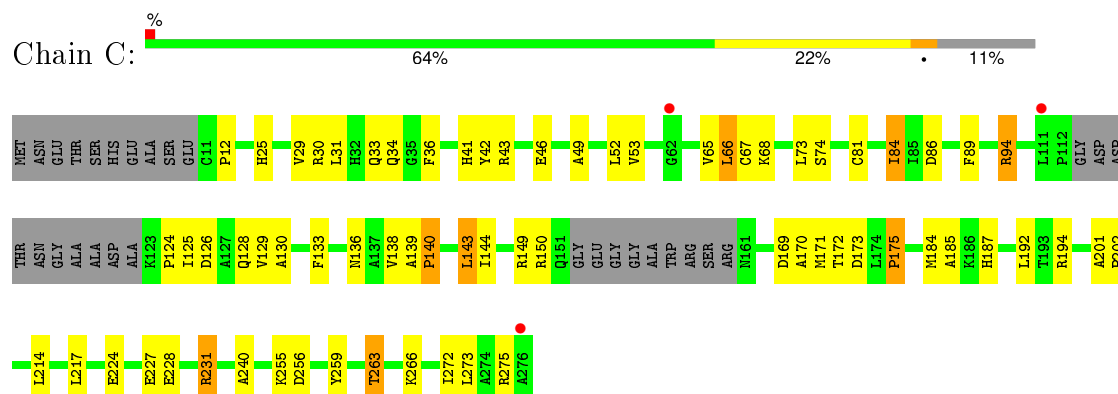
#### • Molecule 1: PTERIDINE REDUCTASE 2



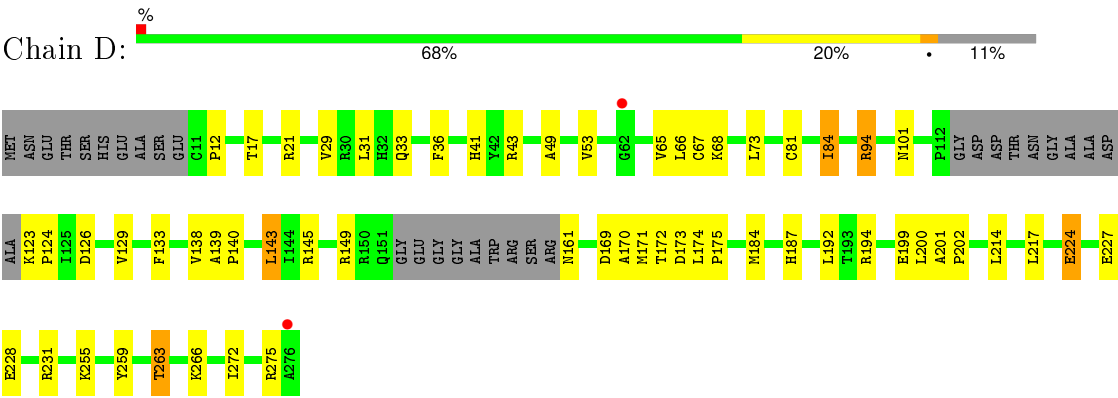
#### • Molecule 1: PTERIDINE REDUCTASE 2



#### • Molecule 1: PTERIDINE REDUCTASE 2



● Molecule 1: PTERIDINE REDUCTASE 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.79 Å 74.79 Å 180.99 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.49 – 2.30 36.62 – 1.77	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.49-2.30) 77.4 (36.62-1.77)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 1.77 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.197 , 0.239 0.202 , 0.245	Depositor DCC
$R_{free}$ test set	2603 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
Estimated twinning fraction	0.014 for -h,-k,l 0.045 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 85572 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, MTX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/1865	0.59	0/2527
1	B	0.35	0/1865	0.60	0/2527
1	C	0.38	0/1865	0.62	0/2527
1	D	0.37	0/1865	0.62	0/2527
All	All	0.36	0/7460	0.61	0/10108

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	1837	0	1874	70	0
1	B	1837	0	1874	62	0
1	C	1837	0	1874	58	0
1	D	1837	0	1874	62	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	0	0
3	A	33	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	20	2	0
3	C	33	0	20	1	0
3	D	33	0	20	2	0
4	A	79	0	0	4	0
4	B	64	0	0	3	0
4	C	98	0	0	3	0
4	D	105	0	0	8	0
All	All	8018	0	7680	221	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 14.

