

Full wwPDB X-ray Structure Validation Report (i)

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:	5CDM
:	2.5A structure of QPT-1 with S.aureus DNA gyrase and DNA
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:	2015-07-04
:	2.50 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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.



Matria	Whole archive	Similar resolution				
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA})$				
R_{free}	130704	4661 (2.50-2.50)				
Clashscore	141614	5346 (2.50-2.50)				
Ramachandran outliers	138981	5231 (2.50-2.50)				
Sidechain outliers	138945	5233 (2.50-2.50)				
RSRZ outliers	127900	4559 (2.50-2.50)				

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	В	190	78%	21%	
1	D	190	% 71%	27%	•
2	А	482	78%	20%	•
2	С	482	81%	18%	•
3	Е	8	50% 50%	%	



Mol	Chain	Length	Quality of chain								
3	F	8	75%	12% 12%							
4	Ι	12	67%	33%							
4	Ν	12	33% 50%	8% 8%							



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2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 23019 atoms, of which 11161 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 B,DNA gyrase subunit B.

Mol	Chain	Residues			Atom	IS		ZeroOcc	AltConf	Trace	
1	В	180	Total	С	Η	Ν	0	\mathbf{S}	0	9	0
I D	105	2937	931	1455	260	282	9	0	<u>ک</u>	0	
1	П	100	Total	С	Η	Ν	0	S	0	4	0
I D	190	2953	937	1459	262	286	9	0	±	0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	544	THR	-	linker	UNP P66937
В	545	GLY	-	linker	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937

• Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues		Atoms							AltConf	Trace
0	2 A	482	Total	С	Η	Ν	0	Р	S	0	4	0
			7668	2373	3845	696	736	1	17			
0	2 C	401	Total	С	Η	Ν	0	Р	S	0	19	0
	401	7803	2406	3926	711	743	1	16		12	0	

• 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*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	3 E 8	8	Total	С	Η	Ν	Ο	Р	0	0	0
5		0	256	78	90	33	47	8	0	0	
2	Б	7	Total	С	Η	Ν	Ο	Р	0	0	0
5 Г	(223	68	79	28	41	7	0		0	

• Molecule 4 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*GP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').



Mol	Chain	Residues		Atoms						AltConf	Trace
4	T	12	Total	С	Η	Ν	Ο	Р	0	0	0
т	4 1		375	116	134	43	71	11	0	0	
4	N	11	Total	С	Η	Ν	Ο	Р	0	0	0
4	4 IN	11	342	106	121	41	64	10	0	0	

• Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

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



Mol	Chain	Residues	At	toms	\mathbf{s}		ZeroOcc	AltConf
6	В	1	Total 14	C 3	Н 8	O 3	0	0
6	А	1	Total 14	C 3	H 8	O 3	0	0





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	А	1	Total 5	0 4	S 1	0	0

• Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total Na 1 1	0	0

• Molecule 9 is (2R,4S,4aS)-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',6'(1'H,3'H)-trione (three-letter code: 54Q) (formula: $C_{17}H_{18}N_4O_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
0	т	1	Total	С	Η	Ν	Ο	0	0	
9 1	1	1	45	17	18	4	6	0	0	
0	N	1	Total	С	Η	Ν	Ο	0	0	
9	IN	1	45	17	18	4	6	0	0	

• Molecule 10 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
10	Ν	1	Total 8	0 6	Р 2	0	1

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
11	А	113	Total O 113 113	0	0
11	D	25	$\begin{array}{cc} \text{Total} & \text{O} \\ 25 & 25 \end{array}$	0	0
11	С	102	Total O 102 102	0	0
11	Ε	13	Total O 13 13	0	0
11	Ι	5	Total O 5 5	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	14	Total O 14 14	0	0
11	Ν	21	TotalO2121	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 B,DNA gyrase subunit B



