

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.22
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	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 (i)

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.



Motria	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R <sub>free</sub>	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	А	482	87%	12%	
1	С	482	90%	9%	
1	R	482	87%	11%	••
1	Т	482	87%	12%	
2	В	188	<sup>2%</sup> 90%	8%	•



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Mol	Chain	Length	Quality of chain		
2	D	188	77% 20	0%	•
2	S	188	88%	11%	•
2	U	188	2% 	9%	••
3	Е	20	75% 2	5%	
3	F	20	65% 35%		
3	V	20	65% 35%		
3	W	20	65% 35%		



#### 5CDO

# 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace	
1	Δ	489	Total	С	Η	Ν	Ο	Р	S	0	4	0
	A	402	7629	2365	3821	693	733	1	16	0	4	0
1	C	480	Total	С	Η	Ν	Ο	Р	S	0	0	0
		400	7623	2358	3832	690	726	1	16	0	0	U
1	D	477	Total	С	Η	Ν	Ο	Р	S	0	1	0
	n 4	411	7503	2336	3752	676	722	1	16			
1	ı T	401	Total	С	Η	Ν	Ο	Р	S	0	0	0
	401	7522	2340	3755	680	731	1	15	0	0	0	

• Molecule 1 is a protein called DNA gyrase subunit A.

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

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
9	В	188	Total	С	Η	Ν	Ο	S	0	0	0
	D	100	2869	912	1413	251	284	9	0		0
0	П	199	Total	С	Η	Ν	Ο	S	0	0	0
	D	100	2861	910	1412	251	279	9	0	0	0
0	c	199	Total	С	Η	Ν	Ο	S	0	0	0
	G	100	2832	904	1395	250	274	9	0	0	0
0	2 U	U 187	Total	С	Η	Ν	Ο	S	0	0	0
			2838	902	1399	253	275	9	0		

There are 144 discrepancies between the modelled and reference sequences:

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



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



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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



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

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

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
2	F	20	Total	С	Η	Ν	Ο	Р	0	0	0
0		20	602	185	210	74	114	19	0	0	0
2	F	20	Total	С	Η	Ν	0	Р	0	0	0
0	Г	20	629	194	222	76	118	19	0		0
2	V	20	Total	С	Η	Ν	Ο	Р	0	0	0
0	v	20	630	194	223	76	118	19	0	0	0
2 W	20	Total	С	Η	Ν	Ο	Р	0	0	0	
3	VV V	20	601	184	210	74	114	19	0 0		0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Т	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Т	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Na 1 1	0	0
5	С	2	Total Na 2 2	0	0
5	R	1	Total Na 1 1	0	0
5	Т	1	Total Na 1 1	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 14	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	Н 8	O 3	0	0
6	D	1	Total 14	С 3	H 8	O 3	0	0
6	D	1	Total 14	С 3	Н 8	O 3	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	T	1	Total	С	Η	0	0	0
0 U		14	3	8	3	0	0	
6	TT	1	Total	С	Η	Ο	0	0
6 U	U		14	3	8	3		

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

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

• 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<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	F	1	Total	С	Η	Ν	Ο	0	0
0		L	45	17	18	4	6	0	0
0	147	1	Total	С	Η	Ν	Ο	0	0
0	VV V		45	17	18	4	6	U	



• 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<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues		Ate	$\mathbf{pms}$			ZeroOcc	AltConf
9	F	1	Total 45	C 17	H 18	N 4	O 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<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	C	1	Total	С	Η	Ν	Ο	0	0
10	c	1	45	17	18	4	6	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	10	Total O 10 10	0	0
11	В	5	Total O 5 5	0	0
11	С	4	Total O 4 4	0	0
11	D	4	Total O 4 4	0	0
11	Е	2	Total O 2 2	0	0
11	F	3	Total O 3 3	0	0
11	R	13	Total O 13 13	0	0
11	S	9	Total O 9 9	0	0
11	Т	15	Total O 15 15	0	0
11	U	7	Total O 7 7	0	0
11	V	4	Total O 4 4	0	0
11	W	6	Total O 6 6	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: DNA gyrase subunit A