All (221) 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:A:171:MSE:HE1	1:A:272:ILE:HB	1.26	1.15
1:C:171:MSE:HE1	1:C:272:ILE:HB	1.42	1.01
1:A:53:VAL:HG21	1:A:66:LEU:HD13	1.42	1.00
1:C:49:ALA:HB1	1:C:66:LEU:HD11	1.42	1.00
1:D:171:MSE:HE1	1:D:272:ILE:HB	1.49	0.94
1:D:49:ALA:HB1	1:D:66:LEU:HD11	1.50	0.93
1:B:171:MSE:HE1	1:B:272:ILE:HB	1.51	0.89
1:B:53:VAL:HG21	1:B:66:LEU:HD13	1.56	0.85
1:A:31:LEU:O	1:A:36:PHE:HB2	1.79	0.82
1:C:53:VAL:HG21	1:C:66:LEU:HD13	1.62	0.81
1:A:81:CYS:O	1:A:84:ILE:HG22	1.81	0.79
1:B:49:ALA:HB1	1:B:66:LEU:HD11	1.64	0.79
1:C:31:LEU:O	1:C:36:PHE:HB2	1.83	0.78
1:A:53:VAL:CG2	1:A:66:LEU:HD13	2.15	0.77
1:A:171:MSE:HE1	1:A:272:ILE:CB	2.13	0.77
1:B:263:THR:HG22	1:D:266:LYS:HE3	1.66	0.77
1:D:81:CYS:O	1:D:84:ILE:HG22	1.86	0.76
1:B:266:LYS:HE3	1:D:263:THR:HG22	1.68	0.75
1:B:81:CYS:O	1:B:84:ILE:HG22	1.88	0.74
1:C:139:ALA:HB3	1:C:140:PRO:HD3	1.70	0.72
1:D:84:ILE:HG21	1:D:143:LEU:HD11	1.71	0.72
1:C:81:CYS:O	1:C:84:ILE:HG22	1.88	0.72
1:D:53:VAL:HG21	1:D:66:LEU:HD13	1.71	0.72
1:A:194:ARG:NH2	1:B:173:ASP:HA	2.05	0.71
1:A:266:LYS:HE3	1:C:263:THR:HG22	1.72	0.71
1:C:46:GLU:HG3	4:C:3281:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HD11	1:C:217:LEU:HD21	1.74	0.69
1:B:12:PRO:HA	1:B:94:ARG:HH11	1.57	0.69
1:C:84:ILE:HG21	1:C:143:LEU:HD11	1.75	0.69
1:A:139:ALA:HB3	1:A:140:PRO:HD3	1.75	0.69
1:B:214:LEU:HD11	1:B:217:LEU:HD21	1.75	0.68
1:A:173:ASP:HA	1:B:194:ARG:NH2	2.08	0.68
1:B:139:ALA:HB3	1:B:140:PRO:HD3	1.76	0.68
1:C:53:VAL:CG2	1:C:66:LEU:HD13	2.23	0.68
1:A:169:ASP:HB3	1:A:172:THR:HG23	1.75	0.68
1:A:173:ASP:HA	1:B:194:ARG:HH22	1.59	0.67
1:C:12:PRO:HA	1:C:94:ARG:HH11	1.59	0.67
1:A:224:GLU:O	1:A:228:GLU:HG3	1.95	0.67
1:A:49:ALA:HB1	1:A:66:LEU:HD11	1.76	0.67
1:B:224:GLU:O	1:B:228:GLU:HG3	1.94	0.67
1:A:12:PRO:HA	1:A:94:ARG:HH11	1.60	0.67
1:B:53:VAL:CG2	1:B:66:LEU:HD13	2.25	0.66
1:A:73:LEU:HD21	1:A:138:VAL:HG21	1.76	0.66
1:D:201:ALA:HB3	1:D:202:PRO:HD3	1.77	0.66
1:A:240:ALA:HB2	1:C:259:TYR:CE2	2.30	0.66
1:A:25:HIS:CE1	1:A:52:LEU:HD13	2.31	0.66
1:B:84:ILE:O	1:B:84:ILE:HD13	1.96	0.65
1:A:227:GLU:HG3	1:A:231:ARG:NH1	2.12	0.64
1:B:214:LEU:HD12	3:B:2278:MTX:HM2	1.80	0.64
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.80	0.64
1:D:29:VAL:O	1:D:33:GLN:HG3	1.97	0.64
1:D:81:CYS:HB3	1:D:143:LEU:HD13	1.81	0.62
1:D:31:LEU:O	1:D:36:PHE:HB2	2.00	0.62
1:C:194:ARG:HH21	1:D:187:HIS:HE1	1.48	0.61
1:C:173:ASP:HA	1:D:194:ARG:NH2	2.16	0.61
1:D:227:GLU:HG3	1:D:231:ARG:NH1	2.14	0.61
1:A:139:ALA:O	1:A:143:LEU:HD22	1.99	0.61