• Molecule 2: DNA gyrase subunit A



Chain C:	81%	18% •
ILE N10 R11 R11 R12 R15 R19 R16 R16 R46 R46 R47 R48 R48 R48 R48 R48 R58 R58 R58 R58 R58 R58 R58 R58 R58 R5	R65 R66 D73 H79 H79 R100 R100 C115 D116 D116 D116 D115 C123 R122 C125 F122 F123	K130 L133 E134 L135 L135 L135 L135 1139 D151
C152 N153 N153 N153 F166 F166 F166 C188 F165 C23 C23 C23 C23 C23 C23 C23 C23 C23 C23	F266 F266 F266 N269 N269 F280 F284 F284 F284 F285 F285 F285 F285 F285 F285 F285 F285	V333 R342 F343 K344 N347 K349 K349 E350
• Molecule 3: DNA (5'-D(P*GP*	AP*GP*CP*GP*TP*AP*C*GF	*GP*CP*CP*GP*TP*AP*CP
*GP*CP*TP*T)-3') Chain E: 50%	50%	
• Molecule 3: DNA (5'-D(P*GP*	AP*GP*CP*GP*TP*AP*C*GF	P*GP*CP*CP*GP*TP*AP*CP
*GP*CP*TP*T)-3') Chain F: 7	5% 12%	12%
• Molecule 4: DNA (5'-D(P*GP*	AP*GP*CP*GP*TP*AP*C*GF	P*GP*CP*CP*GP*TP*AP*CP
*GP*CP*TP*T)-3') Chain I: 67%	33%	
C2009 C2013 C2013 T2019 T2020		
• Molecule 4: DNA $(5'-D(P^*GP^* GP^*CP^*TP^*T)-3')$	AP*GP*CP*GP*TP*AP*C*GP	*GP*CP*CP*GP*TP*AP*CP

Chain N:	33%	50%	8%	8%
62009 62010 72011 72013 62013 62013 62015 72019 72019 72019				



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 61	Depositor	
Cell constants	93.88Å 93.88Å 412.48Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	36.78 - 2.50	Depositor	
Resolution (A)	36.79 - 2.50	EDS	
% Data completeness	95.3 (36.78-2.50)	Depositor	
(in resolution range)	95.3 (36.79 - 2.50)	EDS	
R _{merge}	(Not available)	Depositor	
R _{sym}	0.10	Depositor	
$< I/\sigma(I) > 1$	$1.75 (at 2.51 \text{\AA})$	Xtriage	
Refinement program	PHENIX	Depositor	
B B.	0.163 , 0.192	Depositor	
Π, Π_{free}	0.163 , 0.185	DCC	
R_{free} test set	3409 reflections $(5.06%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	45.7	Xtriage	
Anisotropy	0.207	Xtriage	
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.36 , 23.0	EDS	
L-test for twinning ²	$< L >=0.39, < L^2>=0.21$	Xtriage	
Estimated twinning fraction	0.213 for h,-h-k,-l	Xtriage	
Reported twinning fraction	0.220 for h,-h-k,-l	Depositor	
Outliers	0 of 67361 reflections	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	23019	wwPDB-VP	
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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, 54Q, MN, SO4, NA, PTR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	В	0.44	0/1513	0.54	0/2043	
1	D	0.42	0/1534	0.56	0/2072	
2	А	0.44	0/3866	0.57	0/5212	
2	С	0.46	0/3952	0.56	0/5320	
3	Е	0.98	0/186	0.86	0/285	
3	F	1.09	0/161	0.91	0/246	
4	Ι	1.09	0/269	0.94	0/414	
4	N	1.12	1/247~(0.4%)	0.97	0/380	
All	All	0.52	1/11728~(0.0%)	0.60	0/15972	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Ν	2013	DG	C3'-O3'	-5.77	1.36	1.44

There are no bond angle outliers.

