



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:18 AM UTC

PDB ID : 5CDO / pdb_00005cdo
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

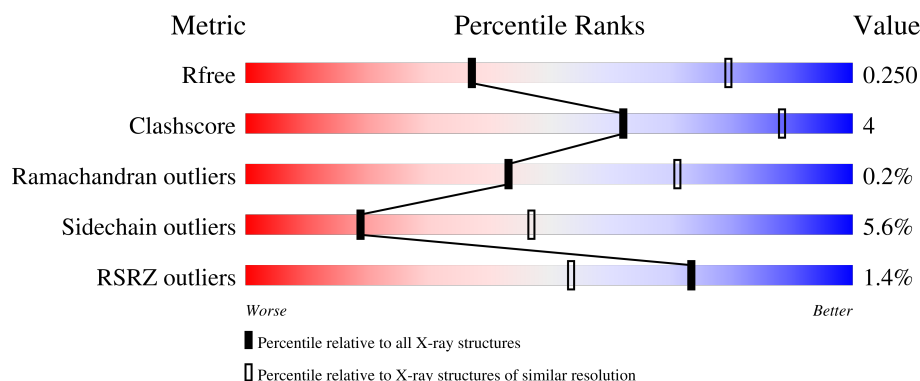
1 Overall quality at a glance

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 $\leq 5\%$. 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	% 84% 15% .
1	C	482	88% 11%
1	R	482	3% 87% 11% ..
1	T	482	% 86% 14%
2	B	188	2% 90% 7% .

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Mol	Chain	Length	Quality of chain
2	D	188	% 76% 22% .
2	S	188	2% 88% 11% .
2	U	188	2% 87% 11% ..
3	E	20	10% 70% 30%
3	F	20	65% 35%
3	V	20	5% 65% 35%
3	W	20	5% 65% 35%

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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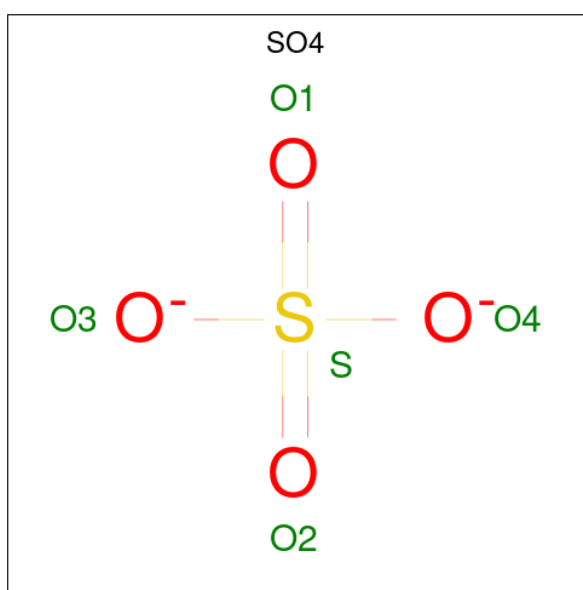
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Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	ASN	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	THR	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	TRP	deletion	UNP P66937
U	?	-	SER	deletion	UNP 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 (CCD ID: SO4) (formula: O₄S).

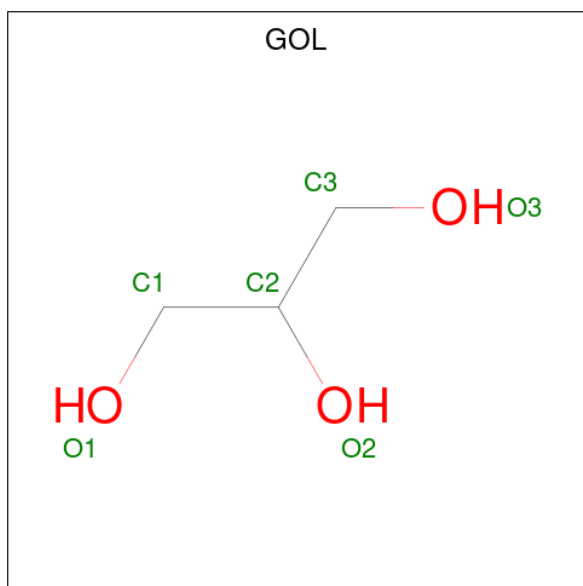


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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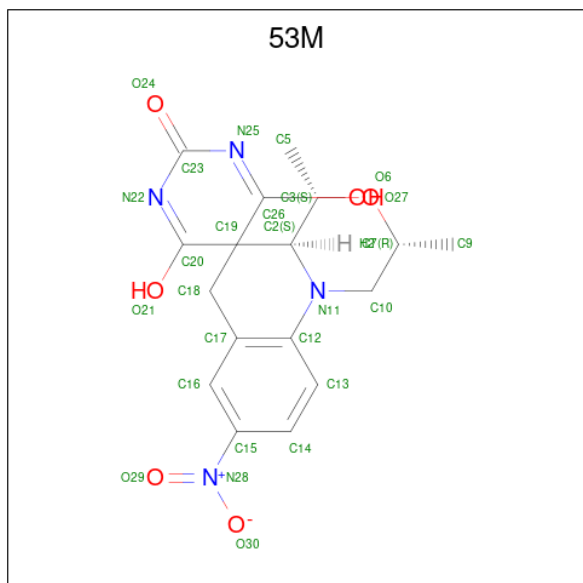
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	U	1	Total	C	H	O	0	0
			14	3	8	3		
6	U	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

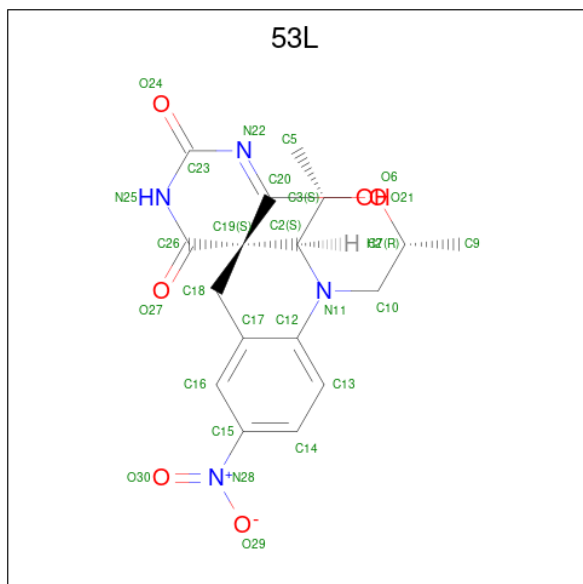
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mn	0	0
			1	1		
7	D	1	Total	Mn	0	0
			1	1		
7	S	1	Total	Mn	0	0
			1	1		
7	U	1	Total	Mn	0	0
			1	1		

- 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 (CCD ID: 53M) (formula: C₁₇H₁₈N₄O₆).