1:C:43:ARG:O	1:C:68:LYS:HE3	2.01	0.60
1:A:84:ILE:O	1:A:84:ILE:HD13	2.02	0.59
1:C:227:GLU:HG3	1:C:231:ARG:NH1	2.16	0.59
1:A:17:THR:O	1:A:101:ASN:HB3	2.02	0.59
1:C:149:ARG:HD3	4:C:3345:HOH:O	2.02	0.58
1:D:224:GLU:O	1:D:228:GLU:HG3	2.03	0.58
1:A:81:CYS:HB3	1:A:143:LEU:HD13	1.86	0.58
1:A:187:HIS:CE1	1:B:194:ARG:HH21	2.20	0.58
1:D:53:VAL:CG2	1:D:66:LEU:HD13	2.33	0.58
1:A:23:ILE:O	1:A:27:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:133:PHE:HB2	2.04	0.58
1:B:43:ARG:O	1:B:68:LYS:HE3	2.04	0.57
1:A:194:ARG:HH22	1:B:173:ASP:HA	1.67	0.57
1:C:194:ARG:HH21	1:D:187:HIS:CE1	2.21	0.57
1:A:124:PRO:O	1:A:128:GLN:HG3	2.04	0.57
1:D:65:VAL:HG22	1:D:66:LEU:N	2.20	0.56
1:A:147:PHE:O	1:A:151:GLN:HG2	2.05	0.56
1:A:255:LYS:HG3	4:A:1332:HOH:O	2.05	0.56
1:B:169:ASP:HB3	1:B:172:THR:HG23	1.88	0.56
1:C:86:ASP:HA	1:C:150:ARG:NH1	2.21	0.56
1:D:43:ARG:NH2	4:D:4345:HOH:O	2.30	0.56
1:C:224:GLU:O	1:C:228:GLU:HG3	2.05	0.56
1:A:263:THR:HG22	1:C:266:LYS:HE3	1.87	0.56
1:D:84:ILE:O	1:D:84:ILE:HD13	2.05	0.56
1:B:124:PRO:O	1:B:128:GLN:HG3	2.06	0.56
1:B:73:LEU:HD21	1:B:138:VAL:HG21	1.88	0.55
1:C:173:ASP:HA	1:D:194:ARG:HH22	1.71	0.55
1:D:214:LEU:HD11	1:D:217:LEU:HD21	1.88	0.55
4:A:1283:HOH:O	1:D:275:ARG:HB2	2.06	0.55
1:C:169:ASP:HB3	1:C:172:THR:HG23	1.90	0.54
1:C:171:MSE:HE1	1:C:272:ILE:CB	2.26	0.54
1:A:275:ARG:HB2	4:D:4283:HOH:O	2.07	0.54
1:D:126:ASP:O	1:D:129:VAL:HG22	2.07	0.54
1:A:43:ARG:O	1:A:68:LYS:HE3	2.08	0.53
1:C:187:HIS:CE1	1:D:194:ARG:HH21	2.25	0.53
1:C:29:VAL:O	1:C:33:GLN:HG3	2.08	0.53
1:D:21:ARG:HD2	4:D:4355:HOH:O	2.07	0.53
1:A:42:TYR:CE2	1:A:46:GLU:HA	2.44	0.53
1:B:81:CYS:SG	1:B:143:LEU:HD13	2.49	0.53
1:B:174:LEU:O	1:C:275:ARG:HD2	2.10	0.52
1:C:84:ILE:O	1:C:84:ILE:HD13	2.08	0.52
1:C:187:HIS:HE1	1:D:194:ARG:HH21	1.57	0.52
1:D:139:ALA:HB3	1:D:140:PRO:HD3	1.91	0.52
1:B:31:LEU:O	1:B:36:PHE:HB2	2.09	0.52
1:A:129:VAL:O	1:A:133:PHE:HB2	2.10	0.52
1:B:65:VAL:HG22	1:B:66:LEU:N	2.24	0.52
1:A:174:LEU:O	1:D:275:ARG:HD2	2.10	0.52
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.92	0.52
1:B:266:LYS:CE	1:D:263:THR:HG22	2.40	0.51
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.25	0.51
1:B:84:ILE:HG21	1:B:143:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HD2	1:D:174:LEU:O	2.10	0.51
1:B:200:LEU:HB3	1:B:205:ILE:HB	1.91	0.51
1:C:125:ILE:HG23	1:C:126:ASP:N	2.26	0.51
4:B:2320:HOH:O	1:C:171:MSE:HG3	2.11	0.50
1:B:29:VAL:O	1:B:33:GLN:HG3	2.10	0.50
1:C:194:ARG:NH2	1:D:173:ASP:HA	2.26	0.50
1:D:169:ASP:HB3	1:D:172:THR:HG23	1.94	0.50
