



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:17 PM GMT

PDB ID : 5CDO
Title : 3.15A structure of QPT-1 with S.aureus DNA gyrase and DNA
Authors : Bax, B.D.; Srikannathasan, V.; Chan, P.F.
Deposited on : 2015-07-04
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

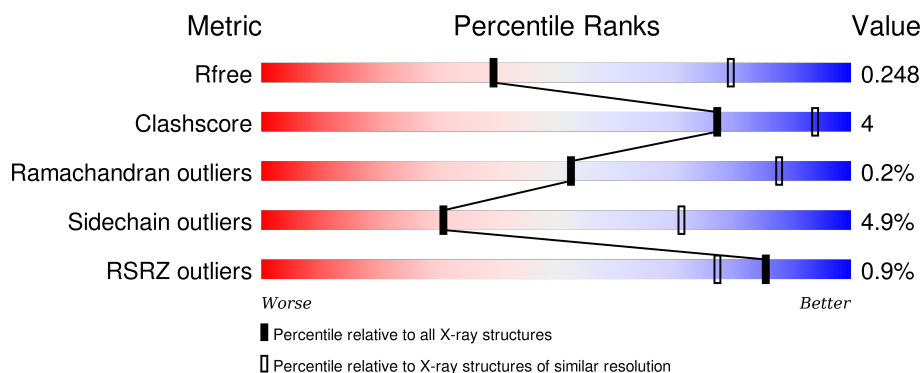
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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 ≥ 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	482	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	C	482	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	R	482	<div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	T	482	<div> <div>88%</div> <div>12%</div> </div>
2	B	188	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	188	
2	S	188	
2	U	188	
3	E	20	
3	F	20	
3	V	20	
3	W	20	

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
5	NA	A	502	-	-	-	X
6	GOL	D	1002	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 44495 atoms, of which 21756 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 gyrase subunit A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	482	Total	C	H	N	O	P	S	0	4	0
			7629	2365	3821	693	733	1	16			
1	C	480	Total	C	H	N	O	P	S	0	0	0
			7623	2358	3832	690	726	1	16			
1	R	477	Total	C	H	N	O	P	S	0	1	0
			7503	2336	3752	676	722	1	16			
1	T	481	Total	C	H	N	O	P	S	0	0	0
			7522	2340	3755	680	731	1	15			

- Molecule 2 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	188	Total	C	H	N	O	S	0	0	0
			2869	912	1413	251	284	9			
2	D	188	Total	C	H	N	O	S	0	0	0
			2861	910	1412	251	279	9			
2	S	188	Total	C	H	N	O	S	0	0	0
			2832	904	1395	250	274	9			
2	U	187	Total	C	H	N	O	S	0	0	0
			2838	902	1399	253	275	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	GLY	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	VAL	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	ARG	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TRP	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	ILE	deletion	UNP P66937
B	544	THR	ALA	linker	UNP P66937
B	545	GLY	ARG	linker	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	GLY	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	VAL	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	ARG	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASN	deletion	UNP P66937
D	?	-	PRO	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937
D	?	-	PRO	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TRP	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	ILE	deletion	UNP P66937
D	544	THR	ALA	linker	UNP P66937
D	545	GLY	ARG	linker	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	THR	deletion	UNP P66937
S	?	-	GLN	deletion	UNP P66937
S	?	-	GLY	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	GLN	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	VAL	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	ASN	deletion	UNP P66937
S	?	-	ASP	deletion	UNP P66937
S	?	-	ARG	deletion	UNP P66937
S	?	-	GLU	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	ASP	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	LYS	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	SER	deletion	UNP P66937
S	?	-	GLU	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	ASN	deletion	UNP P66937
S	?	-	PRO	deletion	UNP P66937
S	?	-	THR	deletion	UNP P66937
S	?	-	PRO	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	TRP	deletion	UNP P66937
S	?	-	SER	deletion	UNP P66937
S	?	-	ILE	deletion	UNP P66937
S	544	THR	ALA	linker	UNP P66937
S	545	GLY	ARG	linker	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	THR	deletion	UNP P66937
U	?	-	GLN	deletion	UNP P66937
U	?	-	GLY	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	GLN	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	VAL	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	ASN	deletion	UNP P66937
U	?	-	ASP	deletion	UNP P66937
U	?	-	ARG	deletion	UNP P66937
U	?	-	GLU	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	ASP	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	SER	deletion	UNP P66937
U	?	-	GLU	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937

