Full wwPDB X-ray Structure Validation Report (i)

Jul 27, 2021 – 03:25 pm BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The following versions of software and data (see references (i)) 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	:	2.22
buster-report	:	1.1.7 (2018)
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)	:	2.22

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.
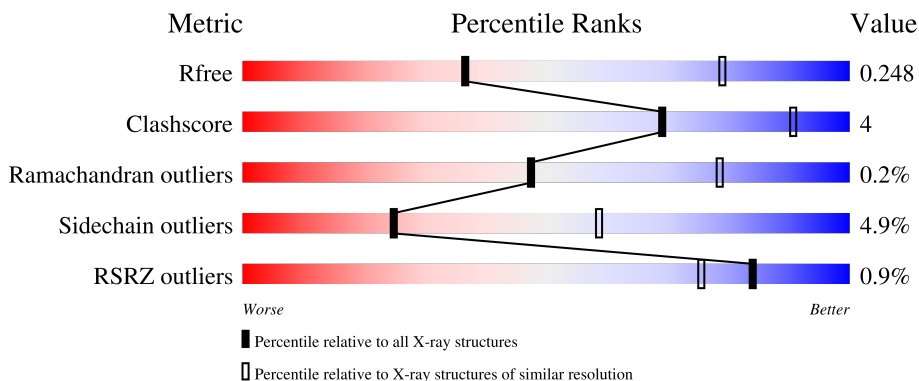
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	% 87% 12% •
1	C	482	90% 9% •
1	R	482	% 87% 11% ••
1	T	482	87% 12%
2	B	188	2% 90% 8% •

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Mol	Chain	Length	Quality of chain
2	D	188	77% 20%
2	S	188	4% 88% 11%
2	U	188	2% 89% 9%
3	E	20	75% 25%
3	F	20	65% 35%
3	V	20	65% 35%
3	W	20	65% 35%

2 Entry composition (i)

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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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: O_4S).
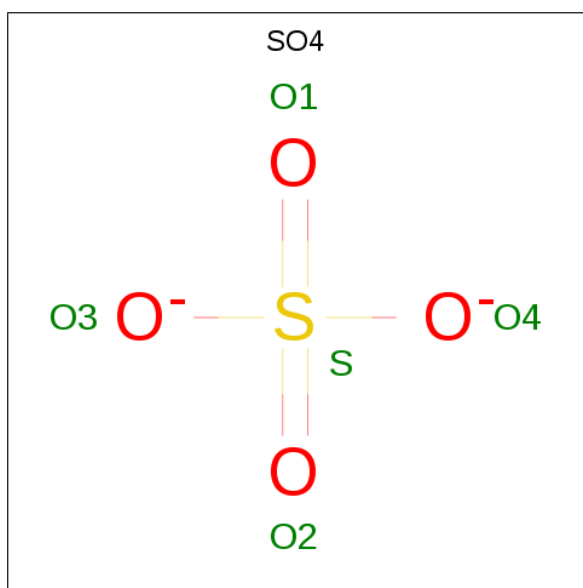
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	T	1	Total 5	O 4	S 1	0	0
4	T	1	Total 5	O 4	S 1	0	0

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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
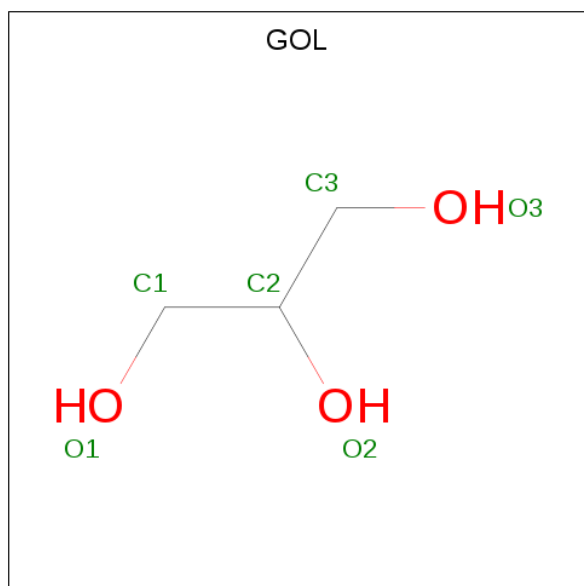
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 3	H 8	O 3	0	0
6	D	1	Total 14	C 3	H 8	O 3	0	0
6	D	1	Total 14	C 3	H 8	O 3	0	0

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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: $C_{17}H_{18}N_4O_6$).
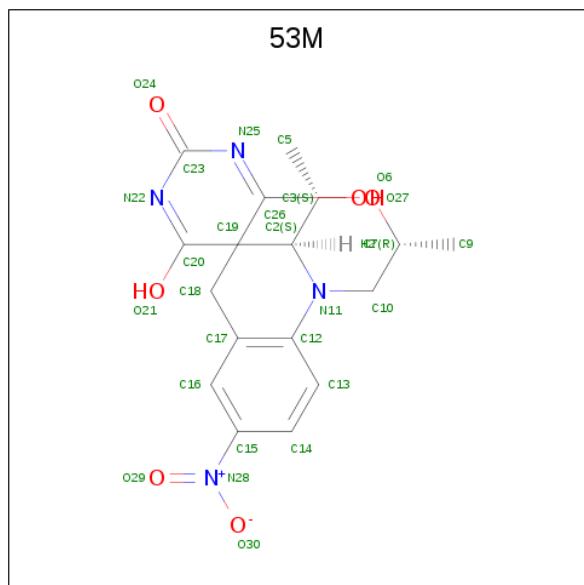
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	H	N	O	0	0
			45	17	18	4	6		
8	W	1	Total	C	H	N	O	0	0
			45	17	18	4	6		

- 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: $C_{17}H_{18}N_4O_6$).
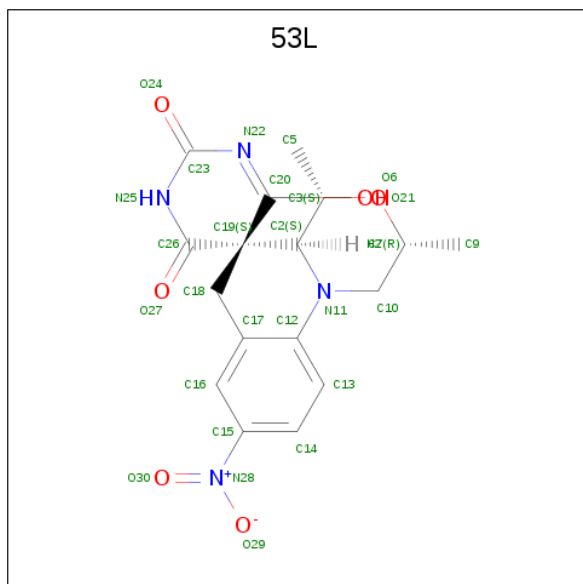
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	F	1	45	17	18	4	6	0	0

- 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: $C_{17}H_{18}N_4O_6$).

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

- Molecule 11 is water.