1:A:137:ALA:C	1:A:140:PRO:HD2	2.32	0.49
1:A:106:TYR:HB2	1:A:107:PRO:HD2	1.94	0.49
1:C:201:ALA:N	1:C:202:PRO:CD	2.75	0.49
1:A:30:ARG:NH1	1:A:34:GLN:OE1	2.46	0.49
1:A:170:ALA:C	1:A:171:MSE:HE2	2.34	0.48
1:D:129:VAL:O	1:D:133:PHE:HB2	2.13	0.48
1:D:12:PRO:HA	1:D:94:ARG:HH11	1.78	0.48
1:C:129:VAL:O	1:C:133:PHE:HB2	2.13	0.48
1:D:214:LEU:HD12	3:D:4278:MTX:HM2	1.94	0.48
1:B:176:LEU:HB2	1:C:275:ARG:NH1	2.29	0.47
1:B:41:HIS:HA	1:B:67:CYS:O	2.14	0.47
1:D:170:ALA:C	1:D:171:MSE:HE2	2.35	0.47
1:A:214:LEU:HD12	3:A:1278:MTX:HM2	1.95	0.47
1:B:171:MSE:HE1	1:B:272:ILE:CB	2.36	0.47
1:C:30:ARG:NH1	1:C:34:GLN:OE1	2.47	0.47
1:B:275:ARG:HB2	4:C:3282:HOH:O	2.15	0.47
1:A:89:PHE:O	1:A:93:GLY:N	2.44	0.47
1:A:51:ARG:O	1:A:55:GLU:HB2	2.15	0.47
1:D:255:LYS:HB3	1:D:255:LYS:NZ	2.30	0.47
1:A:41:HIS:HA	1:A:67:CYS:O	2.15	0.46
1:A:214:LEU:HD11	1:A:217:LEU:HD21	1.97	0.46
1:D:161:ASN:N	4:D:4288:HOH:O	2.48	0.46
1:A:259:TYR:CE2	1:C:240:ALA:HB2	2.51	0.46
1:C:140:PRO:O	1:C:144:ILE:HG13	2.15	0.46
1:C:89:PHE:CE1	1:C:94:ARG:HA	2.50	0.46
1:B:126:ASP:O	1:B:129:VAL:HG22	2.16	0.46
1:D:145:ARG:O	1:D:149:ARG:HG3	2.16	0.46
1:A:217:LEU:HD13	1:A:226:GLN:HG2	1.97	0.46
1:A:171:MSE:CE	1:A:272:ILE:HB	2.19	0.46
1:A:89:PHE:CE1	1:A:94:ARG:HA	2.50	0.46
1:C:73:LEU:HD12	1:C:130:ALA:HA	1.97	0.46
1:A:84:ILE:HG21	1:A:143:LEU:HD11	1.97	0.45
1:A:194:ARG:HH21	1:B:187:HIS:CE1	2.33	0.45
1:A:194:ARG:HH21	1:B:187:HIS:HE1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLU:HG3	4:A:1311:HOH:O	2.16	0.45
1:B:173:ASP:O	1:B:175:PRO:HD3	2.17	0.45
1:A:126:ASP:O	1:A:129:VAL:HG22	2.17	0.45
1:A:173:ASP:C	1:A:175:PRO:HD3	2.37	0.45
1:A:11:CYS:O	1:A:94:ARG:HD2	2.16	0.45
1:C:214:LEU:CD1	3:C:3278:MTX:HM2	2.47	0.45
1:B:214:LEU:CD1	3:B:2278:MTX:HM2	2.45	0.45
1:A:187:HIS:HE1	1:B:194:ARG:HH21	1.64	0.45
1:A:25:HIS:ND1	1:A:52:LEU:HD22	2.32	0.45
1:D:43:ARG:NE	4:D:4345:HOH:O	2.43	0.45
1:B:39:VAL:HG22	1:B:65:VAL:CG1	2.46	0.44
1:D:81:CYS:CB	1:D:143:LEU:HD13	2.44	0.44
1:D:17:THR:O	1:D:101:ASN:HB3	2.16	0.44
1:D:65:VAL:HG22	1:D:66:LEU:H	1.81	0.44
1:C:41:HIS:HA	1:C:67:CYS:O	2.18	0.44
1:D:84:ILE:C	1:D:84:ILE:HD13	2.38	0.44
1:C:65:VAL:HG22	1:C:66:LEU:N	2.32	0.44
1:B:125:ILE:HG23	1:B:126:ASP:N	2.33	0.44
1:B:240:ALA:HB2	1:D:259:TYR:CE2	2.53	0.44
1:B:25:HIS:CE1	1:B:52:LEU:HD13	2.53	0.43
1:C:255:LYS:NZ	1:C:255:LYS:HB3	2.33	0.43
1:A:145:ARG:O	1:A:149:ARG:HG3	2.17	0.43
1:B:170:ALA:C	1:B:171:MSE:HE2	2.39	0.43
1:B:43:ARG:HG2	1:B:44:HIS:CE1	2.54	0.43
1:D:171:MSE:HE1	1:D:272:ILE:CB	2.35	0.43
1:D:214:LEU:CD1	3:D:4278:MTX:HM2	2.49	0.43