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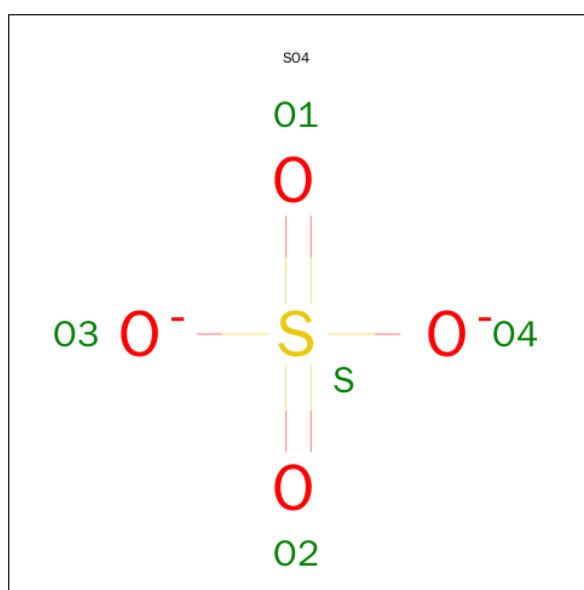
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Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	ASN	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	THR	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	TRP	deletion	UNP P66937
U	?	-	SER	deletion	UNP P66937
U	?	-	ILE	deletion	UNP P66937
U	544	THR	ALA	linker	UNP P66937
U	545	GLY	ARG	linker	UNP P66937

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	20	Total	C	H	N	O	P	0	0	0
			602	185	210	74	114	19			
3	F	20	Total	C	H	N	O	P	0	0	0
			629	194	222	76	118	19			
3	V	20	Total	C	H	N	O	P	0	0	0
			630	194	223	76	118	19			
3	W	20	Total	C	H	N	O	P	0	0	0
			601	184	210	74	114	19			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

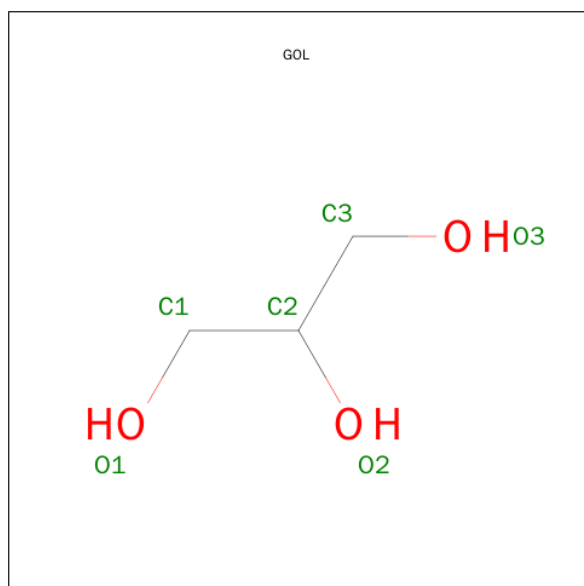


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	T	1	Total O S 5 4 1	0	0
4	T	1	Total O S 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0
5	T	1	Total Na 1 1	0	0
5	C	2	Total Na 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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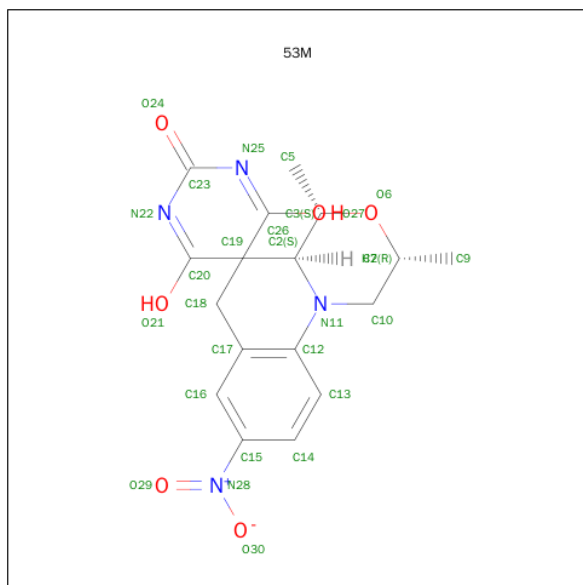
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	U	1	Total	C	H	O	0	0
			14	3	8	3		
6	U	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