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

3 Residue-property plots ⓘ

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.
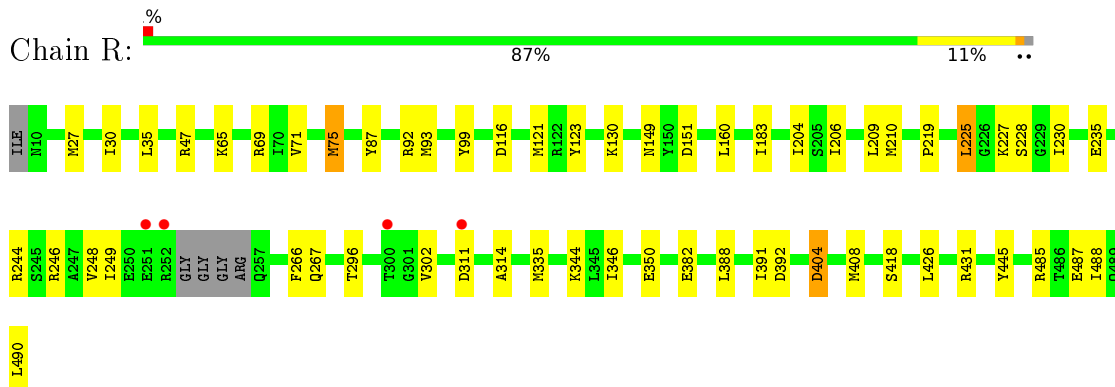
• Molecule 1: DNA gyrase subunit A
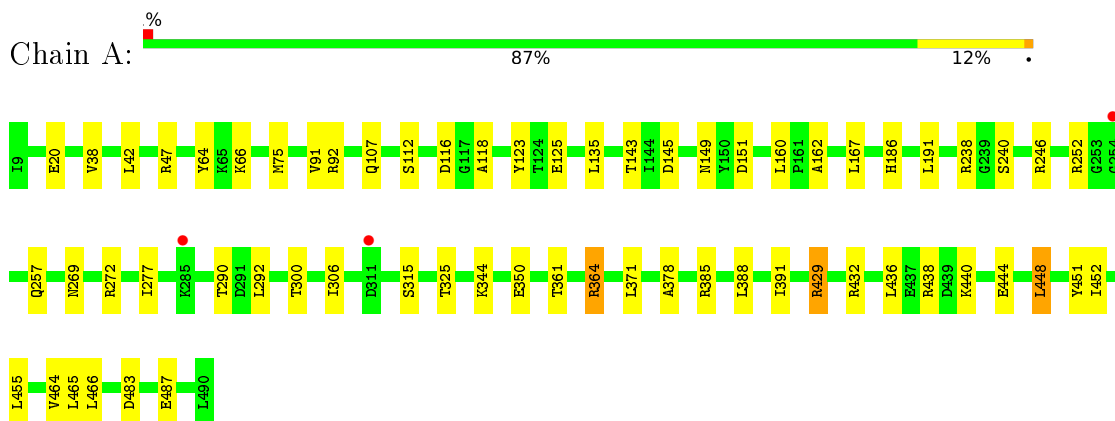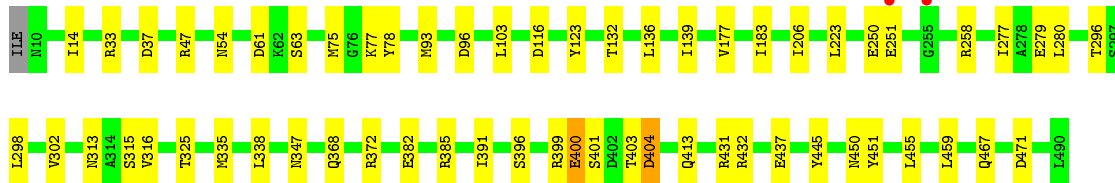
Chain A:

• Molecule 1: DNA gyrase subunit A
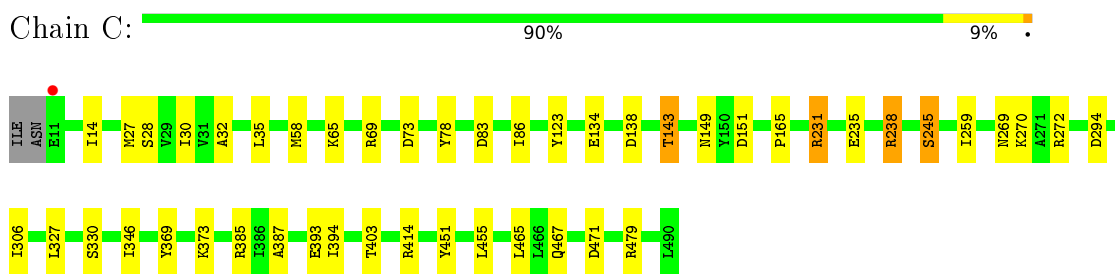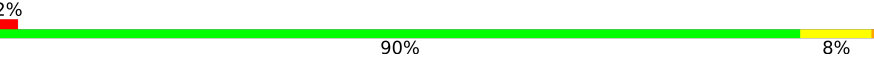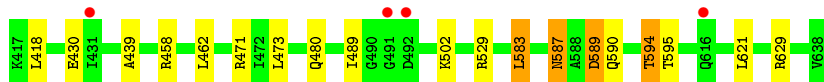
Chain C:

• Molecule 1: DNA gyrase subunit A

Chain R:

• Molecule 1: DNA gyrase subunit A

Chain T:

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

Chain B:

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

Chain D:
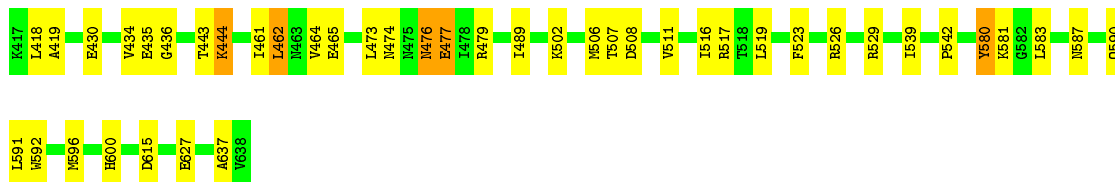
• Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B

Chain S:

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

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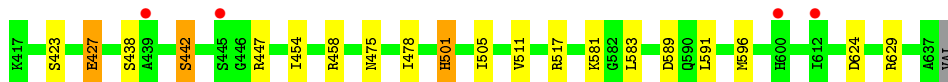
• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*T)-3')

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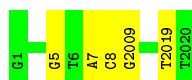
• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP
*GP*CP*TP*T)-3')

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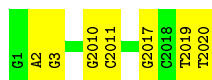
• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP
*GP*CP*TP*T)-3')
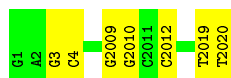
Chain V:

• 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')

Chain W:
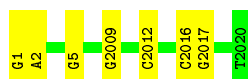
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	2.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215　,　0.246 0.218　,　0.248	Depositor DCC
R_{free} test set	2513 reflections (4.03%)	wwPDB-VP
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 , 40.5	EDS
L-test for twinning[2]	$<|L|> = 0.43$, $<L^2> = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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(^{o})	Ideal(^{o})
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.