1:C:73:LEU:HD21	1:C:138:VAL:HG21	2.01	0.43
1:D:255:LYS:HG3	4:D:4322:HOH:O	2.19	0.43
1:A:111:LEU:HD22	1:A:111:LEU:N	2.34	0.43
1:B:201:ALA:N	1:B:202:PRO:CD	2.82	0.43
1:D:73:LEU:HD21	1:D:138:VAL:HG21	2.01	0.42
1:A:52:LEU:O	1:A:56:LEU:HG	2.18	0.42
1:D:17:THR:HA	1:D:41:HIS:HB3	2.00	0.42
1:B:11:CYS:N	4:B:2288:HOH:O	2.51	0.42
1:C:41:HIS:CG	1:C:42:TYR:N	2.85	0.42
1:D:41:HIS:HA	1:D:67:CYS:O	2.19	0.42
1:B:37:ARG:HD2	1:B:92:PHE:CD1	2.54	0.42
1:B:275:ARG:CZ	1:C:171:MSE:HB3	2.50	0.42
1:C:25:HIS:CE1	1:C:52:LEU:HD13	2.55	0.42
1:A:169:ASP:HB3	1:A:172:THR:CG2	2.48	0.42
1:B:123:LYS:HA	1:B:124:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD11	1:B:242:ALA:HB2	2.01	0.42
1:D:43:ARG:O	1:D:68:LYS:HE3	2.19	0.41
1:A:133:PHE:HZ	1:A:184:MSE:HE2	1.84	0.41
1:A:86:ASP:HA	1:A:150:ARG:NH1	2.35	0.41
1:D:43:ARG:CZ	4:D:4345:HOH:O	2.68	0.41
1:B:266:LYS:O	1:D:263:THR:HG21	2.21	0.41
1:B:173:ASP:C	1:B:175:PRO:HD3	2.40	0.41
1:B:30:ARG:NH1	1:B:34:GLN:OE1	2.53	0.41
1:D:173:ASP:C	1:D:175:PRO:HD3	2.40	0.41
1:C:184:MSE:SE	1:D:192:LEU:HD13	2.71	0.41
1:D:199:GLU:HG3	4:D:4312:HOH:O	2.20	0.41
1:C:66:LEU:HD12	1:C:66:LEU:HA	1.86	0.41
1:A:84:ILE:C	1:A:84:ILE:HD13	2.41	0.41
1:D:201:ALA:N	1:D:202:PRO:CD	2.84	0.41
1:C:173:ASP:C	1:C:175:PRO:HD3	2.41	0.41
1:C:136:ASN:HB2	1:C:185:ALA:HB1	2.03	0.41
1:A:20:ALA:HB3	4:A:1291:HOH:O	2.21	0.41
1:D:123:LYS:HA	1:D:124:PRO:HD3	1.87	0.41
1:C:170:ALA:C	1:C:171:MSE:HE2	2.41	0.40
1:C:124:PRO:O	1:C:128:GLN:HG3	2.21	0.40
1:B:30:ARG:HH11	1:B:30:ARG:HG3	1.87	0.40
1:B:14:ALA:HA	1:B:97:VAL:O	2.21	0.40
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.82	0.40
1:C:214:LEU:HD11	1:C:217:LEU:CD2	2.48	0.40
1:B:255:LYS:HB3	1:B:255:LYS:NZ	2.36	0.40
1:B:243:ALA:N	4:B:2309:HOH:O	2.49	0.40
1:A:125:ILE:HG23	1:A:126:ASP:N	2.36	0.40
1:C:192:LEU:HD13	1:D:184:MSE:SE	2.71	0.40
1:A:12:PRO:CA	1:A:94:ARG:HH11	2.32	0.40
1:D:139:ALA:N	1:D:140:PRO:CD	2.85	0.40
1:B:52:LEU:O	1:B:56:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/276 (87%)	229 (95%)	12 (5%)	0	100	100
1	B	241/276 (87%)	233 (97%)	8 (3%)	0	100	100
1	C	241/276 (87%)	228 (95%)	12 (5%)	1 (0%)	39	48
1	D	241/276 (87%)	229 (95%)	12 (5%)	0	100	100
All	All	964/1104 (87%)	919 (95%)	44 (5%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	PRO

### 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	190/206 (92%)	180 (95%)	10 (5%)	28	37
1	B	190/206 (92%)	182 (96%)	8 (4%)	36	49
1	C	190/206 (92%)	180 (95%)	10 (5%)	28	37
1	D	190/206 (92%)	184 (97%)	6 (3%)	46	62