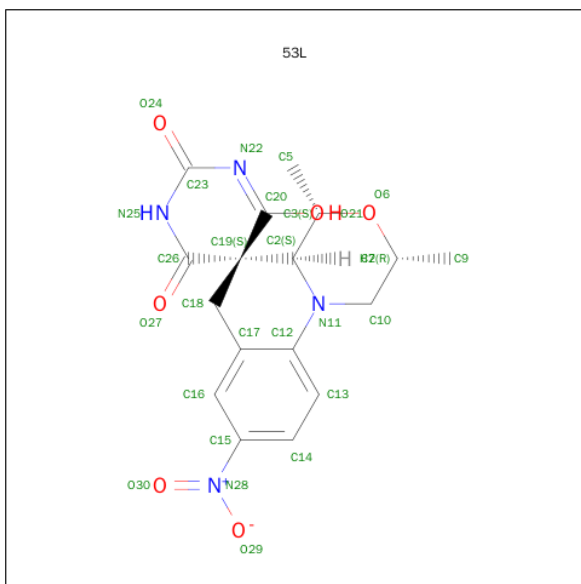
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mn	0	0
			1	1		
7	D	1	Total	Mn	0	0
			1	1		
7	S	1	Total	Mn	0	0
			1	1		
7	U	1	Total	Mn	0	0
			1	1		

- Molecule 8 is (2R,4S,4aS)-4',6'-dihydroxy-2,4-dimethyl-8-nitro-1,2,4,4a-tetrahydro-2'H,6H-spiro[1,4-oxazino[4,3-a]quinoline-5,5'-pyrimidin]-2'-one (three-letter code: 53M) (formula: C₁₇H₁₈N₄O₆).



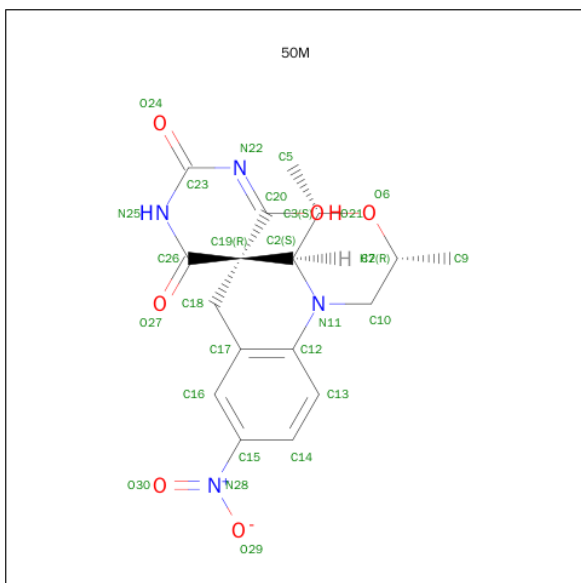
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	H	N	O	0	0
			45	17	18	4	6		
8	W	1	Total	C	H	N	O	0	0
			45	17	18	4	6		

- Molecule 9 is (2R,4S,4aS,5S)-6'-hydroxy-2,4-dimethyl-8-nitro-1,2,4,4a-tetrahydro-2'H,6H-spiro[1,4-oxazino[4,3-a]quinoline-5,5'-pyrimidine]-2',4'(3'H)-dione (three-letter code: 53L) (formula: C₁₇H₁₈N₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	F	1	45	17	18	4	6	0	0