All (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
2:S:439:ALA:O	2:S:443:THR:OG1	2.11	0.69
8:W:2101:53M:H52	8:W:2101:53M:C20	2.23	0.68
3:E:7:DA:N3	11:E:2201:HOH:O	2.26	0.68
1:A:92[A]:ARG:NH1	3:E:5:DG:OP1	2.28	0.67
2:B:621:LEU:O	2:B:629:ARG:NH1	2.30	0.64
2:D:465:GLU:OE2	2:D:526:ARG:NE	2.31	0.62
3:W:2012:DC:H2"	8:W:2101:53M:O29	1.99	0.62
9:F:2101:53L:H52	9:F:2101:53L:C26	2.30	0.62
1:A:112:SER:OG	1:A:116:ASP:OD1	2.18	0.61
3:V:2009:DG:H2'	3:V:2010:DG:C8	2.36	0.61
1:A:149:ASN:ND2	1:A:151:ASP:OD1	2.34	0.61
8:E:2101:53M:C26	8:E:2101:53M:C5	2.79	0.60
1:T:47:ARG:NH1	4:T:502:SO4:O4	2.36	0.59
2:U:629:ARG:NE	3:W:2017:DG:OP1	2.30	0.59
2:B:629:ARG:NE	3:F:2017:DG:OP1	2.36	0.58
1:C:149:ASN:ND2	1:C:151:ASP:OD1	2.37	0.58
1:A:47:ARG:NH1	6:A:503:GOL:O2	2.33	0.57
2:U:438:SER:O	2:U:442:SER:OG	2.23	0.56
3:W:2012:DC:C2'	8:W:2101:53M:O29	2.53	0.56
1:A:436:LEU:HD12	1:C:403:THR:HG22	1.88	0.56
10:S:6002:50M:C20	10:S:6002:50M:H52	2.35	0.56
3:V:2012:DC:H42	3:W:2009:DG:H1	1.52	0.55
3:W:2012:DC:C2	8:W:2101:53M:H14	2.41	0.55
8:W:2101:53M:C20	8:W:2101:53M:C5	2.85	0.55
1:C:83:ASP:HA	1:C:86:ILE:HD12	1.88	0.54
2:D:473:LEU:HD21	2:D:489:ILE:HD11	1.88	0.54
1:C:269:ASN:HB3	1:C:272:ARG:HB3	1.90	0.54
1:A:186:HIS:HB2	1:A:191:LEU:HD11	1.90	0.53
1:R:92:ARG:NH1	3:W:5:DG:OP1	2.42	0.53
1:R:431:ARG:NH1	1:T:404:ASP:OD2	2.40	0.53
1:A:38:VAL:HA	1:A:167:LEU:HD22	1.90	0.53
1:T:368:GLN:HG3	1:T:459:LEU:HD21	1.91	0.53
1:C:467:GLN:NE2	1:C:471:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:2101:53L:C26	9:F:2101:53L:C5	2.86	0.52
1:A:42:LEU:HD12	1:A:47:ARG:HG3	1.91	0.52
1:R:116:ASP:N	1:R:116:ASP:OD1	2.43	0.52
2:D:435:GLU:HB2	2:D:507:THR:HA	1.92	0.52
1:R:227:LYS:HE3	1:R:488:ILE:HG21	1.92	0.51
1:C:231:ARG:NH2	1:C:235:GLU:OE2	2.44	0.51
3:E:2009:DG:C4	8:E:2101:53M:O21	2.64	0.51
1:T:296:THR:HG23	1:T:302:VAL:HA	1.94	0.50
3:V:3:DG:H2"	3:V:4:DC:C6	2.46	0.50
1:A:371:LEU:HD11	1:A:452:ILE:HG23	1.93	0.49
3:F:2019:DT:H2"	3:F:2020:DT:C5'	2.42	0.49
1:R:249:ILE:HG12	1:R:314:ALA:HB3	1.95	0.49
2:S:427:GLU:HA	2:S:501:HIS:CG	2.47	0.49
10:S:6002:50M:C20	10:S:6002:50M:C5	2.91	0.49
2:D:443:THR:HG23	2:D:596:MET:SD	2.53	0.49
3:V:2020:DT:H3	3:W:1:DG:H2'	1.77	0.49
2:B:473:LEU:HD21	2:B:489:ILE:HD11	1.94	0.49
1:T:177:VAL:HG22	3:W:2016:DC:H4'	1.93	0.49
1:T:183:ILE:HG12	1:T:335:MET:HG2	1.94	0.49
1:A:429:ARG:NH2	4:A:501:SO4:O3	2.46	0.49
1:A:388:LEU:HA	1:A:391:ILE:HG12	1.94	0.49
1:T:61:ASP:OD1	1:T:61:ASP:N	2.45	0.49
3:V:2019:DT:H3	3:W:2:DA:H61	1.60	0.49
1:R:149:ASN:ND2	1:R:151:ASP:OD1	2.45	0.49
1:R:296:THR:HG23	1:R:302:VAL:HA	1.94	0.49
1:A:361:THR:HA	1:A:364:ARG:HD2	1.94	0.48
1:R:225:LEU:HD21	1:R:244:ARG:HB2	1.95	0.48
1:A:436:LEU:HD22	1:A:440:LYS:HE3	1.96	0.48
2:D:592:TRP:HA	2:D:596:MET:HB2	1.95	0.48
3:F:2:DA:H2"	3:F:3:DG:C8	2.47	0.48
2:B:430:GLU:HB3	2:B:502:LYS:HB2	1.95	0.48
1:C:369:TYR:CE1	1:C:373:LYS:HE3	2.49	0.48
2:B:462:LEU:HD11	2:B:471:ARG:HE	1.79	0.47
1:R:30:ILE:HG23	1:R:35:LEU:HD12	1.96	0.47
2:S:443:THR:HB	2:S:454:ILE:HG21	1.95	0.47
1:R:346:ILE:HB	1:R:350:GLU:HB2	1.95	0.47
1:C:270:LYS:NZ	1:C:294:ASP:OD2	2.46	0.47
2:S:433:LEU:HD23	2:S:455:LEU:HB3	1.96	0.47
1:R:204:ILE:HG21	1:R:209:LEU:HD21	1.96	0.47
1:T:103:LEU:O	1:T:132:THR:OG1	2.29	0.47
1:C:245:SER:OG	1:C:327:LEU:O	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ARG:HH22	3:E:2019:DT:P	2.38	0.47
2:D:476:ASN:N	6:D:1002:GOL:O3	2.45	0.47
1:R:183:ILE:HG12	1:R:335:MET:HG2	1.97	0.47
1:A:143:THR:N	11:A:604:HOH:O	2.49	0.46
1:C:27:MET:SD	2:D:637:ALA:HB1	2.55	0.46
1:A:252:ARG:HB3	1:T:467:GLN:HG2	1.98	0.46
2:D:434:VAL:HA	2:D:506:MET:O	2.16	0.46
2:S:434:VAL:HG11	2:S:443:THR:HG21	1.97	0.46
1:A:91:VAL:HG11	1:A:118:ALA:HB2	1.97	0.46
1:C:259:ILE:HB	1:C:306:ILE:HB	1.97	0.46
2:D:461:ILE:HD13	2:D:477:GLU:HB3	1.97	0.45