All	All	760/824 (92%)	726 (96%)	34 (4%)	34	46

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	66	LEU
1	A	84	ILE
1	A	143	LEU
1	A	200	LEU
1	A	224	GLU
1	A	231	ARG

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	263	THR
1	A	273	LEU
1	B	84	ILE
1	B	94	ARG
1	B	143	LEU
1	B	200	LEU
1	B	224	GLU
1	B	256	ASP
1	B	263	THR
1	B	273	LEU
1	C	66	LEU
1	C	74	SER
1	C	84	ILE
1	C	94	ARG
1	C	140	PRO
1	C	143	LEU
1	C	231	ARG
1	C	256	ASP
1	C	263	THR
1	C	273	LEU
1	D	84	ILE
1	D	94	ARG
1	D	143	LEU
1	D	200	LEU
1	D	224	GLU
1	D	263	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	187	HIS
1	B	50	GLN
1	B	187	HIS
1	C	50	GLN
1	C	187	HIS
1	D	25	HIS
1	D	50	GLN
1	D	187	HIS
1	D	204	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	NDP	A	1277	-	42,52,52	1.54	4 (9%)	55,80,80	1.72	12 (21%)
3	MTX	A	1278	-	27,35,35	2.76	4 (14%)	30,49,49	1.48	4 (13%)
2	NDP	B	2277	-	42,52,52	1.49	4 (9%)	55,80,80	1.78	12 (21%)
3	MTX	B	2278	-	27,35,35	2.82	5 (18%)	30,49,49	1.54	5 (16%)
2	NDP	C	3277	-	42,52,52	1.53	6 (14%)	55,80,80	1.85	12 (21%)
3	MTX	C	3278	-	27,35,35	2.69	5 (18%)	30,49,49	1.49	2 (6%)
2	NDP	D	4277	-	42,52,52	1.56	6 (14%)	55,80,80	1.80	12 (21%)
3	MTX	D	4278	-	27,35,35	2.61	4 (14%)	30,49,49	1.55	5 (16%)

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	NDP	A	1277	-	-	1/30/77/77	0/5/5/5
3	MTX	A	1278	-	-	0/19/25/25	0/3/3/3
2	NDP	B	2277	-	-	0/30/77/77	0/5/5/5
3	MTX	B	2278	-	-	0/19/25/25	0/3/3/3
2	NDP	C	3277	-	-	1/30/77/77	0/5/5/5
3	MTX	C	3278	-	-	0/19/25/25	0/3/3/3
2	NDP	D	4277	-	-	1/30/77/77	0/5/5/5
3	MTX	D	4278	-	-	0/19/25/25	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3277	NDP	C4N-C5N	-5.51	1.37	1.49
2	A	1277	NDP	C4N-C5N	-5.47	1.37	1.49
2	D	4277	NDP	C4N-C5N	-5.46	1.37	1.49
2	B	2277	NDP	C4N-C5N	-5.28	1.37	1.49
2	D	4277	NDP	P2B-O2X	-2.24	1.46	1.54
2	D	4277	NDP	PA-O1A	-2.24	1.43	1.51
2	A	1277	NDP	PA-O1A	-2.22	1.43	1.51
2	C	3277	NDP	PA-O1A	-2.22	1.43	1.51
2	B	2277	NDP	PA-O1A	-2.18	1.43	1.51
2	C	3277	NDP	C3B-C2B	-2.07	1.48	1.53
2	C	3277	NDP	P2B-O2X	-2.00	1.47	1.54
3	A	1278	MTX	C13-C14	2.00	1.43	1.39
3	D	4278	MTX	C13-C14	2.08	1.43	1.39
3	C	3278	MTX	C4-N3	2.12	1.38	1.33
3	B	2278	MTX	C4-N3	2.16	1.38	1.33
3	C	3278	MTX	C13-C14	2.16	1.43	1.39
3	B	2278	MTX	C2-N3	2.25	1.39	1.35
2	D	4277	NDP	C4A-N3A	2.54	1.39	1.35
2	C	3277	NDP	C6N-C5N	2.68	1.38	1.33
2	B	2277	NDP	C6N-C5N	2.70	1.38	1.33
2	D	4277	NDP	C6N-C5N	2.84	1.38	1.33
3	A	1278	MTX	C6-N5	2.90	1.38	1.32
3	C	3278	MTX	C6-N5	2.91	1.38	1.32
3	B	2278	MTX	C6-N5	2.92	1.38	1.32