- Molecule 10 is (2R,4S,4aS,5R)-6'-hydroxy-2,4-dimethyl-8-nitro-1,2,4,4a-tetrahydro-2'H,6H-spiro[1,4-oxazino[4,3-a]quinoline-5,5'-pyrimidine]-2',4'(3'H)-dione (three-letter code: 50M) (formula: C₁₇H₁₈N₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	S	1	Total	C	H	N	O	0	0
			45	17	18	4	6		

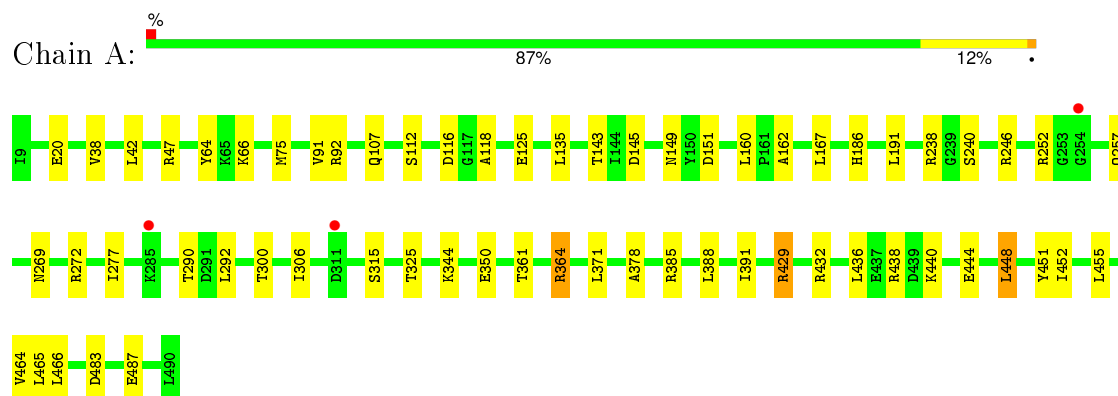
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	10	Total	O	0	0
			10	10		
11	B	5	Total	O	0	0
			5	5		
11	C	4	Total	O	0	0
			4	4		
11	D	4	Total	O	0	0
			4	4		
11	E	2	Total	O	0	0
			2	2		
11	F	3	Total	O	0	0
			3	3		
11	R	13	Total	O	0	0
			13	13		
11	S	9	Total	O	0	0
			9	9		
11	T	15	Total	O	0	0
			15	15		
11	U	7	Total	O	0	0
			7	7		
11	V	4	Total	O	0	0
			4	4		
11	W	6	Total	O	0	0
			6	6		

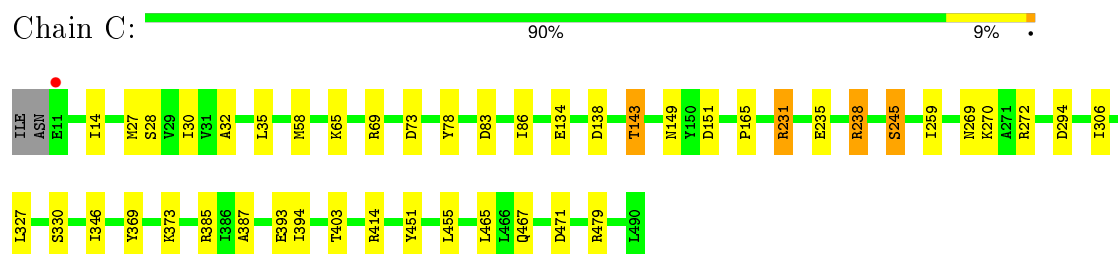
3 Residue-property plots

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.

