



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 09:56 AM EDT

PDB ID : 3SYZ  
Title : Crystal structure of the large fragment of DNA polymerase I from *Thermus Aquaticus* in an open binary complex with dNaM as templating nucleobase  
Authors : Betz, K.; Diederichs, K.; Marx, A.  
Deposited on : 2011-07-18  
Resolution : 1.95 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

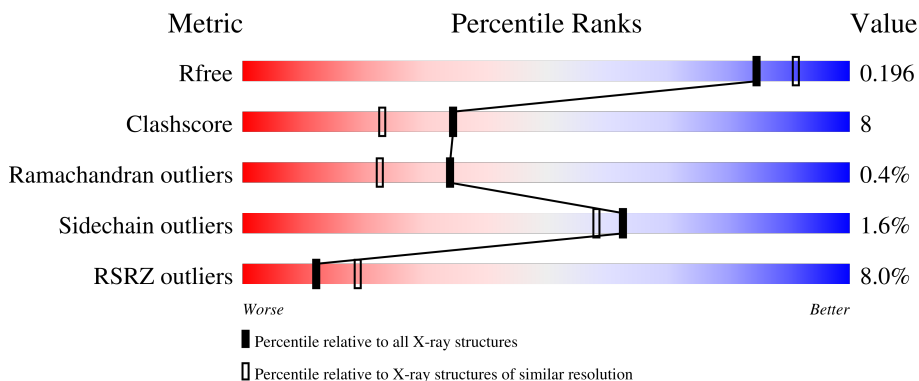
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

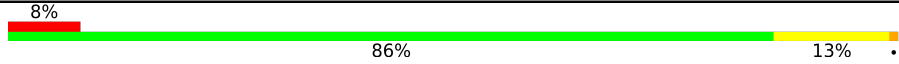


The reported resolution of this entry is 1.95 Å.

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	540	
2	B	12	
3	C	16	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9785 atoms, of which 4480 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 DNA polymerase I, thermostable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	540	8711	2751	4381	779	788	12	0	11	0

- Molecule 2 is a DNA chain called (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	12	252	114	12	48	67	11	0	0	0

- Molecule 3 is a DNA chain called (5'-D(\*AP\*AP\*AP\*(BMN)P\*GP\*GP\*CP\*GP\*CP\*CP\*GP\*TP\*GP\*GP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	16	331	162	61	93	15	0	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

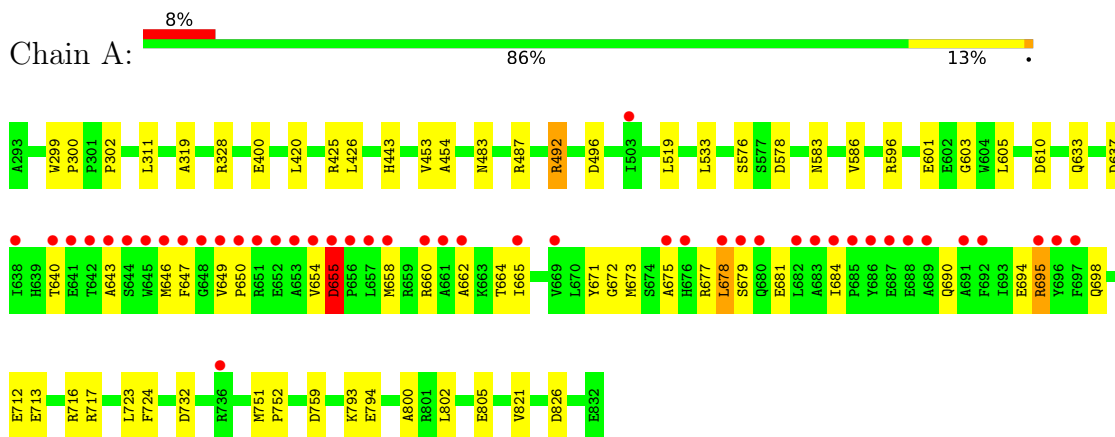
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	268	Total 268	O 268	0	0
7	B	26	Total 26	O 26	0	0
7	C	30	Total 30	O 30	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

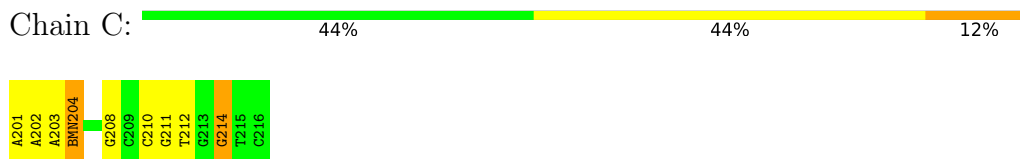
- Molecule 1: DNA polymerase I, thermostable