2	A	1277	NDP	C6N-C5N	2.92	1.38	1.33
3	D	4278	MTX	C6-N5	2.97	1.38	1.32
2	D	4277	NDP	C2N-C3N	4.10	1.44	1.34
2	C	3277	NDP	C2N-C3N	4.17	1.44	1.34
2	B	2277	NDP	C2N-C3N	4.32	1.45	1.34
2	A	1277	NDP	C2N-C3N	4.43	1.45	1.34
3	D	4278	MTX	C7-C6	5.61	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2278	MTX	C7-C6	6.71	1.50	1.39
3	C	3278	MTX	C7-C6	6.86	1.50	1.39
3	A	1278	MTX	C7-C6	6.97	1.50	1.39
3	C	3278	MTX	C7-N8	10.61	1.50	1.31
3	D	4278	MTX	C7-N8	10.91	1.50	1.31
3	A	1278	MTX	C7-N8	11.04	1.50	1.31
3	B	2278	MTX	C7-N8	11.45	1.51	1.31

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3278	MTX	N1-C2-N3	-5.12	119.64	127.44
3	D	4278	MTX	N1-C2-N3	-5.04	119.77	127.44
2	D	4277	NDP	N3A-C2A-N1A	-4.79	125.23	128.89
2	B	2277	NDP	N3A-C2A-N1A	-4.79	125.23	128.89
3	B	2278	MTX	N1-C2-N3	-4.79	120.15	127.44
3	A	1278	MTX	N1-C2-N3	-4.77	120.18	127.44
2	C	3277	NDP	N3A-C2A-N1A	-4.67	125.32	128.89
2	B	2277	NDP	C3N-C2N-N1N	-4.67	116.46	123.14
2	C	3277	NDP	C3N-C2N-N1N	-4.64	116.50	123.14
2	D	4277	NDP	C3N-C2N-N1N	-4.53	116.65	123.14
2	A	1277	NDP	N3A-C2A-N1A	-4.49	125.45	128.89
2	A	1277	NDP	C3N-C2N-N1N	-4.45	116.77	123.14
2	D	4277	NDP	O5B-C5B-C4B	-2.86	98.58	109.12
2	C	3277	NDP	O2B-P2B-O1X	-2.83	100.04	107.11
2	B	2277	NDP	O5B-C5B-C4B	-2.75	98.98	109.12
2	C	3277	NDP	O5B-C5B-C4B	-2.71	99.13	109.12
2	A	1277	NDP	O7N-C7N-N7N	-2.67	116.13	122.76
2	A	1277	NDP	O5B-C5B-C4B	-2.65	99.33	109.12
2	B	2277	NDP	O7N-C7N-N7N	-2.65	116.19	122.76
2	D	4277	NDP	C4N-C5N-C6N	-2.61	118.28	122.58
2	C	3277	NDP	C4B-O4B-C1B	-2.55	106.92	109.72
2	A	1277	NDP	C4B-O4B-C1B	-2.55	106.92	109.72
2	D	4277	NDP	O7N-C7N-N7N	-2.54	116.44	122.76
2	B	2277	NDP	O2B-P2B-O1X	-2.53	100.78	107.11
2	C	3277	NDP	O7N-C7N-N7N	-2.44	116.69	122.76
2	C	3277	NDP	C4N-C5N-C6N	-2.41	118.60	122.58
2	A	1277	NDP	C4N-C5N-C6N	-2.41	118.61	122.58
2	A	1277	NDP	O2B-P2B-O1X	-2.39	101.14	107.11
2	B	2277	NDP	C4N-C5N-C6N	-2.38	118.65	122.58
2	B	2277	NDP	C4B-O4B-C1B	-2.35	107.14	109.72
2	D	4277	NDP	C4B-O4B-C1B	-2.29	107.21	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4277	NDP	O2B-P2B-O1X	-2.01	102.08	107.11
3	A	1278	MTX	C6-N5-C4A	2.05	121.97	117.62
2	A	1277	NDP	O4B-C1B-N9A	2.13	112.56	108.10
3	B	2278	MTX	C7-N8-C8A	2.17	119.49	116.93
3	B	2278	MTX	C6-N5-C4A	2.18	122.24	117.62
3	D	4278	MTX	C6-N5-C4A	2.20	122.27	117.62
3	A	1278	MTX	N8-C8A-N1	2.39	119.57	116.14
3	B	2278	MTX	C9-C6-N5	2.46	121.13	117.11
3	D	4278	MTX	C7-N8-C8A	2.46	119.83	116.93
3	C	3278	MTX	N8-C8A-N1	2.48	119.69	116.14
3	D	4278	MTX	N8-C8A-N1	2.48	119.69	116.14