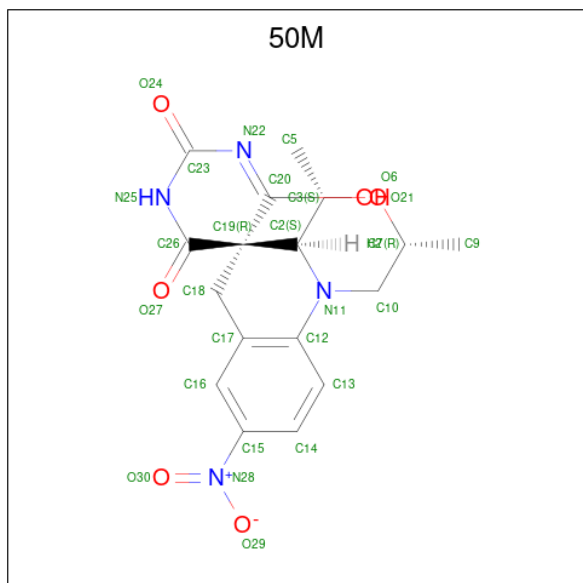
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	H	N	O	0	0
			45	17	18	4	6		
8	W	1	Total	C	H	N	O	0	0
			45	17	18	4	6		

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



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

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



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

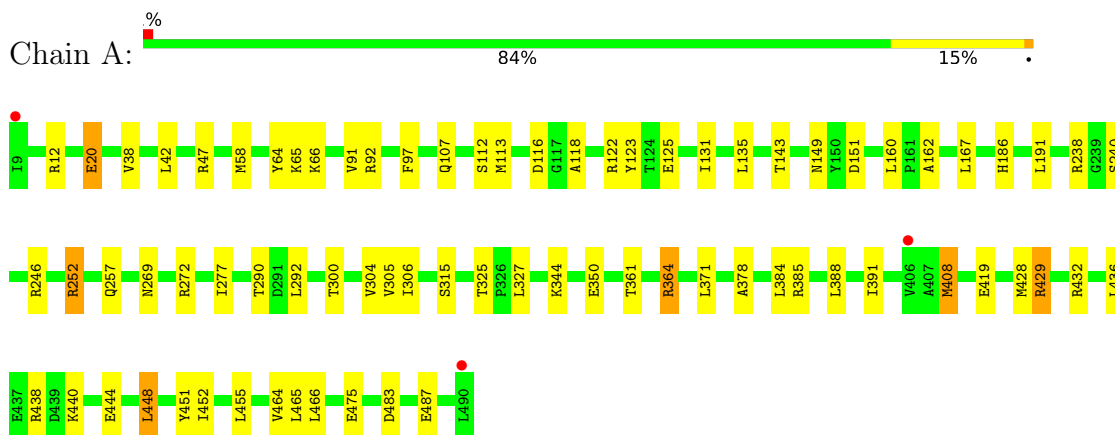
- Molecule 11 is water.

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		

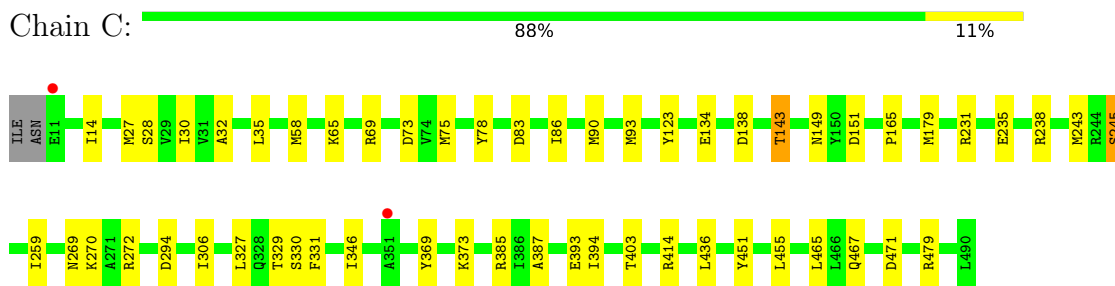
3 Residue-property plots [i](#)

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.