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	В	1482	1455	1449	28	0
1	D	1494	1459	1442	35	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	3823	3845	3831	61	2
2	С	3877	3926	3872	56	2
3	Е	166	90	90	3	0
3	F	144	79	79	1	0
4	Ι	241	134	134	4	0
4	Ν	221	121	122	9	0
5	В	1	0	0	0	0
5	D	1	0	0	0	0
6	А	6	8	8	0	0
6	В	6	8	7	2	0
7	А	5	0	0	0	0
8	А	1	0	0	0	0
9	Ι	27	18	18	3	0
9	Ν	27	18	18	4	0
10	Ν	8	0	0	3	0
11	А	113	0	0	1	0
11	В	35	0	0	1	0
11	С	102	0	0	5	0
11	D	25	0	0	1	0
11	Е	13	0	0	0	0
11	F	14	0	0	0	0
11	Ι	5	0	0	0	0
11	N	21	0	0	0	0
All	All	11858	11161	11070	188	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:TYR:OH	1:B:615:ASP:OD1	1.92	0.87
1:B:425:SER:OG	1:B:427:GLU:OE1	1.94	0.86
2:C:204:ILE:O	2:C:349:LYS:NZ	2.09	0.85
2:A:252:ARG:NH1	2:A:308:VAL:O	2.16	0.78
2:A:389:ASP:OD1	2:A:438:ARG:NH2	2.18	0.77
1:B:631:GLN:NE2	1:B:634:GLU:OE1	2.23	0.71
1:D:587:ASN:ND2	1:D:590:GLN:OE1	2.25	0.69
1:D:420:ASP:OD2	1:D:499:ARG:NH1	2.26	0.68
1:D:470:ASP:OD2	11:D:801:HOH:O	2.12	0.67
2:C:344:LYS:NZ	2:C:350:GLU:OE1	2.27	0.67



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Atom-1	Atom-2	Interatomic	Clash
	7100HI 2	distance (Å)	overlap (Å)
4:I:2019:DT:O4	3:F:2:DA:N1	2.29	0.66
1:B:477:GLU:OE1	6:B:1002:GOL:O1	2.11	0.66
2:C:437:GLU:OE2	11:C:501:HOH:O	2.13	0.65
2:A:299:ARG:NH2	1:D:446:GLY:O	2.30	0.65
2:C:354:HIS:O	11:C:502:HOH:O	2.15	0.65
2:A:321:LEU:O	2:A:325:THR:OG1	2.10	0.64
2:C:445:TYR:CE2	2:C:449:LEU:HD11	2.34	0.63
2:C:115:GLY:HA3	2:C:269:ASN:ND2	2.14	0.63
2:C:283:ASP:HB2	2:C:285:LYS:CD	2.29	0.62
2:A:116:ASP:OD1	2:A:116:ASP:N	2.32	0.62
2:A:114:ASP:O	2:A:269:ASN:ND2	2.32	0.62
2:A:12:ARG:HH12	2:A:16:SER:HB3	1.65	0.62
2:C:64:TYR:HB3	2:C:125:GLU:HB3	1.79	0.62
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.30	0.61
1:D:430:GLU:HB3	1:D:502:LYS:HB2	1.83	0.61
2:C:66:LYS:HE3	2:C:125:GLU:HG3	1.81	0.61
4:N:2019:DT:HO3'	10:N:2101[A]:DT:P	2.25	0.60
2:A:64:TYR:HB3	2:A:125:GLU:HB3	1.84	0.60
1:B:447:ARG:HG2	1:B:454:ILE:HD11	1.83	0.60
1:B:476:ASN:OD1	1:B:479:ARG:NH2	2.35	0.59
4:N:2016:DC:H2"	4:N:2017:DG:H5'	1.85	0.59
1:B:605:GLN:N	2:A:10:ASN:O	2.36	0.58
2:C:292:LEU:CD1	2:C:306:ILE:HG12	2.34	0.58
4:N:2019:DT:O3'	10:N:2101[A]:DT:P	2.62	0.57
2:C:324:GLN:NE2	11:C:506:HOH:O	2.37	0.57
1:D:470:ASP:OD1	1:D:471:ARG:N	2.38	0.57
1:B:624:ASP:OD1	1:B:625:VAL:N	2.38	0.57
1:D:469:LEU:HG	1:D:473:LEU:HD11	1.86	0.56
1:D:443:THR:HG23	1:D:596:MET:SD	2.46	0.56
2:A:299:ARG:HH11	2:A:299:ARG:HG3	1.71	0.56
1:B:501:HIS:ND1	11:B:1103:HOH:O	2.33	0.56
2:A:298:LEU:HB2	2:A:299:ARG:NH1	2.22	0.54
2:A:256:ARG:HG2	2:A:310:LYS:HB2	1.90	0.54
1:D:448:ASP:OD1	1:D:450[B]:ARG:HG3	2.07	0.53
1:D:633:ILE:O	1:D:637:ALA:HB2	2.08	0.53
1:B:443:THR:HG22	1:B:454:ILE:HD11	1.91	0.53
2:A:92:ARG:NH2	3:E:6:DT:OP2	2.42	0.53
2:C:475:GLU:OE2	2:C:479:ARG:NH2	2.42	0.52
2:A:112:SER:HB2	2:A:116:ASP:OD1	2.09	0.52
1:D:479[B]:ARG:HG3	1:D:479[B]:ARG:HH11	1.75	0.52
1:D:607:LYS:HE3	2:C:11:GLU:CB	2.40	0.52