Chain T:	87%	12%	
11E N10 114 114 114 114 114 114 114 114 114 1	M75 477 477 477 477 477 477 493 493 493 1103 1116 1116 1116 1132 1132 1133	V177 133 133 133 1206 1223 1223 251 255 255 255 255 255 255 255 255 255	7952
1299 1299 1311 1311 1325 1335 1335 1335 1335 1335	9368 7372 8372 8385 8385 8385 8396 8400 8400 8400 8400 8400 8400 8400 840	R433 R432 E437 E437 Y455 Y455 L455 L455 C455 L455 C455 L455 C455 L455 C455 L455 C455 C	
• Molecule 2: DNA g	yrase subunit B,DNA gyrase s	subunit B	
Chain B:	90%	8% •	
K417 L418 L418 R400 A409 A409 A409 A409 L418 L417 L417 L417	480 1489 1489 1489 1489 1489 1588 1588 1588 1588 1588 1589 1589 15	46 16 16 16 16 16 16 16 16 16 16 16 16 16	
• Molecule 2: DNA g	yrase subunit B,DNA gyrase s	subunit B	
Chain D:	77%	20% •	
R417         R417           1418         419           4419         443           1434         1434           1435         1443           1443         1444           1461         1463           1463         1463           1463         1463           1463         1463           1463         1463           1463         1463	V464 E465 E465 1474 1474 1474 1476 1476 1476 1476 1476	1101 1101 1101 1101 1101 1101 11020 11020 11020 11020 11021 11021 11021 11021 11021 11021	d590
1591 M596 M596 H600 H600 D615 B627 M637 V638			
• Molecule 2: DNA g	yrase subunit B,DNA gyrase s	subunit B	
Chain S:	88%	11% •	
K417 E427 E427 F431 F432 F432 F432 C436 C436 C436 C436 C436 C436 C436 C436	1454 1455 1455 1455 1459 1502 1503 1503 1503 1503 1503 1503 1503 1503	T595 1612 0616 0624 V638 V638	
• Molecule 2: DNA g	yrase subunit B,DNA gyrase s	subunit B	
Chain U:	89%	9% ••	
K417 5423 5423 5428 5428 6448 6446 6446 6446	R4-88 R4-88 14-76	12-31 155 96 156 12 166 29 166 37 17AL	
• Molecule 3: DNA ( *GP*CP*TP*T)-3')	5'-D(P*GP*AP*GP*CP*GP*	*TP*AP*C*GP*GP*CP*CP*	GP*TP*AP*CP
Chain E:	75%	25%	
61 65 16 76 47 47 6209 62099 12019 12020			



• 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: 65% 35%



• 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:	65%	35%

**11 12** 

• 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.	050/	250/
Unam vv.	65%	35%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	90.47Å 170.21Å 124.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $102.75^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{A})$	58.41 - 3.15	Depositor
Resolution (A)	58.41 - 3.15	EDS
% Data completeness	98.0 (58.41-3.15)	Depositor
(in resolution range)	98.1(58.41 - 3.15)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.47 (at 3.13 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
D D.	0.215 , $0.246$	Depositor
$\Pi, \Pi_{free}$	0.218 , $0.248$	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 <sup>2</sup>	$ \langle L  \rangle = 0.43, \langle L^2 \rangle = 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.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.26	0/3854	0.50	0/5195	
1	С	0.26	0/3821	0.51	1/5149~(0.0%)	
1	R	0.25	0/3779	0.49	0/5098	
1	Т	0.25	0/3797	0.50	0/5126	
2	В	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	Е	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	$1/3\overline{1252}\ (0.0\%)$	

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	С	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3808	3821	3801	29	0
1	С	3791	3832	3832	21	0
1	R	3751	3752	3752	27	0
1	Т	3767	3755	3755	25	0
2	В	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	Е	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	Т	10	0	0	1	0
5	A	1	0	0	0	0
5	С	2	0	0	0	0
5	R	1	0	0	0	0
5	Т	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	В	5	0	0	0	0
11	С	4	0	0	0	0
	D	4	0	0	0	0
	E	2	0	0	1	0
	F	3	0	0	0	0
	R	13	0	0	0	0
11	S	9	0	0	0	0
	Т	15	0	0	0	0
11	U	7	0	0	0	0
	V	4	0	0	0	0
	W	6	0	0	0	0
	All	22739	21756	21735	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 4.