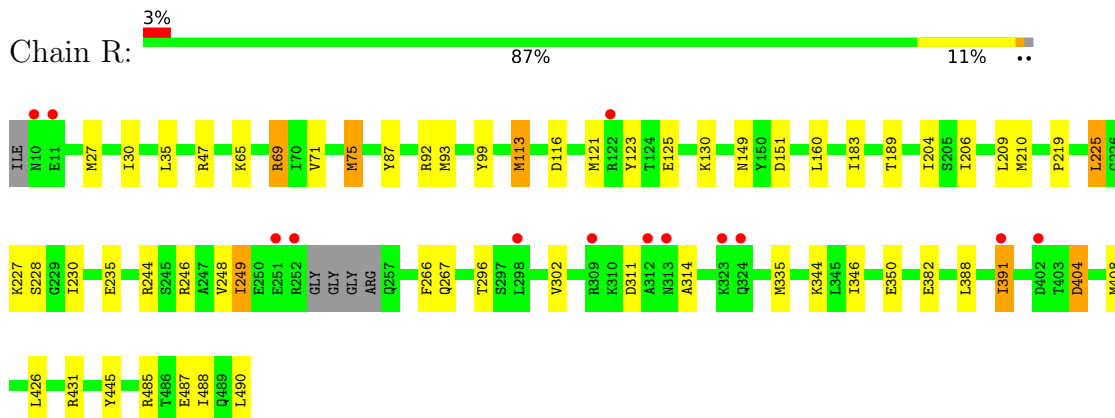
• Molecule 1: DNA gyrase subunit A



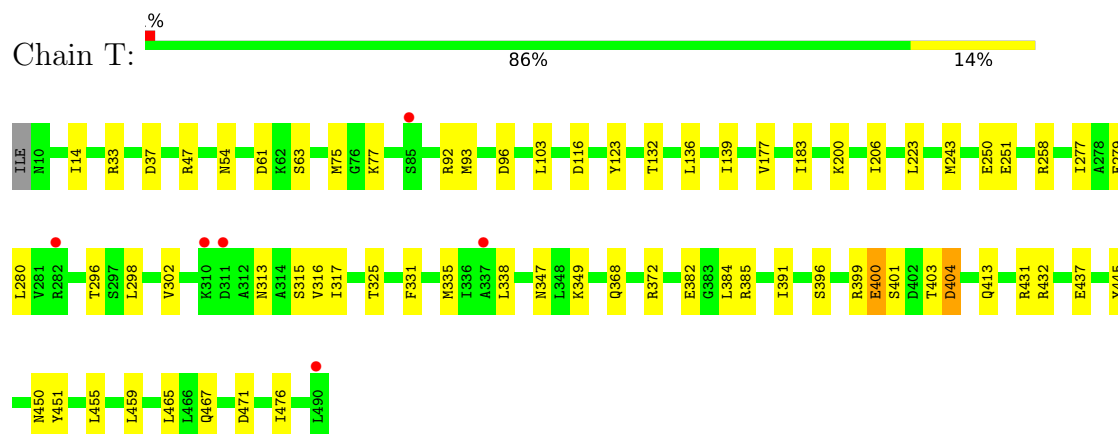
• Molecule 1: DNA gyrase subunit A



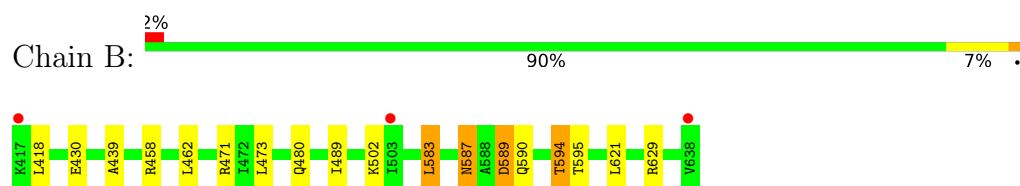
• Molecule 1: DNA gyrase subunit A



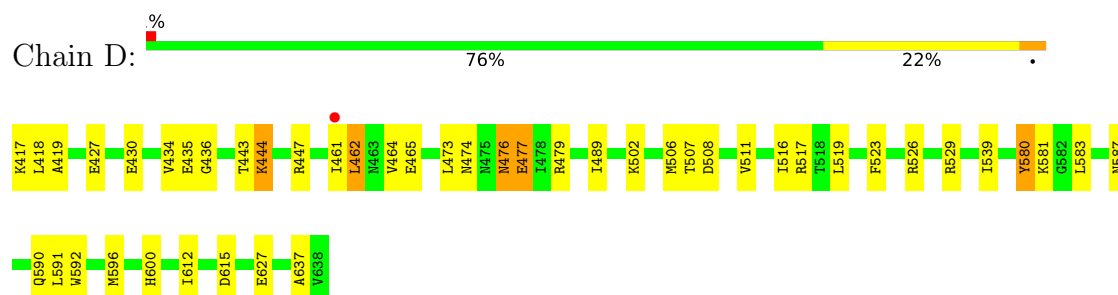
- Molecule 1: DNA gyrase subunit A



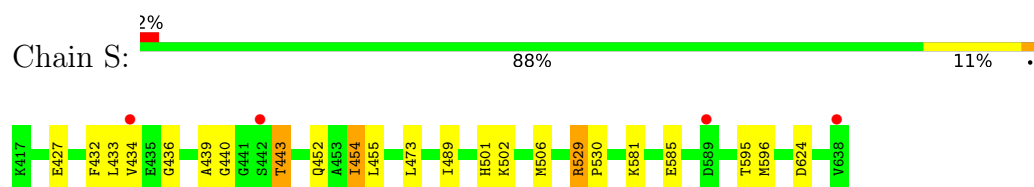
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



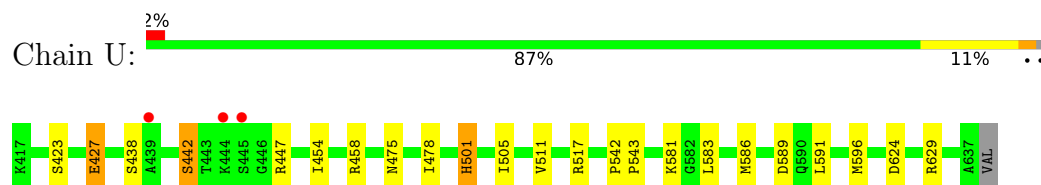
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



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



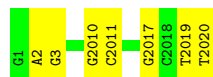
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



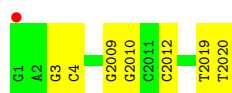
- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



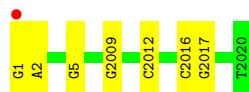
- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



- 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) 98.0 (58.41-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.246 0.218 , 0.250	Depositor DCC
R_{free} test set	2513 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3854	0.72	0/5195
1	C	0.37	0/3821	0.73	0/5149
1	R	0.36	0/3779	0.71	0/5098
1	T	0.36	0/3797	0.74	0/5126
2	B	0.37	0/1479	0.72	0/2000
2	D	0.40	0/1472	0.75	0/1990
2	S	0.35	0/1460	0.69	0/1974
2	U	0.36	0/1462	0.73	1/1977 (0.1%)
3	E	0.25	0/438	0.47	0/673
3	F	0.36	0/455	0.56	0/699
3	V	0.26	0/455	0.50	0/699
3	W	0.34	0/437	0.55	0/672
All	All	0.36	0/22909	0.71	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(°)
2	U	542	PRO	O-C-N	5.13	123.67	121.31

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	37	0
1	C	3791	3832	3832	25	0
1	R	3751	3752	3752	29	0
1	T	3767	3755	3755	26	0
2	B	1456	1413	1413	8	0
2	D	1449	1412	1412	22	0
2	S	1437	1395	1395	11	0
2	U	1439	1399	1399	7	0
3	E	392	210	211	6	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	183	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 (183) 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:122:ARG:HB3	1:C:75:MET:HE1	1.77	0.67
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:A:97:PHE:HB3	1:A:113:MET:HE2	1.84	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
1:A:408:MET:HE1	1:A:419:GLU:HG3	1.87	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:R:113:MET:HE3	1:R:302:VAL:HG21	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:S:452:GLN:NE2	2:S:596:MET:HE2	2.27	0.50
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
1:A:344:LYS:NZ	1:A:350:GLU:OE1	2.34	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:A:384:LEU:HD22	1:A:428:MET:HE2	1.94	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:C:90:MET:HA	1:C:93:MET:HE3	1.95	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
1:C:243:MET:HE2	1:C:331:PHE:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:U:543:PRO:HD2	2:U:586:MET:HE1	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
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
2:S:432:PHE:CE2	2:S:596:MET:HE3	2.51	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:T:243:MET:HE2	1:T:331:PHE:HB2	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:277:ILE:HG12	1:A:325:THR:HG21	2.01	0.43
2:D:447:ARG:HB3	2:D:596:MET:HE1	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:A:58:MET:HE3	1:A:65:LYS:HG3	2.01	0.42
1:A:408:MET:HE3	1:A:408:MET:HB3	1.94	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
1:A:12:ARG:HH22	1:A:20:GLU:CD	2.27	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:R:75:MET:HE2	1:R:75:MET:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:C	3:E:2017:DG:H4'	2.45	0.41
1:R:219:PRO:HA	1:R:485:ARG:HH11	1.86	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
2:U:447:ARG:HB3	2:U:596:MET:HE1	2.02	0.41
1:A:325:THR:C	1:A:327:LEU:H	2.29	0.40
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
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%)	43	71
1	R	473/482 (98%)	449 (95%)	24 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	478/482 (99%)	460 (96%)	17 (4%)	1 (0%)	43	71
2	B	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
2	D	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	11	39
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%)	43	71

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 ⓘ

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%)	385 (94%)	23 (6%)	19	47
1	C	407/416 (98%)	394 (97%)	13 (3%)	34	61
1	R	399/416 (96%)	382 (96%)	17 (4%)	26	54
1	T	401/416 (96%)	373 (93%)	28 (7%)	14	40
2	B	152/157 (97%)	144 (95%)	8 (5%)	20	49
2	D	150/157 (96%)	136 (91%)	14 (9%)	8	29
2	S	146/157 (93%)	137 (94%)	9 (6%)	16	44
2	U	148/157 (94%)	136 (92%)	12 (8%)	11	35
All	All	2211/2292 (96%)	2087 (94%)	124 (6%)	19	47

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	66	LYS
1	A	107	GLN
1	A	131	ILE
1	A	160	LEU
1	A	240	SER
1	A	252	ARG
1	A	257	GLN
1	A	290	THR
1	A	300	THR
1	A	304	VAL
1	A	305	VAL
1	A	315	SER
1	A	364	ARG
1	A	408	MET
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	475	GLU
1	A	483	ASP
2	B	418	LEU
2	B	458	ARG
2	B	480	GLN
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	245	SER
1	C	329	THR
1	C	330	SER
1	C	346	ILE
1	C	385	ARG
1	C	393	GLU
1	C	414	ARG
1	C	436	LEU