- Molecule 2: (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*(DOC))-3')



- Molecule 3: (5'-D(\*AP\*AP\*AP\*(BMN)P\*GP\*GP\*CP\*GP\*CP\*CP\*GP\*TP\*GP\*GP\*TP\*C)-3')



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.53Å 108.53Å 90.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.54 – 1.95 46.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.54-1.95) 99.8 (46.54-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.160 , 0.201 0.157 , 0.196	Depositor DCC
$R_{free}$ test set	2256 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, DOC, GOL, BMN, FMT

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	0.34	0/4450	0.49	0/6027
2	B	0.81	0/249	1.35	3/382 (0.8%)
3	C	0.73	0/345	1.29	2/529 (0.4%)
All	All	0.41	0/5044	0.66	5/6938 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	DC	O4'-C1'-N1	7.97	113.58	108.00
3	C	212	DT	O4'-C1'-N1	-7.24	102.94	108.00
2	B	108	DG	O4'-C1'-N9	5.99	112.19	108.00
2	B	108	DG	C1'-O4'-C4'	-5.34	104.76	110.10
3	C	214	DG	C1'-O4'-C4'	-5.25	104.85	110.10

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	4330	4381	4396	68	1
2	B	240	12	134	3	0
3	C	331	0	185	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	7	6	2	0
5	A	30	40	40	3	0
5	C	30	40	40	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	268	0	0	14	1
7	B	26	0	0	0	0
7	C	30	0	0	4	0
All	All	5305	4480	4801	81	1

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 8.