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:447:ARG:HD3	1:D:454:ILE:HD12	1.92	0.52
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.45	0.52
1:B:592:TRP:HA	1:B:596:MET:HB2	1.90	0.51
2:A:363:VAL:HG21	2:A:469:VAL:HG22	1.92	0.51
4:N:2012:DC:C2	9:N:2102:54Q:H12	2.45	0.51
2:C:15:THR:O	2:C:19:ARG:HG3	2.09	0.51
2:A:135:LEU:HD23	2:A:162:ALA:HA	1.93	0.51
1:D:515:HIS:HB2	2:C:25:TYR:CD1	2.45	0.51
2:C:283:ASP:HB2	2:C:285:LYS:HD3	1.92	0.51
1:B:476:ASN:N	6:B:1002:GOL:O2	2.30	0.51
2:A:355:TYR:O	2:A:358:HIS:HB3	2.11	0.50
1:D:447:ARG:HD3	1:D:454:ILE:CD1	2.42	0.50
2:A:103:LEU:HB3	2:A:132:THR:OG1	2.12	0.50
2:A:270:LYS:NZ	2:A:294:ASP:OD2	2.41	0.50
1:D:443:THR:HG22	1:D:454:ILE:CD1	2.42	0.50
2:A:466:LEU:HD23	2:A:470:ARG:NH2	2.27	0.49
2:C:137:ARG:NH2	11:C:512:HOH:O	2.44	0.49
4:N:2017:DG:H1'	4:N:2018:DC:H5'	1.94	0.49
1:D:442:SER:HB3	1:D:591:LEU:HD12	1.93	0.49
1:D:444:LYS:HA	1:D:447:ARG:HG2	1.93	0.49
2:C:283:ASP:HB2	2:C:285:LYS:HD2	1.93	0.49
2:A:44:PRO:O	2:A:48:ARG:HG3	2.11	0.49
2:A:59:THR:OG1	2:A:61:ASP:OD1	2.22	0.49
2:C:101:TYR:CZ	2:C:188:LEU:HB2	2.47	0.49
2:A:237:GLY:HA2	2:A:335:MET:HE2	1.96	0.48
2:A:381:LEU:HD22	2:A:441:ILE:HG23	1.96	0.48
9:N:2102:54Q:H3	9:N:2102:54Q:C14	2.42	0.48
2:A:149:ASN:ND2	2:A:151:ASP:OD1	2.47	0.48
2:A:329:THR:HG22	2:A:330:SER:N	2.29	0.48
2:A:395:ILE:O	2:A:399:ARG:HG3	2.13	0.48
2:C:367:THR:HG22	2:C:459:LEU:HD11	1.96	0.48
1:B:511:VAL:HB	2:A:25:TYR:HA	1.96	0.48
2:C:151:ASP:OD1	2:C:153:ASN:HB2	2.13	0.48
2:A:377:ARG:CG	2:A:448:LEU:HD11	2.45	0.47
2:A:320:ASN:O	2:A:324:GLN:HG3	2.14	0.47
9:I:2101:54Q:C14	9:I:2101:54Q:H3	2.45	0.47
2:C:116:ASP:OD1	2:C:116:ASP:N	2.48	0.47
2:A:291:ASP:HB3	2:A:307:ASP:HB2	1.95	0.47
4:N:2012:DC:H1'	9:N:2102:54Q:O5	2.15	0.47
1:D:434:VAL:HG12	1:D:435:GLU:N	2.30	0.47
4:I:2018:DC:H2"	4:I:2019:DT:H71	1.96	0.47