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Mol	Chain	Res	Type
1	C	465	LEU
2	D	417	LYS
2	D	418	LEU
2	D	427	GLU
2	D	444	LYS
2	D	477	GLU
2	D	511	VAL
2	D	529	ARG
2	D	580	TYR
2	D	581	LYS
2	D	590	GLN
2	D	600	HIS
2	D	612	ILE
2	D	615	ASP
2	D	627	GLU
1	R	27	MET
1	R	69	ARG
1	R	75	MET
1	R	113	MET
1	R	125	GLU
1	R	130	LYS
1	R	189	THR
1	R	210	MET
1	R	225	LEU
1	R	228	SER
1	R	248	VAL
1	R	249	ILE
1	R	311	ASP
1	R	391	ILE
1	R	404	ASP
1	R	408	MET
1	R	490	LEU
2	S	443	THR
2	S	454	ILE
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
1	T	14	ILE

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Mol	Chain	Res	Type
1	T	63	SER
1	T	75	MET
1	T	77	LYS
1	T	92	ARG
1	T	93	MET
1	T	139	ILE
1	T	200	LYS
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	317	ILE
1	T	349	LYS
1	T	384	LEU
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
1	T	465	LEU
1	T	476	ILE
2	U	423	SER
2	U	427	GLU
2	U	442	SER
2	U	454	ILE
2	U	458	ARG
2	U	501	HIS
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	257	GLN
2	B	501	HIS
1	C	187	ASN
1	C	334	ASN
2	D	605	GLN
1	R	320	ASN
2	S	480	GLN
2	S	600	HIS
1	T	257	GLN
2	U	501	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	R	123	3,1	15,16,17	1.17	1 (6%)	17,22,24	0.73	1 (5%)
1	PTR	A	123	3,1	15,16,17	1.34	1 (6%)	17,22,24	0.55	0
1	PTR	C	123	3,1	15,16,17	1.34	1 (6%)	17,22,24	0.65	1 (5%)
1	PTR	T	123	3,1	15,16,17	1.13	1 (6%)	17,22,24	0.58	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
1	PTR	R	123	3,1	-	2/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	123	3,1	-	1/10/11/13	0/1/1/1
1	PTR	C	123	3,1	-	0/10/11/13	0/1/1/1
1	PTR	T	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	-4.49	1.30	1.40
1	A	123	PTR	OH-CZ	-4.24	1.31	1.40
1	R	123	PTR	OH-CZ	-4.08	1.31	1.40
1	T	123	PTR	OH-CZ	-3.92	1.31	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	PTR	O2P-P-OH	2.33	112.22	105.32
1	R	123	PTR	O2P-P-OH	2.25	111.97	105.32

There are no chirality outliers.

All (4) 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
1	R	123	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
6	GOL	U	5003	-	5,5,5	0.31	0	5,5,5	0.40	0
8	53M	W	2101	-	27,30,30	1.14	2 (7%)	27,47,47	1.55	6 (22%)
4	SO4	T	502	-	4,4,4	0.25	0	6,6,6	0.09	0
6	GOL	D	1002	-	5,5,5	0.25	0	5,5,5	0.26	0
6	GOL	U	5002	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	D	1003	-	5,5,5	0.43	0	5,5,5	0.23	0
10	50M	S	6002	-	28,30,30	1.28	3 (10%)	32,47,47	2.01	11 (34%)
8	53M	E	2101	-	27,30,30	1.14	3 (11%)	27,47,47	1.53	5 (18%)
6	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.40	0
9	53L	F	2101	-	28,30,30	1.39	3 (10%)	32,47,47	1.54	7 (21%)
4	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	T	501	-	4,4,4	0.26	0	6,6,6	0.08	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	U	5003	-	-	2/4/4/4	-
8	53M	W	2101	-	-	0/2/55/55	0/3/4/4
6	GOL	U	5002	-	-	2/4/4/4	-
6	GOL	D	1002	-	-	4/4/4/4	-
6	GOL	D	1003	-	-	4/4/4/4	-
10	50M	S	6002	-	-	2/2/55/55	0/4/4/4
8	53M	E	2101	-	-	0/2/55/55	0/3/4/4
6	GOL	A	503	-	-	1/4/4/4	-
9	53L	F	2101	-	-	2/2/55/55	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	2101	53L	C19-C26	-3.77	1.48	1.52
10	S	6002	50M	C19-C26	-3.19	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	2101	53L	C18-C19	-3.18	1.48	1.54
10	S	6002	50M	C18-C19	-2.83	1.49	1.54
9	F	2101	53L	C19-C2	-2.78	1.52	1.56
8	W	2101	53M	C18-C19	-2.69	1.49	1.54
8	E	2101	53M	C18-C19	-2.48	1.50	1.54
8	E	2101	53M	C19-C2	-2.41	1.52	1.56
8	W	2101	53M	C19-C2	-2.27	1.52	1.56
10	S	6002	50M	C19-C2	-2.20	1.52	1.56
8	E	2101	53M	O6-C7	-2.15	1.40	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S	6002	50M	C19-C26-N25	-5.23	112.31	117.72
9	F	2101	53L	C19-C26-N25	-3.79	113.79	117.72
8	E	2101	53M	C20-C19-C26	-3.66	108.47	112.82
10	S	6002	50M	C16-C17-C12	3.47	122.20	118.95
10	S	6002	50M	O30-N28-C15	-3.40	114.14	118.82
8	W	2101	53M	C7-C10-N11	-3.27	100.97	111.31
9	F	2101	53L	C16-C17-C12	3.15	121.90	118.95
8	E	2101	53M	C16-C17-C12	3.08	121.83	118.95
10	S	6002	50M	C7-O6-C3	-2.95	107.83	112.25
10	S	6002	50M	C18-C19-C26	-2.84	102.32	108.36
10	S	6002	50M	O27-C26-N25	2.77	125.08	120.59
8	W	2101	53M	O6-C7-C9	2.74	112.00	106.88
10	S	6002	50M	C14-C15-N28	-2.66	117.01	119.34
8	W	2101	53M	C7-O6-C3	-2.63	108.31	112.25
10	S	6002	50M	C9-C7-C10	-2.61	105.82	112.39
10	S	6002	50M	C16-C15-N28	2.51	120.90	118.74
9	F	2101	53L	O27-C26-N25	2.47	124.58	120.59
8	E	2101	53M	C18-C17-C16	-2.43	116.03	121.18
8	W	2101	53M	C20-C19-C26	-2.40	109.98	112.82
8	E	2101	53M	C7-O6-C3	-2.29	108.82	112.25
8	W	2101	53M	C18-C17-C16	-2.23	116.45	121.18
8	E	2101	53M	C9-C7-C10	-2.22	106.80	112.39
10	S	6002	50M	C2-C19-C26	2.22	116.73	109.20
10	S	6002	50M	C18-C17-C16	-2.21	116.49	121.18
8	W	2101	53M	O29-N28-C15	-2.18	115.82	118.82
9	F	2101	53L	C14-C15-N28	-2.18	117.44	119.34
9	F	2101	53L	C7-O6-C3	-2.13	109.07	112.25
9	F	2101	53L	C18-C17-C16	-2.12	116.69	121.18
9	F	2101	53L	C9-C7-C10	-2.01	107.32	112.39

There are no chirality outliers.