All (81) 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:660:ARG:HD2	3:C:201:DA:H2'	1.56	0.85
2:B:103:DC:H2''	2:B:104:DC:H5'	1.59	0.83
1:A:601:GLU:OE2	7:A:861:HOH:O	2.01	0.79
1:A:643:ALA:HB1	1:A:654:VAL:HG11	1.64	0.78
1:A:671:TYR:CD1	3:C:204:BMN:H38B	2.19	0.76
1:A:732:ASP:OD2	7:A:871:HOH:O	2.06	0.73
3:C:203:DA:H2''	5:C:3:GOL:H31	1.71	0.73
1:A:724:PHE:CD2	7:A:276:HOH:O	2.44	0.71
1:A:717:ARG:NH2	7:A:895:HOH:O	2.24	0.69
2:B:102:DA:H2'	2:B:103:DC:C6	2.29	0.66
3:C:210:DC:H2'	3:C:211:DG:C8	2.33	0.64
1:A:713:GLU:HG3	1:A:716:ARG:NH2	2.13	0.63
3:C:201:DA:H5'	7:C:25:HOH:O	1.98	0.63
1:A:646:MET:O	1:A:647:PHE:CB	2.47	0.62
2:B:103:DC:H2''	2:B:104:DC:C5'	2.28	0.61
3:C:208:DG:N7	5:C:5:GOL:H12	2.19	0.57
1:A:647:PHE:CB	1:A:658:MET:SD	2.94	0.56
1:A:400:GLU:OE2	7:A:901:HOH:O	2.18	0.55
1:A:453:VAL:HB	5:A:834:GOL:H2	1.86	0.55
1:A:633[B]:GLN:OE1	7:A:243:HOH:O	2.18	0.55
1:A:605:LEU:HG	1:A:793:LYS:HG2	1.88	0.55
1:A:643:ALA:CB	1:A:654:VAL:HG11	2.33	0.55
1:A:712:GLU:HG2	7:A:884:HOH:O	2.06	0.55
1:A:649:VAL:CB	1:A:650:PRO:HA	2.38	0.54
1:A:299:TRP:CG	1:A:300:PRO:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:GLU:O	1:A:698:GLN:HG3	2.09	0.53
1:A:713:GLU:HB3	7:A:895:HOH:O	2.08	0.52
1:A:454:ALA:HB2	5:A:834:GOL:H31	1.90	0.52
1:A:603:GLY:O	1:A:793:LYS:HG3	2.08	0.52
1:A:672:GLY:HA3	5:A:2:GOL:H11	1.91	0.52
1:A:671:TYR:CG	3:C:204:BMN:H38B	2.45	0.52
1:A:647:PHE:CB	1:A:658:MET:HG3	2.40	0.51
1:A:673:MET:HB2	1:A:678:LEU:HD21	1.93	0.50
1:A:679:SER:HA	1:A:684:ILE:HG13	1.93	0.50
1:A:643:ALA:HB1	1:A:654:VAL:CG1	2.40	0.50
1:A:578:ASP:HA	5:C:1:GOL:H2	1.93	0.49
1:A:805:GLU:OE2	7:A:273:HOH:O	2.19	0.49
1:A:660:ARG:CD	3:C:201:DA:H2'	2.35	0.49
3:C:202:DA:C2	3:C:204:BMN:H38A	2.48	0.49
1:A:664:THR:O	3:C:204:BMN:H21	2.13	0.49
1:A:637:ASP:OD2	1:A:640:THR:OG1	2.15	0.49
1:A:647:PHE:CB	1:A:658:MET:CG	2.91	0.49
1:A:677:ARG:O	1:A:681:GLU:HB2	2.13	0.48
1:A:695:ARG:HB2	1:A:695:ARG:NH1	2.28	0.48
1:A:519:LEU:HB2	1:A:533:LEU:HD21	1.95	0.48
1:A:655:ASP:C	1:A:655:ASP:OD2	2.52	0.48
1:A:671:TYR:CE1	3:C:204:BMN:H38B	2.47	0.48
1:A:717:ARG:CZ	7:A:895:HOH:O	2.62	0.48
1:A:610[B]:ASP:OD2	7:A:886:HOH:O	2.20	0.47
1:A:633[B]:GLN:NE2	7:A:194:HOH:O	2.46	0.47
1:A:492:ARG:O	1:A:496:ASP:HB2	2.14	0.47
1:A:673:MET:SD	1:A:677:ARG:HD3	2.54	0.47
1:A:662:ALA:HA	1:A:665:ILE:HG22	1.97	0.46
1:A:576:SER:O	3:C:208:DG:H4'	2.15	0.46
1:A:679:SER:HB2	1:A:684:ILE:O	2.14	0.46
1:A:654:VAL:O	1:A:655:ASP:CB	2.63	0.46
1:A:695:ARG:HB2	1:A:695:ARG:CZ	2.46	0.46
1:A:311:LEU:HB3	1:A:319:ALA:HB1	1.99	0.45
1:A:425:ARG:NH2	1:A:723:LEU:O	2.49	0.45
1:A:662:ALA:O	1:A:665:ILE:CG2	2.64	0.45
1:A:299:TRP:CD2	1:A:300:PRO:HA	2.52	0.45
1:A:426[A]:LEU:CD2	7:A:125:HOH:O	2.65	0.45
1:A:802:LEU:C	1:A:802:LEU:HD13	2.38	0.44
1:A:443:HIS:HD1	4:A:5:FMT:C	2.29	0.44
3:C:204:BMN:C38	7:C:222:HOH:O	2.64	0.44
1:A:302:PRO:HG2	1:A:328:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:DG:N7	5:C:2:GOL:O1	2.36	0.43
1:A:800:ALA:HB1	1:A:821:VAL:HG21	2.00	0.43
1:A:426[A]:LEU:HD22	7:A:125:HOH:O	2.18	0.43
1:A:654:VAL:O	1:A:655:ASP:CG	2.57	0.43
3:C:203:DA:H2	7:C:223:HOH:O	2.02	0.43
5:C:5:GOL:H11	7:C:220:HOH:O	2.17	0.43
1:A:673:MET:HB2	1:A:678:LEU:CD2	2.49	0.43
1:A:662:ALA:O	1:A:665:ILE:HG22	2.20	0.42
1:A:675:ALA:CB	1:A:690:GLN:HG2	2.48	0.42
3:C:202:DA:H2	3:C:204:BMN:H38A	1.84	0.42
1:A:724:PHE:CD2	1:A:759:ASP:HB3	2.54	0.42
1:A:483:ASN:HA	4:A:3:FMT:H	2.02	0.42
1:A:596[B]:ARG:NH2	1:A:826:ASP:OD2	2.53	0.42
1:A:751:MET:HB3	1:A:752:PRO:HD3	2.00	0.41
1:A:649:VAL:CB	1:A:650:PRO:CA	2.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794[A]:GLU:OE1	7:A:879:HOH:O[5_554]	2.10	0.10

## 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	549/540 (102%)	527 (96%)	20 (4%)	2 (0%)	34 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	VAL

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Mol	Chain	Res	Type
1	A	655	ASP