5CDM

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:164:PHE:HB2	2:A:165:PRO:HD2	1.97	0.47
2:C:369:TYR:CD1	2:C:369:TYR:C	2.88	0.47
1:B:443:THR:O	1:B:447:ARG:HG2	2.15	0.46
4:I:2012:DC:C2	9:I:2101:54Q:H12	2.50	0.46
2:A:48:ARG:HD3	2:A:78:TYR:CB	2.45	0.46
1:D:516:ILE:HA	1:D:519:LEU:HD12	1.97	0.46
2:C:252:ARG:HD3	2:C:258:ARG:HB3	1.98	0.46
1:D:420:ASP:OD1	1:D:500:TYR:OH	2.25	0.46
2:A:192:ILE:HD13	2:A:477:ARG:HB2	1.98	0.46
2:A:410:SER:O	2:A:414:ARG:HG3	2.16	0.46
1:D:598:PRO:HA	1:D:601:ARG:HG2	1.97	0.46
1:B:444:LYS:HA	1:B:454:ILE:CD1	2.46	0.45
2:A:332:GLY:O	11:A:601:HOH:O	2.20	0.45
2:C:381:LEU:HD23	2:C:384:LEU:HD12	1.98	0.45
1:B:502:LYS:HG2	1:B:538:TYR:CE1	2.52	0.45
4:N:2013:DG:C2	9:N:2102:54Q:H15	2.51	0.45
2:C:159:VAL:HG22	2:C:160:LEU:N	2.31	0.45
1:B:637:ALA:HB1	1:B:639:TYR:CE2	2.51	0.45
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.51	0.45
1:B:515:HIS:CD2	2:A:25:TYR:CD2	3.05	0.45
2:A:84:SER:O	2:A:88:GLU:HB2	2.17	0.45
1:D:542:PRO:HB2	1:D:543:PRO:HD2	1.99	0.45
1:D:503:ILE:N	1:D:503:ILE:HD12	2.32	0.45
4:I:2013:DG:C2	9:I:2101:54Q:H15	2.52	0.45
2:A:296:THR:HG23	2:A:302:VAL:HA	1.99	0.44
2:C:115:GLY:HA3	2:C:269:ASN:HD21	1.79	0.44
1:D:544:THR:HG22	1:D:545:GLY:N	2.32	0.44
3:E:1:DG:H2'	3:E:2:DA:C4	2.53	0.44
2:C:12:ARG:HH22	2:C:20:GLU:CD	2.21	0.44
2:A:87:TYR:O	2:A:91:VAL:HG23	2.17	0.44
2:A:313:ASN:O	2:A:317:ILE:HG13	2.18	0.44
2:C:364:ARG:O	2:C:368:GLN:HG3	2.18	0.44
2:C:280:LEU:HD23	2:C:285:LYS:HE2	2.00	0.43
2:C:120:ALA:HB3	2:C:123:PTR:HD1	2.00	0.43
2:C:347:ASN:ND2	2:C:350:GLU:OE2	2.51	0.43
2:C:391:ILE:O	2:C:395:ILE:HG12	2.18	0.43
4:N:2019:DT:O3'	10:N:2101[B]:DT:P	2.77	0.43
2:A:396:SER:O	2:A:400:GLU:HG3	2.19	0.43
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.54	0.43
2:C:100:ARG:HB2	2:C:185:PRO:HB2	2.00	0.43
2:C:434:THR:O	2:C:438:ARG:HD3	2.19	0.43