All (17) 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
10	S	6002	50M	C16-C15-N28-O30
9	F	2101	53L	C14-C15-N28-O30
9	F	2101	53L	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

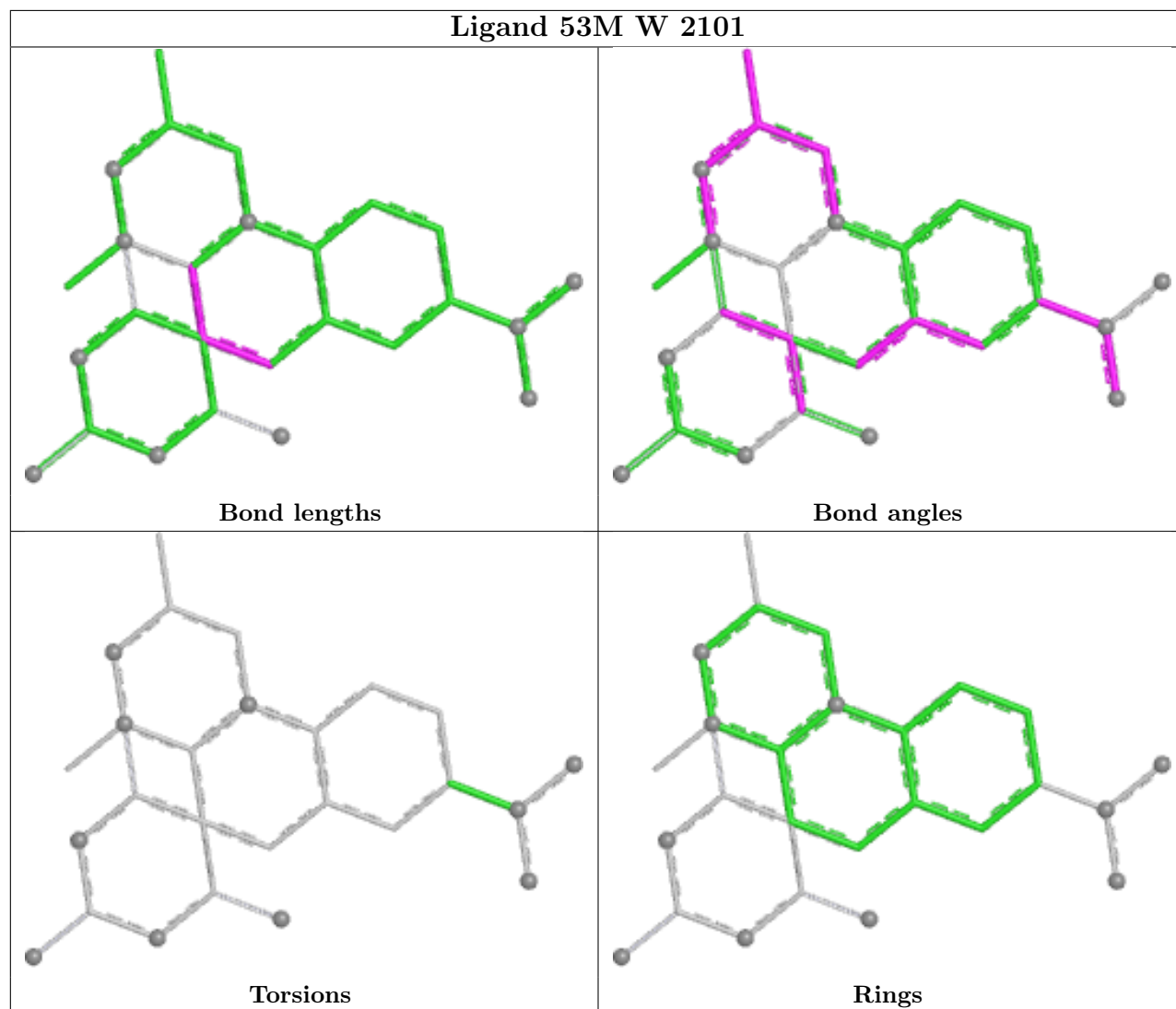
There are no ring outliers.

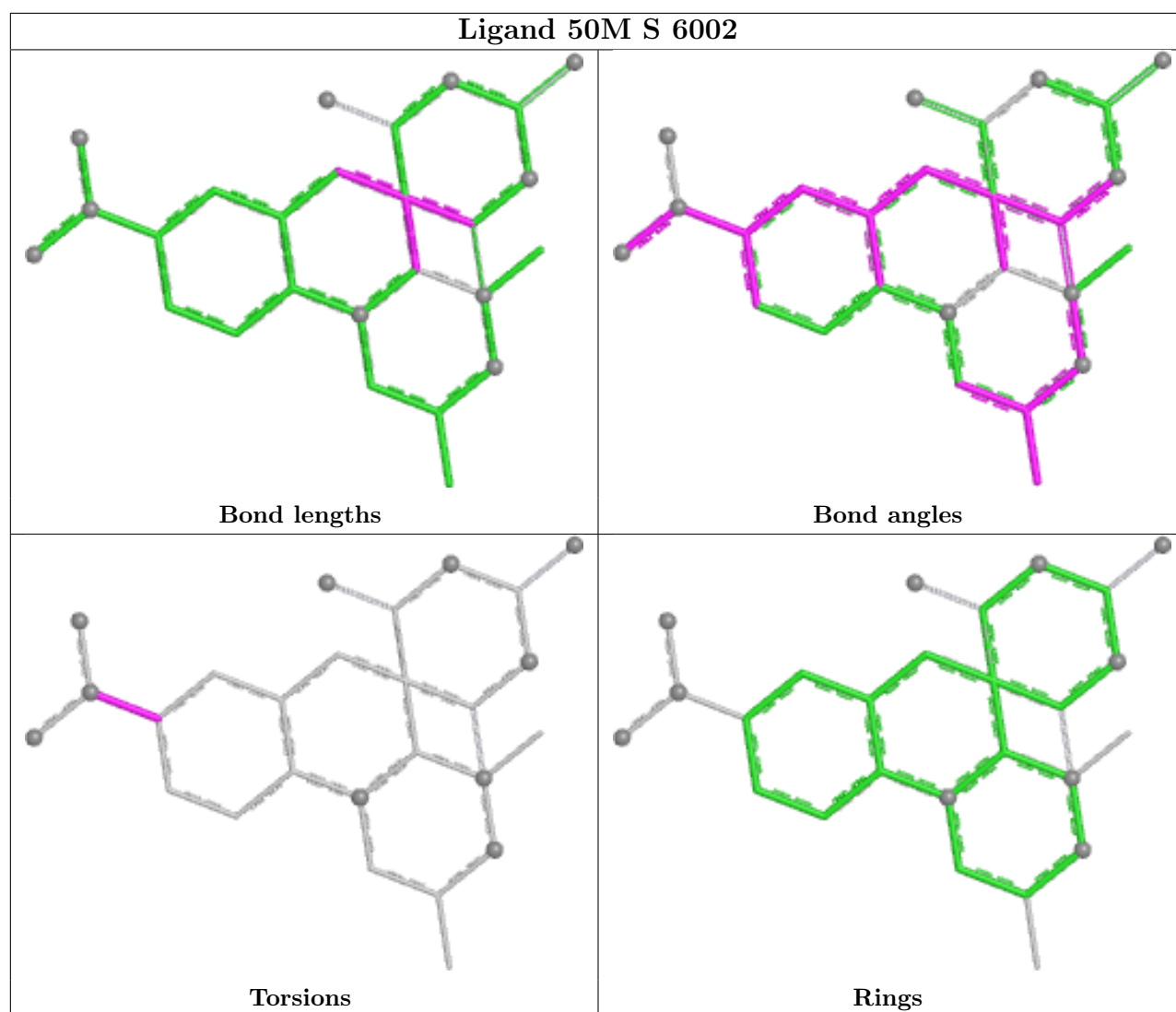
8 monomers are involved in 20 short contacts:

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

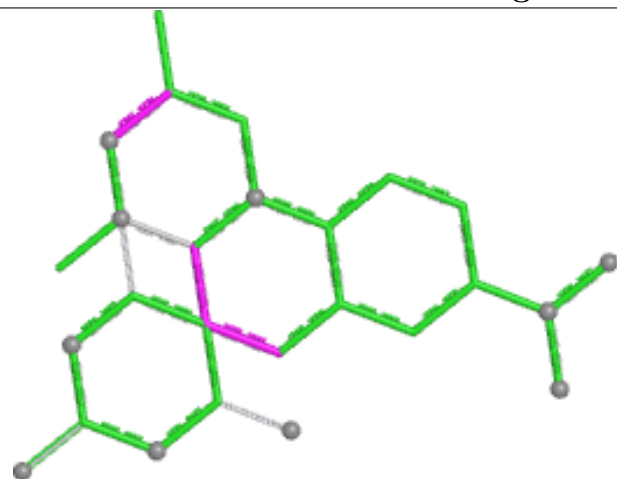
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

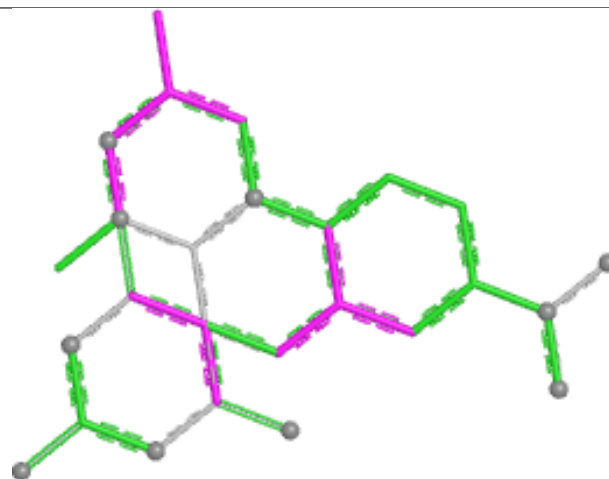




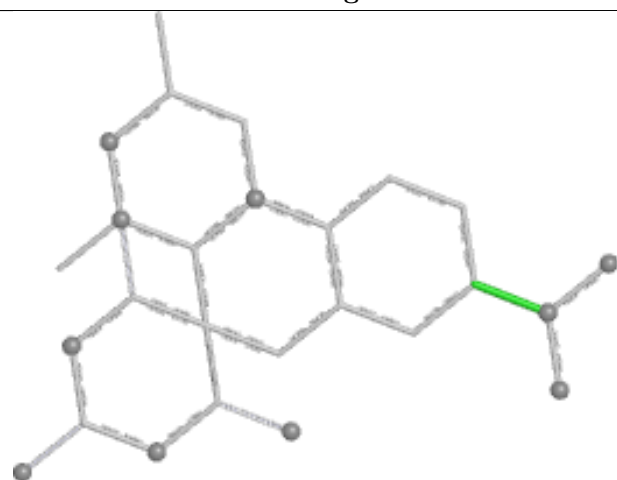
Ligand 53M E 2101



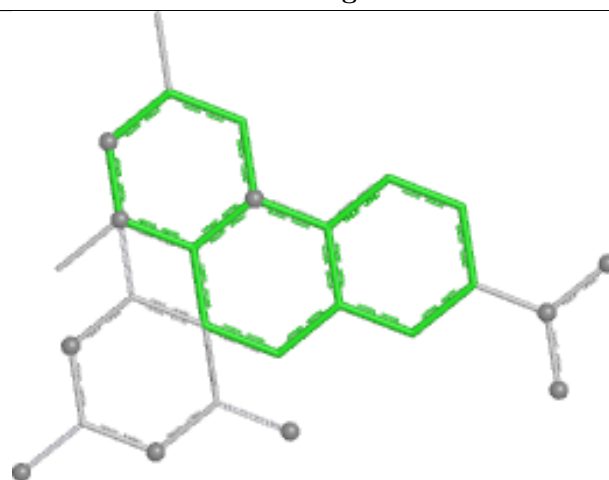
Bond lengths



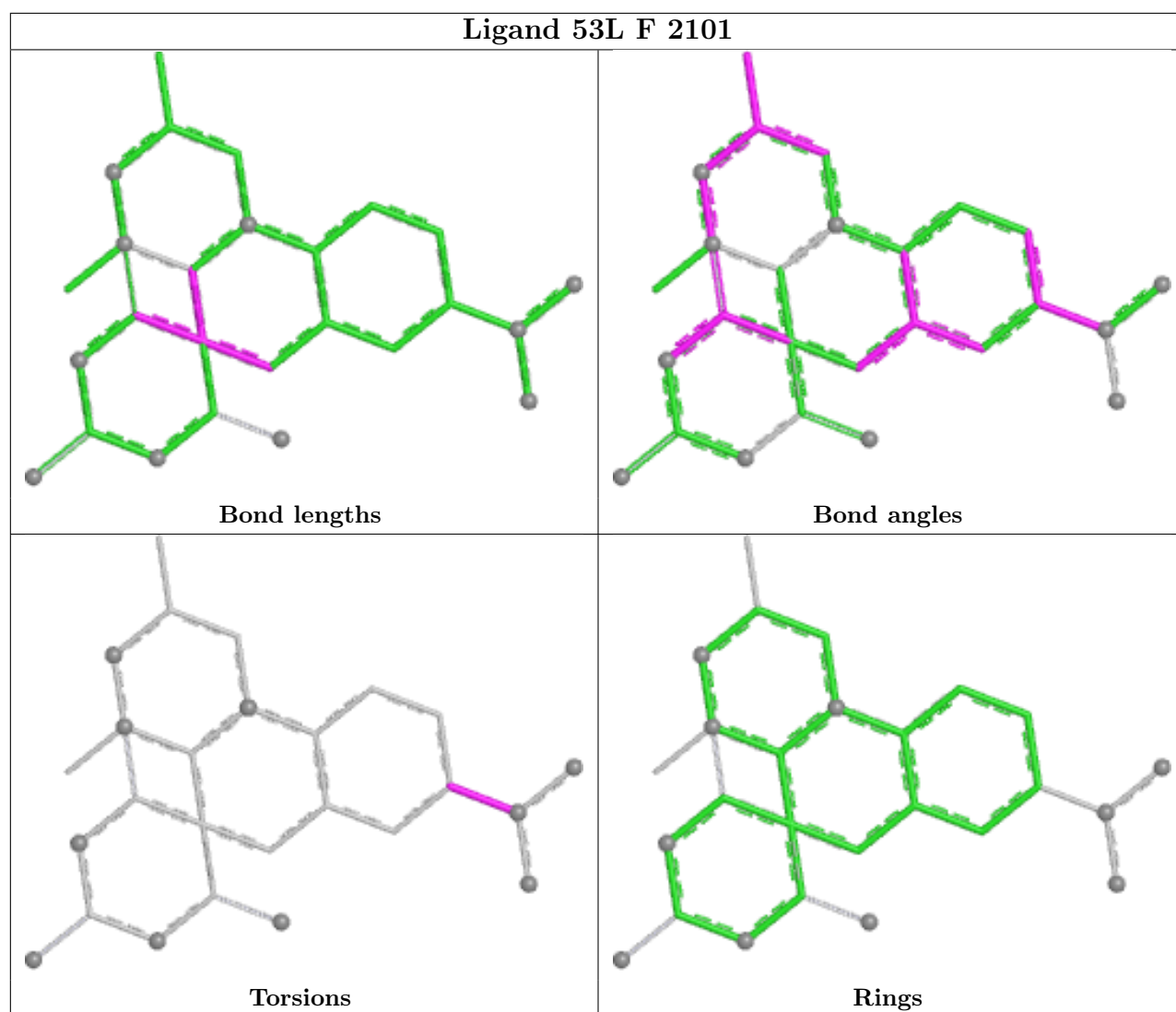
Bond angles



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

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, 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%)	-0.04	3 (0%) 85 72	19, 46, 69, 90	2 (0%)
1	C	479/482 (99%)	-0.12	2 (0%) 88 78	25, 41, 64, 95	0
1	R	476/482 (98%)	0.04	13 (2%) 56 35	20, 43, 104, 151	1 (0%)
1	T	480/482 (99%)	-0.09	6 (1%) 75 55	25, 42, 82, 115	0
2	B	188/188 (100%)	0.20	3 (1%) 70 50	30, 60, 84, 98	0
2	D	188/188 (100%)	0.18	1 (0%) 87 75	32, 60, 81, 90	0
2	S	188/188 (100%)	0.40	4 (2%) 63 42	32, 69, 95, 108	0
2	U	187/188 (99%)	0.18	3 (1%) 70 50	36, 62, 78, 88	0
3	E	20/20 (100%)	0.33	2 (10%) 12 7	32, 38, 59, 64	0
3	F	20/20 (100%)	0.32	0 100 100	33, 38, 50, 51	0
3	V	20/20 (100%)	0.38	1 (5%) 34 20	35, 44, 65, 73	0
3	W	20/20 (100%)	0.25	1 (5%) 34 20	33, 41, 70, 73	0
All	All	2747/2760 (99%)	0.04	39 (1%) 73 53	19, 47, 84, 151	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	251	GLU	4.0
1	R	10	ASN	4.0
1	R	313	ASN	3.8
1	R	309	ARG	3.7
3	E	2020	DT	3.3
1	T	490	LEU	3.2
2	S	442	SER	3.2
1	A	9	ILE	3.1
1	R	252	ARG	3.0
2	S	434	VAL	3.0
1	R	122[A]	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	R	11	GLU	2.9
2	S	638	VAL	2.8
1	T	310	LYS	2.6
2	U	444	LYS	2.6
2	U	445	SER	2.6
2	B	638	VAL	2.6
1	R	298	LEU	2.5
1	C	351	ALA	2.5