### 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	446/441 (101%)	439 (98%)	7 (2%)	62 58

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

Mol	Chain	Res	Type
1	A	420	LEU
1	A	487	ARG
1	A	492	ARG
1	A	583	ASN
1	A	655	ASP
1	A	678	LEU
1	A	695	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	583	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DOC	B	112	3,2	16,19,20	3.00	7 (43%)	20,26,29	1.14	1 (5%)
3	BMN	C	204	3	22,25,26	1.49	2 (9%)	31,35,38	1.81	6 (19%)

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	DOC	B	112	3,2	-	0/7/18/19	0/2/2/2
3	BMN	C	204	3	-	3/9/23/24	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	O2-C2	7.13	1.36	1.23
2	B	112	DOC	C2-N3	5.99	1.48	1.36
3	C	204	BMN	C6-C1	4.56	1.48	1.39
2	B	112	DOC	C5-C4	4.29	1.52	1.42
2	B	112	DOC	C4-N4	4.04	1.43	1.33
3	C	204	BMN	C4-C3	3.00	1.49	1.42
2	B	112	DOC	C6-C5	2.45	1.40	1.35
2	B	112	DOC	O4'-C1'	-2.40	1.36	1.42
2	B	112	DOC	C2-N1	2.09	1.44	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	BMN	C2'-C1'-C1	-6.06	106.05	114.72
3	C	204	BMN	O37-C6-C5	-3.92	120.17	125.24
3	C	204	BMN	O37-C6-C1	3.62	119.29	115.83
3	C	204	BMN	C2-C1-C6	2.65	120.83	117.06
3	C	204	BMN	O4'-C1'-C1	2.45	112.21	109.74
3	C	204	BMN	O4'-C1'-C2'	2.42	107.46	103.57
2	B	112	DOC	O4'-C1'-C2'	2.22	109.07	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	204	BMN	C2-C1-C1'-C2'
3	C	204	BMN	C6-C1-C1'-C2'
3	C	204	BMN	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	204	BMN	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z  > 2$
4	FMT	A	1	-	2,2,2	0.68	0	1,1,1	0.39	0
5	GOL	A	6	-	5,5,5	0.30	0	5,5,5	0.52	0
5	GOL	C	7	-	5,5,5	0.34	0	5,5,5	0.39	0
4	FMT	A	836	-	2,2,2	0.64	0	1,1,1	0.35	0
5	GOL	C	1	-	5,5,5	0.38	0	5,5,5	0.21	0
4	FMT	A	5	-	2,2,2	0.71	0	1,1,1	0.44	0
4	FMT	A	3	-	2,2,2	0.70	0	1,1,1	0.43	0
5	GOL	A	9	-	5,5,5	0.38	0	5,5,5	0.09	0
5	GOL	C	5	-	5,5,5	0.33	0	5,5,5	0.35	0
4	FMT	A	835	-	2,2,2	0.69	0	1,1,1	0.42	0
5	GOL	A	833	-	5,5,5	0.36	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	C	3	-	5,5,5	0.34	0	5,5,5	0.42	0
5	GOL	C	2	-	5,5,5	0.32	0	5,5,5	0.19	0
5	GOL	A	2	-	5,5,5	0.39	0	5,5,5	0.29	0
5	GOL	A	834	-	5,5,5	0.40	0	5,5,5	0.37	0
4	FMT	A	7	-	2,2,2	0.67	0	1,1,1	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	6	-	-	0/4/4/4	-
5	GOL	C	7	-	-	1/4/4/4	-
5	GOL	C	1	-	-	2/4/4/4	-
5	GOL	A	9	-	-	4/4/4/4	-
5	GOL	C	5	-	-	4/4/4/4	-
5	GOL	A	833	-	-	3/4/4/4	-
5	GOL	C	3	-	-	1/4/4/4	-
5	GOL	C	2	-	-	2/4/4/4	-
5	GOL	A	2	-	-	2/4/4/4	-
5	GOL	A	834	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	833	GOL	O1-C1-C2-C3
5	A	9	GOL	O1-C1-C2-C3
5	C	2	GOL	O1-C1-C2-C3
5	C	5	GOL	O1-C1-C2-C3
5	C	1	GOL	O1-C1-C2-C3
5	A	834	GOL	C1-C2-C3-O3
5	A	9	GOL	C1-C2-C3-O3
5	A	2	GOL	O1-C1-C2-C3
5	C	5	GOL	C1-C2-C3-O3
5	A	833	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	834	GOL	O2-C2-C3-O3
5	A	9	GOL	O1-C1-C2-O2
5	C	2	GOL	O1-C1-C2-O2
5	C	5	GOL	O1-C1-C2-O2
5	C	5	GOL	O2-C2-C3-O3
5	C	1	GOL	O1-C1-C2-O2
5	A	833	GOL	C1-C2-C3-O3
5	C	7	GOL	O1-C1-C2-C3
5	A	2	GOL	O1-C1-C2-O2
5	A	9	GOL	O2-C2-C3-O3
5	C	3	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	GOL	1	0
4	A	5	FMT	1	0
4	A	3	FMT	1	0
5	C	5	GOL	2	0
5	C	3	GOL	1	0
5	C	2	GOL	1	0
5	A	2	GOL	1	0
5	A	834	GOL	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