3	A	1278	MTX	C9-C6-N5	2.51	121.22	117.11
3	D	4278	MTX	C9-C6-N5	2.57	121.31	117.11
2	B	2277	NDP	O4B-C1B-N9A	2.67	113.68	108.10
3	B	2278	MTX	N8-C8A-N1	2.67	119.96	116.14
2	A	1277	NDP	O4B-C1B-C2B	2.88	111.81	106.60
2	D	4277	NDP	O4B-C1B-N9A	2.89	114.15	108.10
2	B	2277	NDP	O4B-C1B-C2B	3.00	112.03	106.60
2	C	3277	NDP	O4B-C1B-C2B	3.21	112.42	106.60
2	A	1277	NDP	O2B-C2B-C3B	3.42	124.80	111.51
2	D	4277	NDP	O4B-C1B-C2B	3.45	112.85	106.60
2	B	2277	NDP	O2B-C2B-C3B	3.48	125.04	111.51
2	C	3277	NDP	O4B-C1B-N9A	3.66	115.75	108.10
2	C	3277	NDP	O2B-C2B-C3B	3.79	126.26	111.51
2	D	4277	NDP	C5N-C4N-C3N	3.85	123.13	112.52
2	C	3277	NDP	C5N-C4N-C3N	3.89	123.24	112.52
2	D	4277	NDP	O2B-C2B-C3B	3.91	126.70	111.51
2	A	1277	NDP	C5N-C4N-C3N	3.96	123.44	112.52
2	B	2277	NDP	C5N-C4N-C3N	3.99	123.52	112.52
2	A	1277	NDP	P2B-O2B-C2B	4.11	131.42	121.56
2	B	2277	NDP	P2B-O2B-C2B	4.31	131.91	121.56
2	D	4277	NDP	P2B-O2B-C2B	4.52	132.41	121.56
2	C	3277	NDP	P2B-O2B-C2B	4.90	133.30	121.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3277	NDP	P2B-O2B-C2B-C3B
2	A	1277	NDP	P2B-O2B-C2B-C3B
2	D	4277	NDP	P2B-O2B-C2B-C3B

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1278	MTX	1	0
3	B	2278	MTX	2	0
3	C	3278	MTX	1	0
3	D	4278	MTX	2	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 [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	244/276 (88%)	-0.13	5 (2%) 68 75	21, 38, 54, 64	0
1	B	244/276 (88%)	-0.22	4 (1%) 74 80	18, 37, 54, 63	0
1	C	244/276 (88%)	-0.34	3 (1%) 81 85	17, 32, 51, 59	0
1	D	244/276 (88%)	-0.45	2 (0%) 87 90	17, 30, 51, 60	0
All	All	976/1104 (88%)	-0.28	14 (1%) 78 83	17, 34, 53, 64	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	5.9
1	D	62	GLY	4.2
1	C	62	GLY	3.5
1	C	276	ALA	3.2
1	B	223	GLN	3.2
1	A	224	GLU	2.8
1	B	276	ALA	2.8
1	D	276	ALA	2.8
1	B	231	ARG	2.4
1	C	111	LEU	2.3
1	B	224	GLU	2.3
1	A	231	ARG	2.2
1	A	220	ALA	2.1
1	A	223	GLN	2.1

### 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. 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
3	MTX	B	2278	33/33	0.88	0.15	2.46	30,43,69,70	0
3	MTX	D	4278	33/33	0.89	0.13	1.56	15,27,61,63	0
3	MTX	C	3278	33/33	0.88	0.13	1.40	16,27,54,56	0
3	MTX	A	1278	33/33	0.89	0.13	0.90	21,37,63,65	0
2	NDP	C	3277	48/48	0.94	0.11	0.44	18,24,37,40	0
2	NDP	A	1277	48/48	0.94	0.11	0.31	26,34,43,44	0
2	NDP	B	2277	48/48	0.94	0.12	0.31	29,32,44,48	0
2	NDP	D	4277	48/48	0.95	0.10	0.11	18,27,37,39	0

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

There are no such residues in this entry.