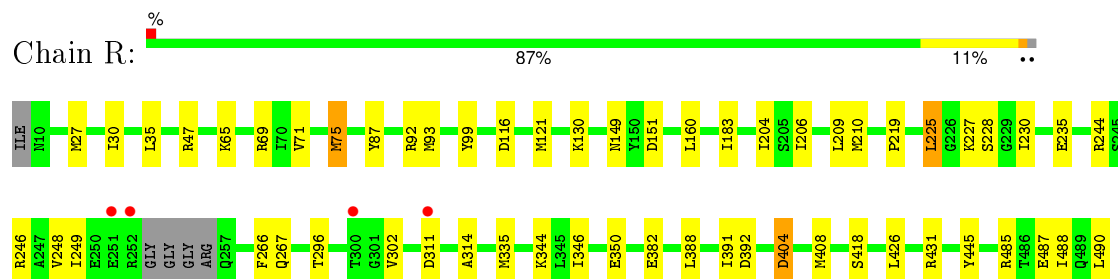
- Molecule 1: DNA gyrase subunit A



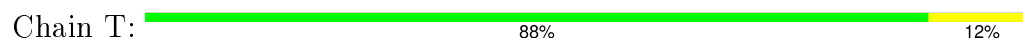
- Molecule 1: DNA gyrase subunit A

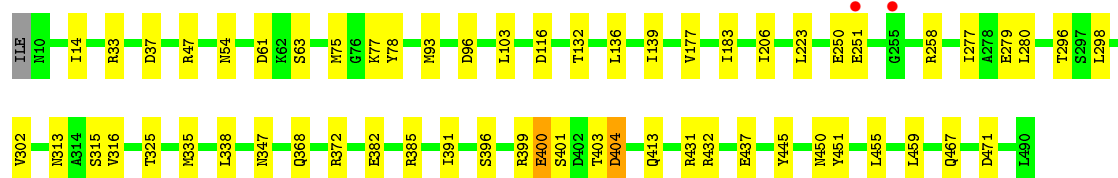


- Molecule 1: DNA gyrase subunit A

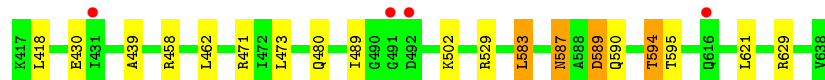
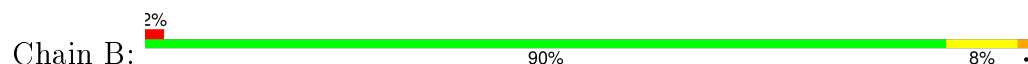


- Molecule 1: DNA gyrase subunit A

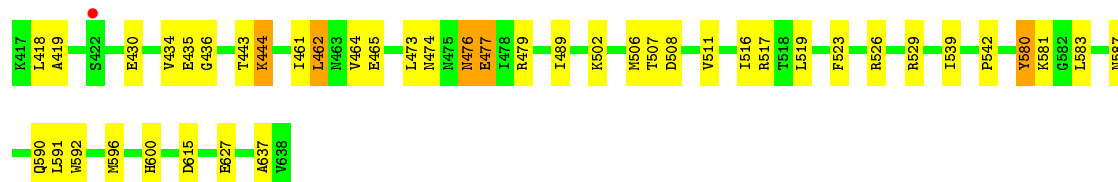




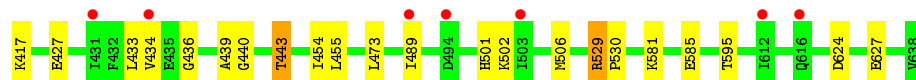
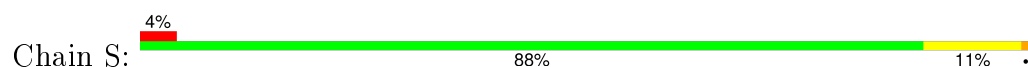
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



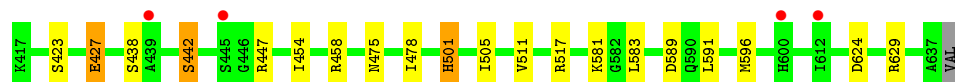
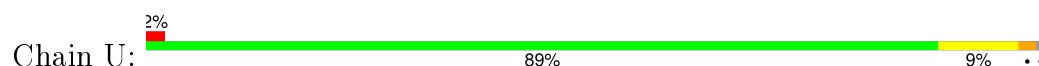
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

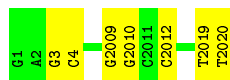


- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')





- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.47Å 170.21Å 124.58Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	58.41 – 3.15 58.41 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.41-3.15) 98.1 (58.41-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.246 0.221 , 0.248	Depositor DCC
R_{free} test set	2511 reflections (4.20%)	DCC
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 62348 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	44495	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 50M, NA, 53M, 53L, SO4, MN, PTR

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	0.26	0/3854	0.50	0/5195
1	C	0.26	0/3821	0.51	1/5149 (0.0%)
1	R	0.25	0/3779	0.49	0/5098
1	T	0.25	0/3797	0.50	0/5126
2	B	0.26	0/1479	0.48	0/2000
2	D	0.28	0/1472	0.53	0/1990
2	S	0.25	0/1460	0.46	0/1974
2	U	0.25	0/1462	0.49	0/1977
3	E	0.63	0/438	0.89	0/673
3	F	0.76	0/455	0.95	0/699
3	V	0.62	0/455	0.93	0/699
3	W	0.76	0/437	0.96	0/672
All	All	0.31	0/22909	0.55	1/31252 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ARG	NE-CZ-NH1	5.53	123.06	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	3808	3821	3801	29	0
1	C	3791	3832	3832	21	0
1	R	3751	3752	3752	27	0
1	T	3767	3755	3755	25	0
2	B	1456	1413	1413	8	0
2	D	1449	1412	1412	21	0
2	S	1437	1395	1395	9	0
2	U	1439	1399	1399	6	0
3	E	392	210	211	5	0
3	F	407	222	224	6	0
3	V	407	223	224	7	0
3	W	391	210	211	10	0
4	A	5	0	0	1	0
4	T	10	0	0	1	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	R	1	0	0	0	0
5	T	1	0	0	0	0
6	A	6	8	8	1	0
6	D	12	16	16	1	0
6	U	12	16	16	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	S	1	0	0	0	0
7	U	1	0	0	0	0
8	E	27	18	16	4	0
8	W	27	18	16	5	0
9	F	27	18	17	3	0
10	S	27	18	17	4	0
11	A	10	0	0	2	0
11	B	5	0	0	0	0
11	C	4	0	0	0	0
11	D	4	0	0	0	0
11	E	2	0	0	1	0
11	F	3	0	0	0	0
11	R	13	0	0	0	0
11	S	9	0	0	0	0
11	T	15	0	0	0	0
11	U	7	0	0	0	0
11	V	4	0	0	0	0
11	W	6	0	0	0	0
All	All	22739	21756	21735	165	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.

The worst 5 of 165 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:GLN:O	2:B:594:THR:OG1	2.03	0.75
1:C:134:GLU:OE1	1:C:479:ARG:NH2	2.19	0.75
8:E:2101:53M:C26	8:E:2101:53M:H52	2.19	0.73
1:R:404:ASP:OD2	1:T:431:ARG:NH2	2.24	0.70
1:A:252:ARG:NH1	1:T:471:ASP:OD2	2.25	0.69

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	483/482 (100%)	460 (95%)	23 (5%)	0	100	100
1	C	477/482 (99%)	443 (93%)	33 (7%)	1 (0%)	52	88
1	R	473/482 (98%)	449 (95%)	24 (5%)	0	100	100
1	T	478/482 (99%)	460 (96%)	17 (4%)	1 (0%)	52	88
2	B	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
2	D	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	17	61
2	S	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
2	U	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
All	All	2654/2680 (99%)	2527 (95%)	123 (5%)	4 (0%)	52	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	476	ASN
1	T	33	ARG

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Mol	Chain	Res	Type
2	D	462	LEU
1	C	165	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	408/416 (98%)	389 (95%)	19 (5%)	32	72
1	C	407/416 (98%)	395 (97%)	12 (3%)	50	83
1	R	399/416 (96%)	386 (97%)	13 (3%)	45	80
1	T	401/416 (96%)	379 (94%)	22 (6%)	27	66
2	B	152/157 (97%)	143 (94%)	9 (6%)	24	63
2	D	150/157 (96%)	138 (92%)	12 (8%)	15	50
2	S	146/157 (93%)	136 (93%)	10 (7%)	20	57
2	U	148/157 (94%)	136 (92%)	12 (8%)	15	49
All	All	2211/2292 (96%)	2102 (95%)	109 (5%)	31	71