2:U:427:GLU:HA	2:U:501:HIS:CG	2.51	0.45
1:R:87:TYR:CD1	1:R:121:MET:HB3	2.51	0.45
1:A:385:ARG:HA	1:A:438:ARG:HH12	1.81	0.45
1:C:238:ARG:HG2	1:C:238:ARG:HH11	1.80	0.45
2:D:587:ASN:O	2:D:591:LEU:HB2	2.16	0.45
1:T:250:GLU:OE2	1:T:258:ARG:NH2	2.49	0.45
2:D:474:ASN:O	2:D:474:ASN:ND2	2.50	0.45
1:A:269:ASN:HB3	1:A:272[B]:ARG:HB2	1.98	0.44
1:A:64:TYR:HB3	1:A:125:GLU:HB3	1.99	0.44
1:C:65:LYS:HE2	1:C:69:ARG:HB3	1.98	0.44
2:D:473:LEU:O	2:D:479:ARG:HD3	2.17	0.44
10:S:6002:50M:H14	3:V:2012:DC:C2	2.52	0.44
1:A:238:ARG:NH1	11:A:605:HOH:O	2.50	0.44
1:R:93:MET:HA	1:R:99:TYR:CD2	2.52	0.44
1:R:227:LYS:HA	1:R:230:ILE:HD12	2.00	0.44
1:T:451:TYR:CE2	1:T:455:LEU:HD11	2.52	0.44
2:U:447:ARG:HB3	2:U:596:MET:HE1	1.99	0.44
2:S:436:GLY:HA2	10:S:6002:50M:O24	2.18	0.44
2:U:505:ILE:HG21	2:U:517:ARG:HG3	1.99	0.44
2:D:517:ARG:HD2	2:D:539:ILE:HD13	2.00	0.44
2:D:436:GLY:HA2	9:F:2101:53L:O24	2.18	0.44
1:C:451:TYR:CE2	1:C:455:LEU:HD11	2.52	0.43
1:T:313:ASN:HB3	1:T:316:VAL:HG23	2.00	0.43
1:R:47:ARG:HG3	1:R:160:LEU:HG	1.99	0.43
1:R:426:LEU:HB3	1:T:431:ARG:HB3	2.00	0.43
1:R:388:LEU:HA	1:R:391:ILE:HG12	2.00	0.43
1:T:277:ILE:HG12	1:T:325:THR:HG21	2.00	0.43
1:C:58:MET:SD	1:C:65:LYS:HD2	2.58	0.43
2:D:464:VAL:HG21	2:D:523:PHE:HA	2.00	0.43
1:T:382:GLU:HG3	1:T:445:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG12	1:A:325:THR:HG21	2.01	0.43
3:E:8:DC:C2	8:E:2101:53M:O27	2.72	0.43
1:C:28:SER:O	1:C:32:ALA:N	2.49	0.42
2:D:516:ILE:HA	2:D:519:LEU:HD12	2.01	0.42
1:R:206:ILE:HD13	1:R:235:GLU:HA	2.00	0.42
1:C:387:ALA:HA	1:C:394:ILE:HG13	2.00	0.42
1:T:37:ASP:HA	1:T:338:LEU:HB2	2.01	0.42
1:T:96:ASP:N	1:T:96:ASP:OD1	2.52	0.42
1:C:138:ASP:O	1:C:143:THR:OG1	2.25	0.42
1:A:135:LEU:HA	1:A:162:ALA:HA	2.00	0.42
2:U:475:ASN:HB3	2:U:478:ILE:HB	2.02	0.42
1:R:382:GLU:HG3	1:R:445:TYR:CE1	2.54	0.42
1:R:344:LYS:HE2	1:R:346:ILE:HG22	2.01	0.42
1:A:444:GLU:O	1:A:448:LEU:HB2	2.20	0.42
2:B:587:ASN:HD21	2:B:589:ASP:HB2	1.84	0.42
2:S:434:VAL:HG21	2:S:440:GLY:HA2	2.02	0.42
2:D:419:ALA:HB2	2:D:444:LYS:HE3	2.02	0.42
1:A:246:ARG:NH2	1:A:487:GLU:OE1	2.51	0.41
1:T:206:ILE:HD11	1:T:347:ASN:ND2	2.35	0.41
1:A:378:ALA:HB2	1:A:448:LEU:HD23	2.03	0.41
1:T:368:GLN:O	1:T:372:ARG:HG3	2.21	0.41
1:A:292:LEU:HD13	1:A:306:ILE:HG12	2.01	0.41
1:C:30:ILE:HG23	1:C:35:LEU:HD12	2.02	0.41
2:S:473:LEU:HD21	2:S:489:ILE:HD11	2.02	0.41
3:V:2020:DT:H2'	3:W:1:DG:O6	2.19	0.41
1:R:219:PRO:HA	1:R:485:ARG:HH11	1.86	0.41
1:A:344:LYS:NZ	1:A:350:GLU:OE1	2.34	0.41
2:D:430:GLU:HB3	2:D:502:LYS:HB2	2.03	0.41
2:D:508:ASP:HA	2:D:583:LEU:HG	2.02	0.41
3:F:2019:DT:H2"	3:F:2020:DT:C4'	2.51	0.41
1:T:54:ASN:HB2	1:T:136:LEU:HD13	2.02	0.41
2:B:439:ALA:CB	2:B:583:LEU:HB3	2.51	0.41
1:T:116:ASP:OD1	1:T:116:ASP:N	2.54	0.41
1:T:396:SER:O	1:T:400:GLU:HG2	2.21	0.41
1:A:451:TYR:CE2	1:A:455:LEU:HD11	2.56	0.40
3:F:2010:DG:H2"	3:F:2011:DC:C6	2.56	0.40
1:R:246:ARG:NH2	1:R:487:GLU:OE1	2.54	0.40
2:D:461:ILE:HD12	2:D:462:LEU:H	1.86	0.40
1:R:65:LYS:HE2	1:R:69:ARG:HB3	2.03	0.40
3:F:2019:DT:H2"	3:F:2020:DT:O5'	2.21	0.40
2:D:580:TYR:N	2:D:580:TYR:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:432:ARG:HA	1:T:437:GLU:HB3	2.02	0.40
1:R:71:VAL:O	1:R:75:MET:HB2	2.21	0.40
1:R:266:PHE:CE2	1:R:267:GLN:HG3	2.57	0.40
2:S:529:ARG:HB3	2:S:530:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/482 (100%)	460 (95%)	23 (5%)	0	100	100
1	C	477/482 (99%)	443 (93%)	33 (7%)	1 (0%)	47	78
1	R	473/482 (98%)	449 (95%)	24 (5%)	0	100	100
1	T	478/482 (99%)	460 (96%)	17 (4%)	1 (0%)	47	78
2	B	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
2	D	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	14	48
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%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	476	ASN
1	T	33	ARG
2	D	462	LEU
1	C	165	PRO