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

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

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	А	483/482~(100%)	460~(95%)	23~(5%)	0	100	100	
1	С	477/482~(99%)	443~(93%)	33~(7%)	1 (0%)	47	78	
1	R	473/482~(98%)	449~(95%)	24~(5%)	0	100	100	
1	Т	478/482~(99%)	460 (96%)	17 (4%)	1 (0%)	47	78	
2	В	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	Т	33	ARG



Continued from previous page...

Mol	Chain	Res	Type		
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	Perce	entiles
1	А	408/416~(98%)	389~(95%)	19~(5%)	26	60
1	С	407/416~(98%)	395~(97%)	12 (3%)	42	72
1	R	399/416~(96%)	386~(97%)	13 (3%)	38	69
1	Т	401/416~(96%)	379~(94%)	22~(6%)	21	54
2	В	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

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

Mol	Chain	Chain Res	
1	R	228	SER
2	S	585	GLU
2	U	442	SER
1	R	311	ASP
2	S	417	LYS

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

Mol	Chain	Res	Type
1	А	412	GLN
1	Т	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).

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	Bond angle		
	туре	Chain	nes	res Link	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	А	123	3,1	15,16,17	1.36	1(6%)	19,22,24	0.55	0	
1	PTR	Т	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	С	123	$^{3,1}$	-	0/10/11/13	0/1/1/1
1	PTR	А	123	$^{3,1}$	-	1/10/11/13	0/1/1/1
1	PTR	Т	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		Observed(Å)	Ideal(Å)
1	С	123	PTR	OH-CZ	-4.44	1.30	1.40
1	А	123	PTR	OH-CZ	-4.20	1.31	1.40
1	R	123	PTR	OH-CZ	-4.03	1.31	1.40
1	Т	123	PTR	OH-CZ	-3.87	1.31	1.40

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Т	123	PTR	CB-CA-C	-2.24	107.27	111.47
1	С	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	А	123	PTR	O-C-CA-CB
1	R	123	PTR	O-C-CA-CB
1	Т	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).

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	ths	B	Bond ang	gles
	туре	Chain	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	Т	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	А	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	А	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%)



Mol Tur	Tune	Chain	Dog	Tink	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	Т	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	А	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	Е	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	-

The worst 5 of 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	50 M	C19-C26	-3.18	1.49	1.53
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	50 M	C18-C19	-2.64	1.49	1.54

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
10	S	6002	50 M	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	50 M	C16-C17-C12	3.54	122.20	118.95
8	Е	2101	53M	C26-C19-C20	-3.47	108.47	112.77
10	S	6002	50 M	O30-N28-C15	-3.29	114.14	118.80

There are no chirality outliers.



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

5 of 18 torsion outliers are listed below:

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
4	Т	502	SO4	1	0
6	А	503	GOL	1	0
8	W	2101	53 M	5	0
4	А	501	SO4	1	0
6	D	1002	GOL	1	0
9	F	2101	53L	3	0
8	Е	2101	53 M	4	0
10	S	6002	50 M	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.

















## 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	А	481/482~(99%)	-0.09	3 (0%) 89 84	25, 42, 62, 81	0
1	С	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	Т	480/482~(99%)	-0.07	2 (0%) 92 89	23, 38, 75, 106	0
2	В	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	Ε	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

The worst 5 of 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	В	492	ASP	3.1
2	S	612	ILE	3.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



Mol	Type	Chain	$\mathbf{Res}$	Atoms	RSCC	$\mathbf{RSR}$	${f B} ext{-factors}({f A}^2)$	$\mathbf{Q}{<}0.9$
1	PTR	С	123	16/17	0.94	0.21	$35,\!42,\!47,\!50$	0
1	PTR	Т	123	16/17	0.94	0.21	$43,\!50,\!56,\!60$	0
1	PTR	А	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

median,  $95^{th}$  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.

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} extsf{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	NA	Т	503	1/1	0.79	0.25	$43,\!43,\!43,\!43$	0
5	NA	С	502	1/1	0.81	0.28	$30,\!30,\!30,\!30$	0
5	NA	А	502	1/1	0.82	0.33	$39,\!39,\!39,\!39$	0
6	GOL	А	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	Е	2101	27/27	0.92	0.24	18,22,25,28	0
4	SO4	Т	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	Т	501	5/5	0.94	0.13	55, 56, 56, 57	0
4	SO4	А	501	5/5	0.95	0.17	$65,\!65,\!66,\!66$	0
5	NA	С	501	1/1	0.96	0.26	19, 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	В	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.