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	600	HIS
1	R	404	ASP
2	U	454	ILE
2	D	615	ASP
1	R	210	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	T	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PTR	A	123	1,3	13,16,17	1.31	2 (15%)	19,22,24	0.72	1 (5%)
1	PTR	C	123	1,3	13,16,17	1.34	1 (7%)	19,22,24	0.78	2 (10%)
1	PTR	R	123	1,3	13,16,17	1.13	1 (7%)	19,22,24	0.85	2 (10%)
1	PTR	T	123	1,3	13,16,17	1.08	1 (7%)	19,22,24	0.76	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	123	1,3	-	0/9/11/13	0/1/1/1
1	PTR	C	123	1,3	-	0/9/11/13	0/1/1/1
1	PTR	R	123	1,3	-	0/9/11/13	0/1/1/1
1	PTR	T	123	1,3	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	PTR	OH-CZ	-4.21	1.30	1.40
1	A	123	PTR	OH-CZ	-3.98	1.31	1.40
1	R	123	PTR	OH-CZ	-3.83	1.31	1.40
1	T	123	PTR	OH-CZ	-3.68	1.31	1.40
1	A	123	PTR	P-O2P	-2.01	1.47	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	PTR	O-C-CA	-2.38	119.35	125.72
1	R	123	PTR	O-C-CA	-2.32	119.51	125.72
1	T	123	PTR	O-C-CA	-2.32	119.51	125.72
1	C	123	PTR	O-C-CA	-2.05	120.22	125.72
1	R	123	PTR	O2P-P-OH	2.04	111.97	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	SO4	A	501	-	4,4,4	0.18	0	6,6,6	0.06	0
6	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.28	0
6	GOL	D	1002	-	5,5,5	0.20	0	5,5,5	0.20	0
6	GOL	D	1003	-	5,5,5	0.43	0	5,5,5	0.19	0
8	53M	E	2101	-	22,30,30	0.97	2 (9%)	23,47,47	1.57	4 (17%)
9	53L	F	2101	-	24,30,30	1.20	2 (8%)	29,47,47	1.73	7 (24%)
10	50M	S	6002	-	24,30,30	1.10	2 (8%)	29,47,47	2.28	10 (34%)
4	SO4	T	501	-	4,4,4	0.16	0	6,6,6	0.07	0
4	SO4	T	502	-	4,4,4	0.18	0	6,6,6	0.08	0
6	GOL	U	5002	-	5,5,5	0.32	0	5,5,5	0.28	0
6	GOL	U	5003	-	5,5,5	0.29	0	5,5,5	0.34	0
8	53M	W	2101	-	22,30,30	0.96	1 (4%)	23,47,47	1.83	6 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	501	-	-	0/0/0/0	0/0/0/0
6	GOL	A	503	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1002	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1003	-	-	0/4/4/4	0/0/0/0
8	53M	E	2101	-	-	0/4/55/55	0/3/4/4
9	53L	F	2101	-	-	0/4/55/55	0/4/4/4
10	50M	S	6002	-	-	0/4/55/55	0/4/4/4
4	SO4	T	501	-	-	0/0/0/0	0/0/0/0
4	SO4	T	502	-	-	0/0/0/0	0/0/0/0
6	GOL	U	5002	-	-	0/4/4/4	0/0/0/0
6	GOL	U	5003	-	-	0/4/4/4	0/0/0/0
8	53M	W	2101	-	-	0/4/55/55	0/3/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	2101	53L	C19-C26	-3.70	1.48	1.52
10	S	6002	50M	C19-C26	-3.13	1.49	1.52
9	F	2101	53L	C18-C19	-2.59	1.48	1.54
10	S	6002	50M	C18-C19	-2.31	1.49	1.54
8	W	2101	53M	C18-C19	-2.20	1.49	1.54