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	408/416 (98%)	389 (95%)	19 (5%)	26	60
1	C	407/416 (98%)	395 (97%)	12 (3%)	42	72
1	R	399/416 (96%)	386 (97%)	13 (3%)	38	69
1	T	401/416 (96%)	379 (94%)	22 (6%)	21	54
2	B	152/157 (97%)	143 (94%)	9 (6%)	19	51
2	D	150/157 (96%)	138 (92%)	12 (8%)	12	39
2	S	146/157 (93%)	136 (93%)	10 (7%)	16	46
2	U	148/157 (94%)	136 (92%)	12 (8%)	11	39
All	All	2211/2292 (96%)	2102 (95%)	109 (5%)	25	59

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	66	LYS
1	A	75	MET
1	A	107	GLN
1	A	145	ASP
1	A	160	LEU
1	A	240	SER
1	A	257	GLN
1	A	290	THR
1	A	300	THR
1	A	315	SER
1	A	364	ARG
1	A	429	ARG
1	A	432	ARG
1	A	448	LEU
1	A	464	VAL
1	A	465	LEU
1	A	466	LEU
1	A	483	ASP

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Mol	Chain	Res	Type
2	B	418	LEU
2	B	458	ARG
2	B	480	GLN
2	B	529	ARG
2	B	583	LEU
2	B	587	ASN
2	B	589	ASP
2	B	594	THR
2	B	595	THR
1	C	14	ILE
1	C	73	ASP
1	C	78	TYR
1	C	143	THR
1	C	231	ARG
1	C	245	SER
1	C	330	SER
1	C	346	ILE
1	C	385	ARG
1	C	393	GLU
1	C	414	ARG
1	C	465	LEU
2	D	418	LEU
2	D	444	LYS
2	D	477	GLU
2	D	511	VAL
2	D	529	ARG
2	D	542	PRO
2	D	580	TYR
2	D	581	LYS
2	D	590	GLN
2	D	600	HIS
2	D	615	ASP
2	D	627	GLU
1	R	27	MET
1	R	75	MET
1	R	130	LYS
1	R	210	MET
1	R	225	LEU
1	R	228	SER
1	R	248	VAL
1	R	311	ASP
1	R	392	ASP

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Mol	Chain	Res	Type
1	R	404	ASP
1	R	408	MET
1	R	418	SER
1	R	490	LEU
2	S	417	LYS
2	S	443	THR
2	S	502	LYS
2	S	506	MET
2	S	529	ARG
2	S	581	LYS
2	S	585	GLU
2	S	595	THR
2	S	624	ASP
2	S	627	GLU
1	T	14	ILE
1	T	63	SER
1	T	75	MET
1	T	77	LYS
1	T	78	TYR
1	T	93	MET
1	T	139	ILE
1	T	223	LEU
1	T	251	GLU
1	T	279	GLU
1	T	280	LEU
1	T	298	LEU
1	T	315	SER
1	T	385	ARG
1	T	391	ILE
1	T	399	ARG
1	T	400	GLU
1	T	401	SER
1	T	403	THR
1	T	404	ASP
1	T	413	GLN
1	T	450	ASN
2	U	423	SER
2	U	427	GLU
2	U	442	SER
2	U	454	ILE
2	U	458	ARG
2	U	501	HIS

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Mol	Chain	Res	Type
2	U	511	VAL
2	U	581	LYS
2	U	583	LEU
2	U	589	ASP
2	U	591	LEU
2	U	624	ASP

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	C	123	3,1	15,16,17	1.35	1 (6%)	19,22,24	0.64	1 (5%)
1	PTR	A	123	3,1	15,16,17	1.36	1 (6%)	19,22,24	0.55	0
1	PTR	T	123	3,1	15,16,17	1.18	1 (6%)	19,22,24	0.75	1 (5%)
1	PTR	R	123	3,1	15,16,17	1.21	1 (6%)	19,22,24	0.71	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	C	123	3,1	-	0/10/11/13	0/1/1/1
1	PTR	A	123	3,1	-	1/10/11/13	0/1/1/1
1	PTR	T	123	3,1	-	1/10/11/13	0/1/1/1
1	PTR	R	123	3,1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	PTR	OH-CZ	-4.44	1.30	1.40
1	A	123	PTR	OH-CZ	-4.20	1.31	1.40
1	R	123	PTR	OH-CZ	-4.03	1.31	1.40
1	T	123	PTR	OH-CZ	-3.87	1.31	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	123	PTR	CB-CA-C	-2.24	107.27	111.47
1	C	123	PTR	O2P-P-OH	2.23	112.22	105.24
1	R	123	PTR	O2P-P-OH	2.15	111.97	105.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	123	PTR	O-C-CA-CB
1	R	123	PTR	O-C-CA-CB
1	T	123	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	T	502	-	4,4,4	0.14	0	6,6,6	0.07	0
6	GOL	D	1003	-	5,5,5	0.42	0	5,5,5	0.21	0
6	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.36	0
8	53M	W	2101	-	29,30,30	1.12	2 (6%)	31,47,47	1.53	6 (19%)
4	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.06	0
6	GOL	D	1002	-	5,5,5	0.25	0	5,5,5	0.22	0
9	53L	F	2101	-	29,30,30	1.35	3 (10%)	35,47,47	1.52	5 (14%)
8	53M	E	2101	-	29,30,30	1.17	3 (10%)	31,47,47	1.47	5 (16%)
4	SO4	T	501	-	4,4,4	0.15	0	6,6,6	0.05	0
10	50M	S	6002	-	29,30,30	1.23	3 (10%)	35,47,47	1.90	10 (28%)
6	GOL	U	5002	-	5,5,5	0.33	0	5,5,5	0.31	0
6	GOL	U	5003	-	5,5,5	0.31	0	5,5,5	0.36	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
6	GOL	D	1003	-	-	4/4/4/4	-
6	GOL	A	503	-	-	2/4/4/4	-
8	53M	W	2101	-	-	0/2/55/55	0/3/4/4
6	GOL	D	1002	-	-	4/4/4/4	-
8	53M	E	2101	-	-	0/2/55/55	0/3/4/4
9	53L	F	2101	-	-	2/2/55/55	0/4/4/4
10	50M	S	6002	-	-	2/2/55/55	0/4/4/4
6	GOL	U	5002	-	-	2/4/4/4	-
6	GOL	U	5003	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	2101	53L	C19-C26	-3.75	1.48	1.53
10	S	6002	50M	C19-C26	-3.18	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	2101	53L	C18-C19	-2.96	1.48	1.54
9	F	2101	53L	C19-C2	-2.89	1.52	1.56
10	S	6002	50M	C18-C19	-2.64	1.49	1.54
8	W	2101	53M	C18-C19	-2.51	1.49	1.54
8	E	2101	53M	C19-C2	-2.50	1.52	1.56
8	W	2101	53M	C19-C2	-2.35	1.52	1.56
8	E	2101	53M	C18-C19	-2.32	1.50	1.54
10	S	6002	50M	C19-C2	-2.28	1.52	1.56
8	E	2101	53M	O6-C7	-2.06	1.40	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S	6002	50M	C19-C26-N25	-5.16	112.31	117.70
9	F	2101	53L	C19-C26-N25	-3.74	113.79	117.70
10	S	6002	50M	C16-C17-C12	3.54	122.20	118.95
8	E	2101	53M	C26-C19-C20	-3.47	108.47	112.77
10	S	6002	50M	O30-N28-C15	-3.29	114.14	118.80
9	F	2101	53L	C16-C17-C12	3.21	121.90	118.95
8	W	2101	53M	C7-C10-N11	-3.20	100.97	111.37
10	S	6002	50M	C14-C15-N28	-3.14	117.01	119.38
8	E	2101	53M	C16-C17-C12	3.14	121.83	118.95
10	S	6002	50M	O27-C26-N25	2.87	125.08	120.50
8	E	2101	53M	C18-C17-C16	-2.66	116.03	121.23
10	S	6002	50M	C18-C19-C26	-2.64	102.32	108.24
9	F	2101	53L	C14-C15-N28	-2.58	117.44	119.38
9	F	2101	53L	O27-C26-N25	2.56	124.58	120.50
10	S	6002	50M	C16-C15-N28	2.45	120.90	118.75
8	W	2101	53M	C18-C17-C16	-2.45	116.45	121.23
10	S	6002	50M	C18-C17-C16	-2.43	116.49	121.23
10	S	6002	50M	C9-C7-C10	-2.42	105.82	112.46
8	W	2101	53M	O6-C7-C9	2.42	112.00	106.88
9	F	2101	53L	C18-C17-C16	-2.33	116.69	121.23
8	W	2101	53M	C26-C19-C20	-2.25	109.98	112.77
8	W	2101	53M	C18-C19-C2	2.25	112.48	107.21
8	E	2101	53M	C14-C15-N28	-2.15	117.76	119.38
8	W	2101	53M	O29-N28-C15	-2.10	115.82	118.80
10	S	6002	50M	C7-O6-C3	-2.08	107.83	112.31
8	E	2101	53M	C9-C7-C10	-2.07	106.80	112.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1002	GOL	O1-C1-C2-C3
6	D	1002	GOL	C1-C2-C3-O3
6	D	1002	GOL	O2-C2-C3-O3
6	D	1003	GOL	O1-C1-C2-C3
6	U	5003	GOL	O1-C1-C2-C3
9	F	2101	53L	C14-C15-N28-O30
9	F	2101	53L	C16-C15-N28-O30
10	S	6002	50M	C16-C15-N28-O30
10	S	6002	50M	C14-C15-N28-O30
6	D	1003	GOL	C1-C2-C3-O3
6	U	5002	GOL	C1-C2-C3-O3
6	D	1002	GOL	O1-C1-C2-O2
6	D	1003	GOL	O1-C1-C2-O2
6	U	5002	GOL	O2-C2-C3-O3
6	U	5003	GOL	O1-C1-C2-O2
6	D	1003	GOL	O2-C2-C3-O3
6	A	503	GOL	O1-C1-C2-O2
6	A	503	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 20 short contacts:

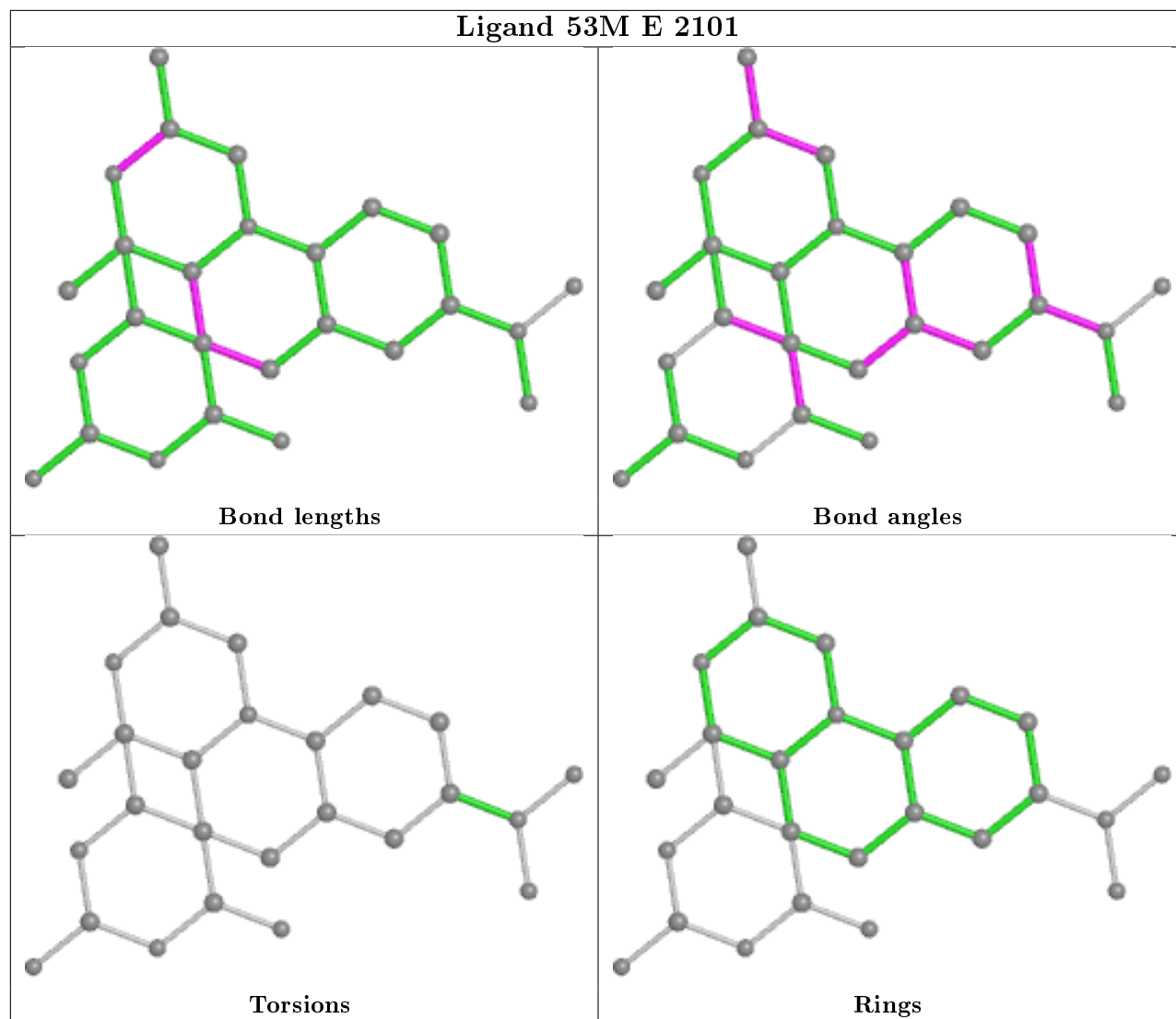| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	502	SO4	1	0
6	A	503	GOL	1	0
8	W	2101	53M	5	0
4	A	501	SO4	1	0
6	D	1002	GOL	1	0
9	F	2101	53L	3	0
8	E	2101	53M	4	0
10	S	6002	50M	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand 53M W 2101