2	U	439	ALA	2.4
2	D	461	ILE	2.4
1	R	312	ALA	2.4
3	V	1	DG	2.4
3	W	1	DG	2.4
2	B	503	ILE	2.3
1	R	402	ASP	2.3
1	T	85	SER	2.3
1	C	11	GLU	2.3
2	B	417	LYS	2.3
3	E	1	DG	2.3
1	T	311	ASP	2.2
2	S	589	ASP	2.2
1	R	323	LYS	2.2
1	R	324	GLN	2.1
1	T	337	ALA	2.1
1	A	406	VAL	2.0
1	T	282	ARG	2.0
1	R	391	ILE	2.0
1	A	490	LEU	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	T	123	16/17	0.93	0.11	43,50,56,60	0
1	PTR	C	123	16/17	0.94	0.11	35,42,47,50	0
1	PTR	R	123	16/17	0.94	0.13	34,40,46,48	0
1	PTR	A	123	16/17	0.94	0.11	32,37,43,44	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

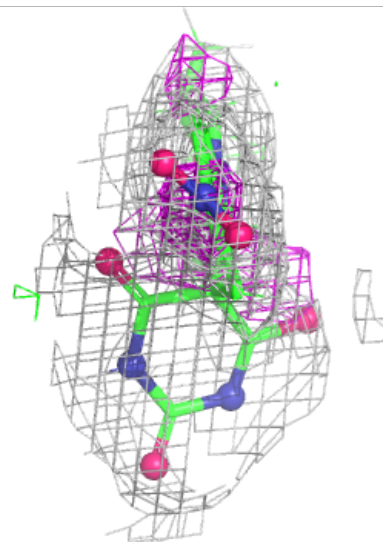
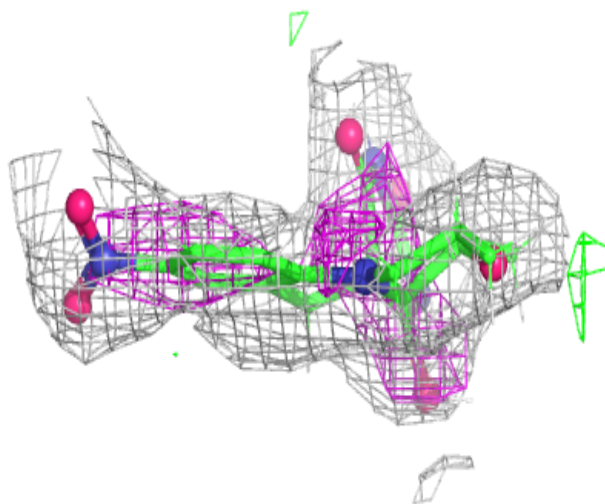
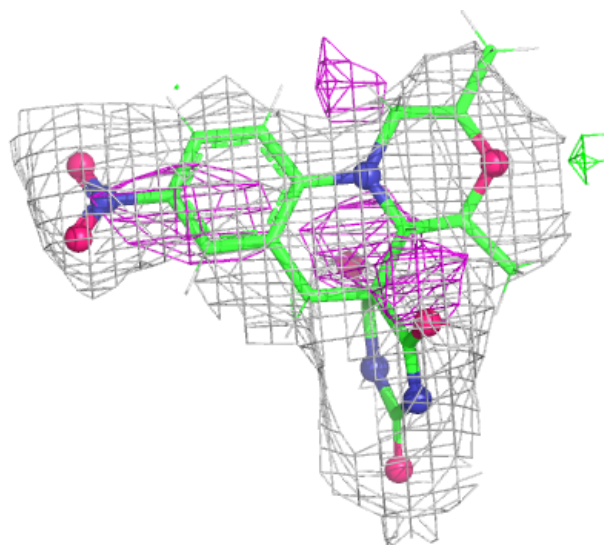
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	U	5002	6/6	0.80	0.13	33,40,42,43	0
6	GOL	D	1003	6/6	0.82	0.14	47,57,58,58	0
5	NA	C	502	1/1	0.83	0.13	30,30,30,30	0
5	NA	A	502	1/1	0.84	0.26	39,39,39,39	0
6	GOL	U	5003	6/6	0.84	0.19	55,66,67,67	0
6	GOL	A	503	6/6	0.86	0.17	30,36,39,39	0
4	SO4	A	501	5/5	0.88	0.12	65,65,66,66	0
10	50M	S	6002	27/27	0.89	0.12	18,21,25,27	0
8	53M	E	2101	27/27	0.90	0.11	18,22,25,28	0
8	53M	W	2101	27/27	0.91	0.10	19,21,25,28	0
9	53L	F	2101	27/27	0.91	0.11	19,21,26,29	0
5	NA	C	501	1/1	0.91	0.25	19,19,19,19	0
6	GOL	D	1002	6/6	0.92	0.16	39,47,49,49	0
5	NA	R	501	1/1	0.92	0.09	40,40,40,40	0
5	NA	T	503	1/1	0.92	0.13	43,43,43,43	0
4	SO4	T	501	5/5	0.92	0.10	55,56,56,57	0
4	SO4	T	502	5/5	0.94	0.14	54,55,56,56	0
7	MN	B	701	1/1	1.00	0.04	37,37,37,37	0
7	MN	D	1001	1/1	1.00	0.04	38,38,38,38	0
7	MN	S	6001	1/1	1.00	0.03	35,35,35,35	0
7	MN	U	5001	1/1	1.00	0.05	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