### 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	540/540 (100%)	0.37	45 (8%) <span style="border: 1px solid red; padding: 2px;">11</span> <span style="border: 1px solid red; padding: 2px;">17</span>	22, 33, 101, 157	0
2	B	11/12 (91%)	-0.40	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	26, 31, 57, 58	0
3	C	15/16 (93%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 33, 62, 133	0
All	All	566/568 (99%)	0.34	45 (7%) <span style="border: 1px solid red; padding: 2px;">12</span> <span style="border: 1px solid red; padding: 2px;">19</span>	22, 34, 100, 157	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	649	VAL	11.7
1	A	644	SER	11.3
1	A	654	VAL	10.3
1	A	648	GLY	8.6
1	A	653	ALA	8.5
1	A	650	PRO	8.3
1	A	652	GLU	8.3
1	A	692	PHE	8.0
1	A	658	MET	7.6
1	A	647	PHE	7.3
1	A	685	PRO	6.6
1	A	643	ALA	6.4
1	A	646	MET	6.4
1	A	688	GLU	6.4
1	A	665	ILE	6.1
1	A	651	ARG	5.8
1	A	645	TRP	5.4
1	A	683	ALA	5.1
1	A	684	ILE	5.0
1	A	642	THR	4.6
1	A	687	GLU	4.4
1	A	657	LEU	4.2
1	A	686	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	655	ASP	3.4
1	A	682	LEU	3.4
1	A	675	ALA	3.1
1	A	680	GLN	3.1
1	A	689	ALA	3.0
1	A	676	HIS	3.0
1	A	669	VAL	2.8
1	A	678	LEU	2.7
1	A	638	ILE	2.6
1	A	695	ARG	2.5
1	A	691	ALA	2.5
1	A	640	THR	2.5
1	A	697	PHE	2.4
1	A	662	ALA	2.4
1	A	679	SER	2.3
1	A	736	ARG	2.3
1	A	661	ALA	2.3
1	A	656	PRO	2.3
1	A	696	TYR	2.2
1	A	660	ARG	2.2
1	A	503	ILE	2.1
1	A	641	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	BMN	C	204	23/24	0.95	0.13	41,58,71,88	0
2	DOC	B	112	18/19	0.98	0.12	25,31,36,40	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	GOL	A	834	6/6	0.75	0.30	33,45,54,54	14
4	FMT	A	836	3/3	0.77	0.29	41,50,60,73	0
4	FMT	A	1	3/3	0.78	0.16	43,57,63,69	0
4	FMT	A	835	3/3	0.78	0.29	43,61,62,75	0
5	GOL	C	5	6/6	0.81	0.22	39,58,69,72	0
5	GOL	C	3	6/6	0.84	0.14	56,69,80,83	0
5	GOL	C	2	6/6	0.85	0.14	55,66,75,79	0
4	FMT	A	3	3/3	0.87	0.14	56,65,73,78	0
5	GOL	C	1	6/6	0.88	0.23	35,72,87,87	0
5	GOL	A	833	6/6	0.88	0.17	44,58,69,78	0
5	GOL	A	9	6/6	0.90	0.17	58,85,97,102	0
5	GOL	C	7	6/6	0.91	0.15	48,66,71,80	0
4	FMT	A	7	3/3	0.91	0.10	50,62,63,75	0
5	GOL	A	2	6/6	0.91	0.23	47,68,82,85	0
6	MG	A	837	1/1	0.91	0.20	64,64,64,64	0
4	FMT	A	5	3/3	0.94	0.08	44,48,58,62	0
5	GOL	A	6	6/6	0.95	0.10	31,37,44,44	0
6	MG	B	1	1/1	0.95	0.06	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.