Bond lengths

Bond angles

Torsions

Rings

Ligand 53L F 2101

Bond lengths

Bond angles

Torsions

Rings

Ligand 53M E 2101

Bond lengths

Bond angles

Torsions

Rings

Ligand 50M S 6002

Bond lengths

Bond angles

Torsions

Rings
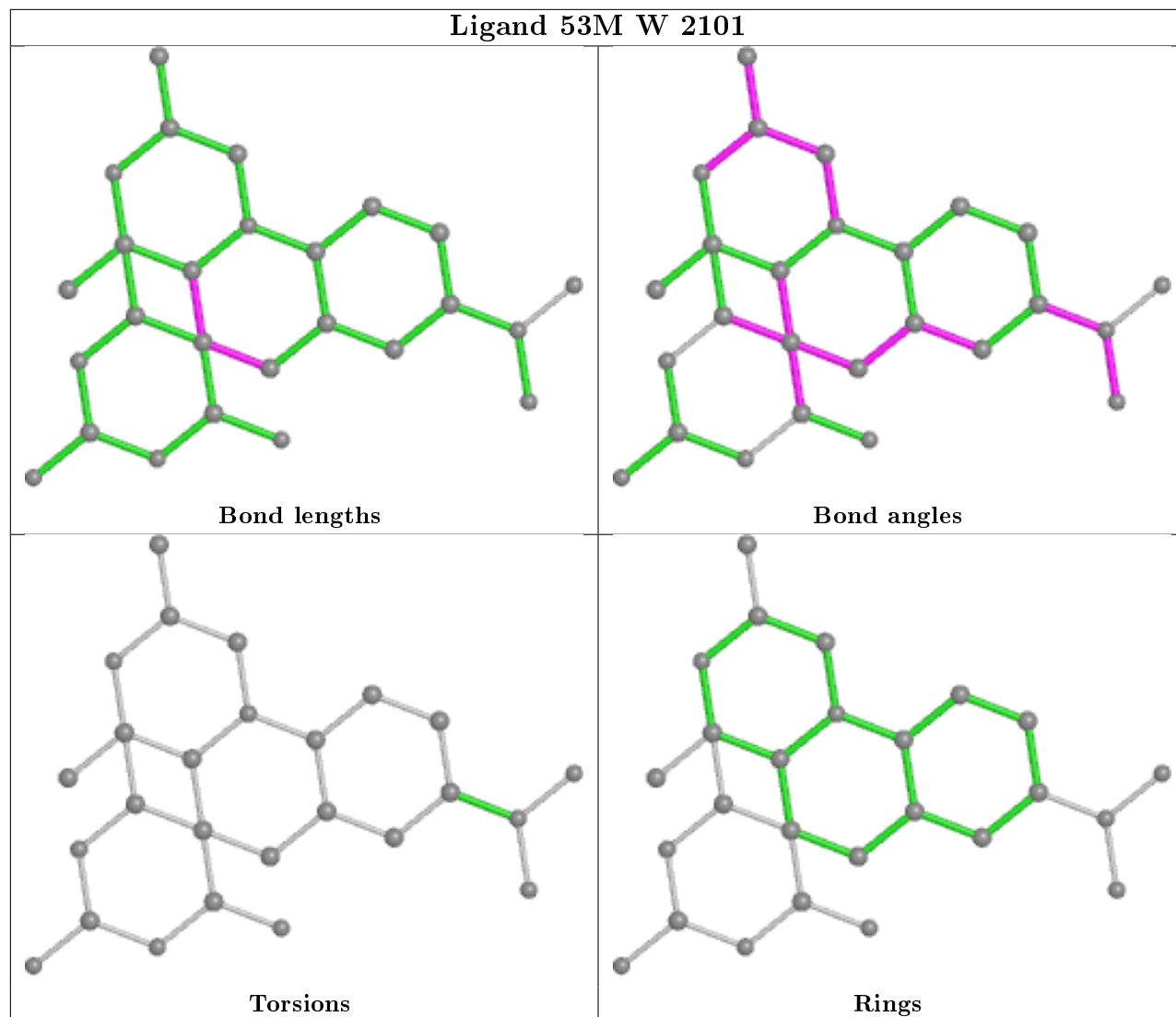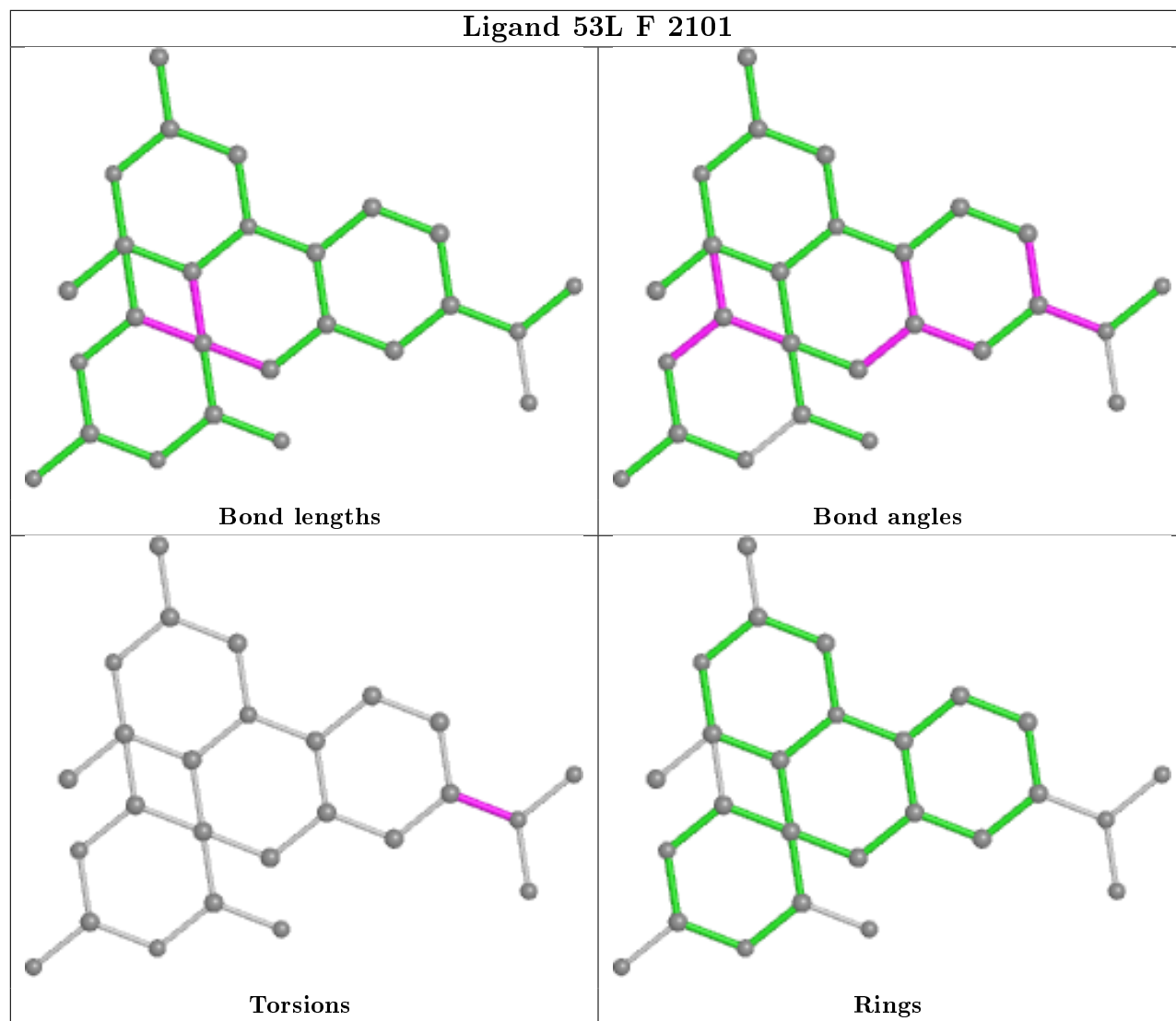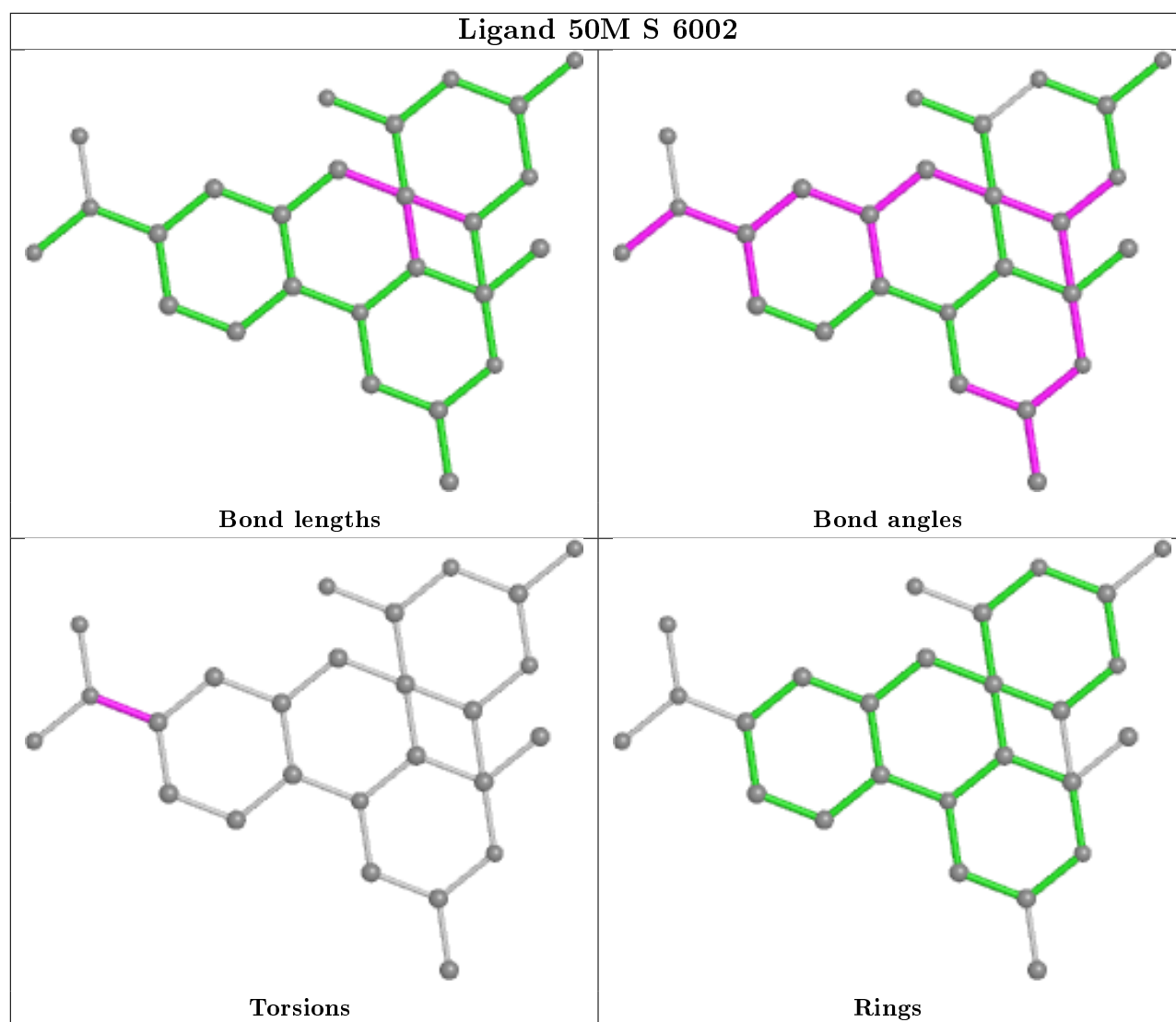
5.7 Other polymers (i)