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S	6002	50M	O30-N28-C15	-6.28	114.14	118.67
10	S	6002	50M	C19-C26-N25	-4.84	112.31	117.58
8	W	2101	53M	C7-C10-N11	-4.01	100.97	109.10
8	W	2101	53M	O29-N28-C15	-3.95	115.82	118.67
10	S	6002	50M	C14-C15-N28	-3.48	117.01	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	SO4	1	0
6	A	503	GOL	1	0
6	D	1002	GOL	1	0
8	E	2101	53M	4	0
9	F	2101	53L	3	0
10	S	6002	50M	4	0
4	T	502	SO4	1	0
8	W	2101	53M	5	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, 95th 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 ²)	Q<0.9
1	A	481/482 (99%)	-0.08	3 (0%) 90 84	25, 42, 62, 81	0
1	C	479/482 (99%)	-0.16	1 (0%) 95 94	22, 37, 59, 87	0
1	R	476/482 (98%)	-0.09	4 (0%) 87 79	24, 39, 94, 135	0
1	T	480/482 (99%)	-0.07	2 (0%) 93 90	23, 38, 75, 106	0
2	B	188/188 (100%)	0.16	4 (2%) 67 50	27, 55, 78, 87	0
2	D	188/188 (100%)	0.16	1 (0%) 91 87	30, 55, 74, 84	0
2	S	188/188 (100%)	0.30	7 (3%) 45 28	29, 63, 89, 95	0
2	U	187/188 (99%)	0.08	4 (2%) 67 50	33, 56, 73, 81	0
3	E	20/20 (100%)	0.09	0 100 100	30, 36, 56, 64	0
3	F	20/20 (100%)	0.22	0 100 100	31, 36, 47, 47	0
3	V	20/20 (100%)	0.09	0 100 100	32, 42, 60, 68	0
3	W	20/20 (100%)	0.08	0 100 100	31, 39, 66, 69	0
All	All	2747/2760 (99%)	-0.02	26 (0%) 85 77	22, 43, 76, 135	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	252	ARG	4.7
2	S	503	ILE	3.3
2	S	431	ILE	3.2
2	B	492	ASP	3.1
2	S	612	ILE	3.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	R	123	16/17	0.96	0.21	-	34,40,46,48	0
1	PTR	A	123	16/17	0.95	0.21	-	32,37,43,44	0
1	PTR	T	123	16/17	0.94	0.21	-	43,50,56,60	0
1	PTR	C	123	16/17	0.94	0.21	-	35,42,47,50	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	D	1002	6/6	0.91	0.33	3.13	39,47,49,49	0
5	NA	A	502	1/1	0.82	0.33	2.02	39,39,39,39	0
6	GOL	A	503	6/6	0.84	0.31	1.95	30,36,39,39	0
8	53M	E	2101	27/27	0.92	0.24	1.35	18,22,25,28	0
6	GOL	U	5002	6/6	0.93	0.25	1.30	33,40,42,43	0
10	50M	S	6002	27/27	0.90	0.23	1.21	18,21,25,27	0
5	NA	C	502	1/1	0.81	0.29	0.96	30,30,30,30	0
5	NA	T	503	1/1	0.79	0.25	0.94	43,43,43,43	0
9	53L	F	2101	27/27	0.93	0.21	0.34	19,21,26,29	0
8	53M	W	2101	27/27	0.92	0.24	0.28	19,21,25,28	0
5	NA	R	501	1/1	0.85	0.23	-0.00	40,40,40,40	0
6	GOL	D	1003	6/6	0.86	0.22	-0.17	47,57,58,58	0
4	SO4	T	502	5/5	0.93	0.19	-0.57	54,55,56,56	0
7	MN	U	5001	1/1	0.99	0.17	-0.93	37,37,37,37	0
7	MN	B	701	1/1	0.99	0.15	-1.50	37,37,37,37	0
6	GOL	U	5003	6/6	0.90	0.14	-1.88	55,66,67,67	0
7	MN	S	6001	1/1	1.00	0.13	-1.89	35,35,35,35	0
7	MN	D	1001	1/1	0.99	0.16	-2.58	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NA	C	501	1/1	0.96	0.26	-	19,19,19,19	0
4	SO4	A	501	5/5	0.95	0.17	-	65,65,66,66	0
4	SO4	T	501	5/5	0.94	0.13	-	55,56,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.