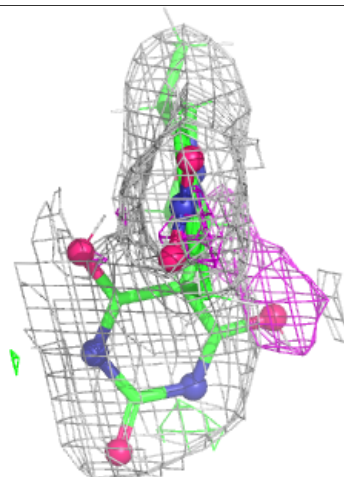
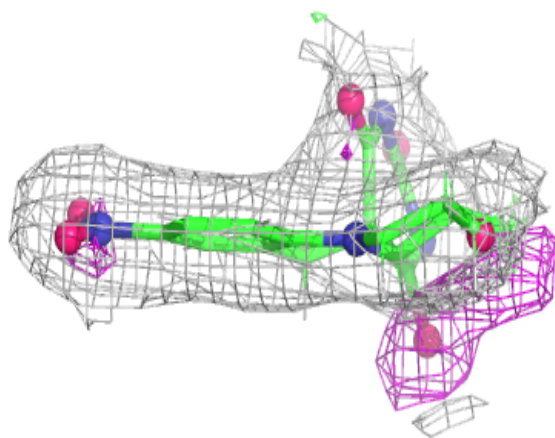
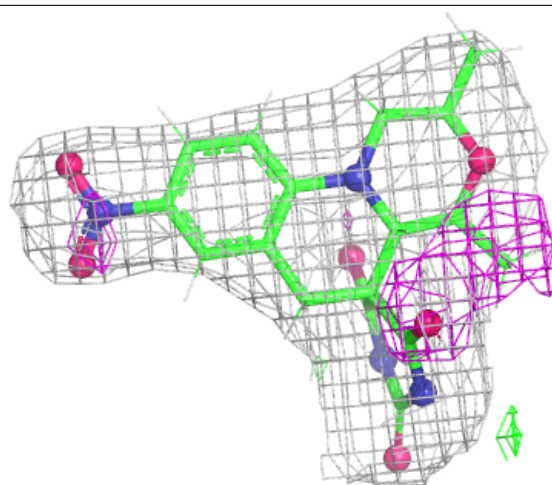
Electron density around 50M S 6002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



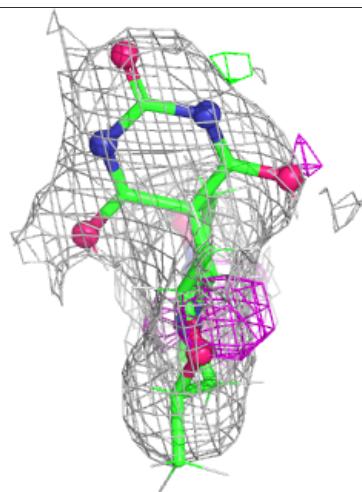
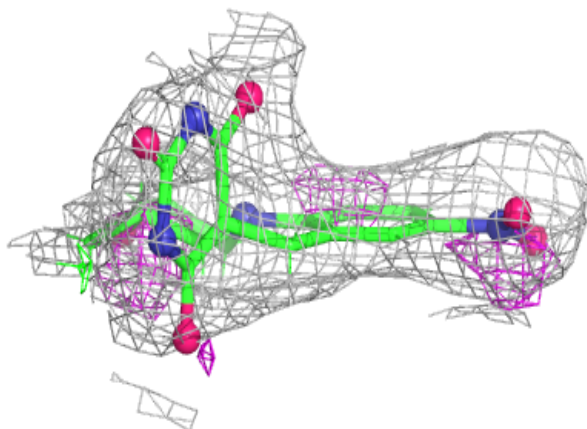
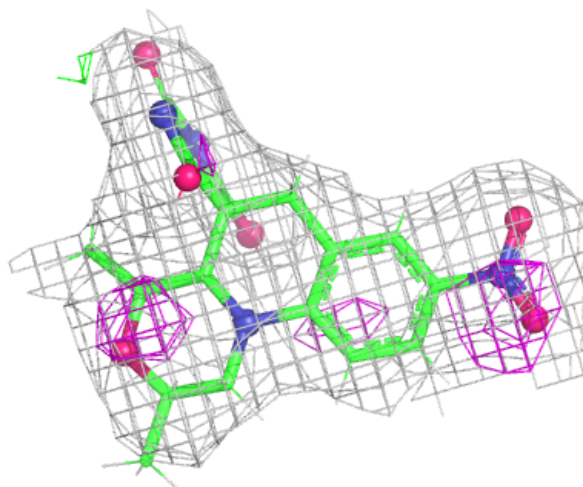
Electron density around 53M E 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



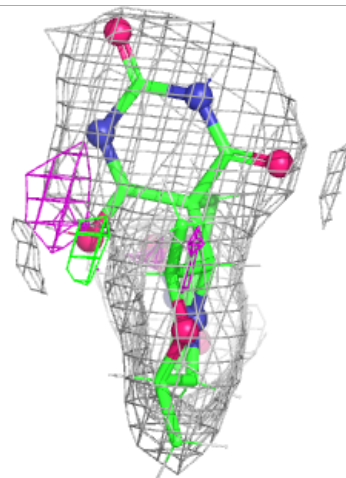
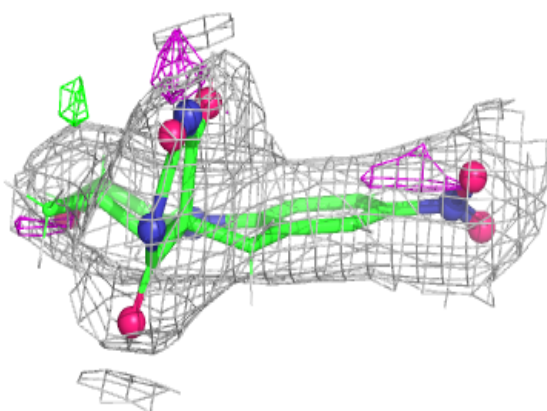
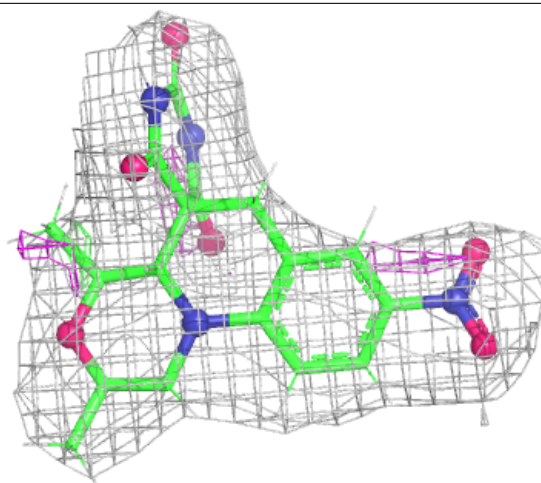
Electron density around 53M W 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 53L F 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.