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%)	-0.09	3 (0%)	89	84	25, 42, 62, 81	0
1	C	479/482 (99%)	-0.16	1 (0%)	95	94	22, 37, 59, 86	0
1	R	476/482 (98%)	-0.09	4 (0%)	86	78	24, 39, 94, 135	0
1	T	480/482 (99%)	-0.07	2 (0%)	92	89	23, 38, 75, 106	0
2	B	188/188 (100%)	0.16	4 (2%)	63	49	27, 55, 78, 87	0
2	D	188/188 (100%)	0.15	0	100	100	30, 55, 74, 84	0
2	S	188/188 (100%)	0.30	7 (3%)	41	25	29, 63, 89, 95	0
2	U	187/188 (99%)	0.08	4 (2%)	63	49	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	25 (0%)	84	75	22, 43, 76, 135	0

All (25) 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
1	R	251	GLU	3.0
2	B	616	GLN	2.9
1	A	254	GLY	2.9
2	S	494	ASP	2.8
2	B	431	ILE	2.7
2	B	491	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	11	GLU	2.4
1	R	311	ASP	2.4
2	U	612	ILE	2.3
2	U	600	HIS	2.2
1	R	300	THR	2.2
2	S	616	GLN	2.1
2	S	489	ILE	2.1
1	A	285	LYS	2.1
2	U	445	SER	2.1
1	T	251	GLU	2.1
2	U	439	ALA	2.1
1	A	311	ASP	2.0
2	S	434	VAL	2.0
1	T	255	GLY	2.0

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. 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	B-factors(Å^2)	Q<0.9
1	PTR	C	123	16/17	0.94	0.21	35,42,47,50	0
1	PTR	T	123	16/17	0.94	0.21	43,50,56,60	0
1	PTR	A	123	16/17	0.95	0.21	32,37,43,44	0
1	PTR	R	123	16/17	0.96	0.21	34,40,46,48	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, 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	B-factors($Å^2$)	Q<0.9
5	NA	T	503	1/1	0.79	0.25	43,43,43,43	0
5	NA	C	502	1/1	0.81	0.28	30,30,30,30	0
5	NA	A	502	1/1	0.82	0.33	39,39,39,39	0
6	GOL	A	503	6/6	0.84	0.31	30,36,39,39	0
5	NA	R	501	1/1	0.86	0.23	40,40,40,40	0
6	GOL	D	1003	6/6	0.86	0.22	47,57,58,58	0
10	50M	S	6002	27/27	0.90	0.23	18,21,25,27	0
6	GOL	U	5003	6/6	0.91	0.13	55,66,67,67	0
6	GOL	D	1002	6/6	0.91	0.33	39,47,49,49	0
8	53M	W	2101	27/27	0.92	0.24	19,21,25,28	0
8	53M	E	2101	27/27	0.92	0.24	18,22,25,28	0
4	SO4	T	502	5/5	0.93	0.19	54,55,56,56	0
9	53L	F	2101	27/27	0.93	0.21	19,21,26,29	0
6	GOL	U	5002	6/6	0.93	0.24	33,40,42,43	0
4	SO4	T	501	5/5	0.94	0.13	55,56,56,57	0
4	SO4	A	501	5/5	0.95	0.17	65,65,66,66	0
5	NA	C	501	1/1	0.96	0.26	19,19,19,19	0
7	MN	D	1001	1/1	0.99	0.16	38,38,38,38	0
7	MN	U	5001	1/1	0.99	0.17	37,37,37,37	0
7	MN	B	701	1/1	0.99	0.15	37,37,37,37	0
7	MN	S	6001	1/1	1.00	0.13	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.