5CDM

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:444:LYS:HG3	1:B:454:ILE:HD12	2.00	0.43
2:A:225:LEU:HD21	2:A:244:ARG:HD2	2.00	0.43
2:C:229:GLY:HA3	2:C:240:SER:O	2.19	0.43
2:A:67:SER:O	2:A:71:VAL:HG23	2.19	0.43
2:C:135:LEU:HG	2:C:164:PHE:CE1	2.54	0.43
1:D:431:ILE:HA	1:D:453:ALA:O	2.19	0.42
1:D:610:ASP:OD1	1:D:611:ALA:N	2.53	0.42
2:A:325:THR:HB	2:A:326:PRO:CD	2.49	0.42
2:C:135:LEU:HG	2:C:164:PHE:HE1	1.84	0.42
2:A:52:GLY:O	2:A:56:GLN:HG3	2.19	0.42
2:C:238[A]:ARG:HA	2:C:333:VAL:O	2.20	0.42
1:B:493:PHE:HE1	1:B:495:LEU:HB2	1.85	0.42
2:C:10:ASN:CG	2:C:11:GLU:H	2.22	0.42
2:C:266:PHE:O	2:C:267:GLN:HB2	2.19	0.42
2:C:283:ASP:CB	2:C:285:LYS:HD2	2.49	0.42
2:C:361:THR:O	2:C:365:ARG:HG3	2.19	0.42
2:A:48:ARG:HD3	2:A:78:TYR:HB3	2.00	0.42
2:C:130:LYS:HA	2:C:133:LEU:HD12	2.01	0.42
2:A:87:TYR:CD1	2:A:121:MET:HB3	2.55	0.42
2:C:56:GLN:NE2	2:C:73:ASP:HB3	2.34	0.42
2:C:475:GLU:CD	2:C:479:ARG:HH21	2.23	0.42
2:C:238[B]:ARG:HA	2:C:333:VAL:O	2.20	0.42
1:B:421:CYS:HA	1:B:449:SER:O	2.20	0.41
2:A:436:LEU:HB3	2:C:402:ASP:O	2.20	0.41
1:D:494:ASP:CG	1:D:497:LYS:HG3	2.40	0.41
1:D:432:PHE:CE2	1:D:596:MET:HE3	2.55	0.41
2:C:368:GLN:O	2:C:372:ARG:HG3	2.20	0.41
1:B:522:THR:OG1	1:B:622:MET:HG3	2.20	0.41
2:A:175:ILE:HD12	3:E:5:DG:C2	2.56	0.41
2:A:280:LEU:HD22	2:A:285:LYS:HB2	2.03	0.41
1:B:427:GLU:H	1:B:427:GLU:CD	2.22	0.41
2:A:14:ILE:HG23	2:A:15:THR:N	2.35	0.41
2:A:96:ASP:O	2:A:219:PRO:HB2	2.20	0.41
1:B:468:ARG:O	1:B:472:ILE:HG13	2.21	0.41
2:A:93:MET:HG2	2:A:99:TYR:CZ	2.55	0.41
1:D:434:VAL:HG23	1:D:454:ILE:HG23	2.02	0.41
2:C:58:MET:HA	2:C:58:MET:CE	2.51	0.41
2:C:100:ARG:HG3	2:C:101:TYR:CE2	2.56	0.41
1:B:432:PHE:HE1	1:B:452:GLN:HG2	1.84	0.41
2:C:280:LEU:HD23	2:C:285:LYS:NZ	2.36	0.41
4:N:2011:DC:C5	4:N:2012:DC:N4	2.89	0.41



5CDM

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:ARG:NH1	2:C:79:HIS:ND1	2.65	0.41
2:A:325:THR:HB	2:A:326:PRO:HD2	2.03	0.41
2:C:431[B]:ARG:C	2:C:433:LEU:H	2.23	0.41
2:A:42:LEU:HD13	2:A:47:ARG:HA	2.02	0.41
2:C:46:HIS:ND1	11:C:505:HOH:O	2.37	0.41
2:A:431:ARG:HB2	2:C:404:ASP:OD2	2.20	0.40
2:A:299:ARG:HG3	2:A:299:ARG:NH1	2.35	0.40
1:B:624:ASP:OD1	1:B:625:VAL:HG23	2.21	0.40
2:A:269:ASN:OD1	2:A:271:ALA:N	2.54	0.40
2:A:432:ARG:HH11	2:A:432:ARG:HG3	1.87	0.40
1:D:626:VAL:O	1:D:629:ARG:HB3	2.21	0.40
2:A:238:ARG:HA	2:A:333:VAL:O	2.22	0.40
1:D:443:THR:HG22	1:D:454:ILE:HD13	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:416:LYS:NZ	2:C:322:TYR:O[1_545]	2.11	0.09
2:A:409:GLU:OE1	2:C:323:LYS:NZ[1_545]	2.16	0.04

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	nalysed Favoured Allowed		Outliers	Perce	ntiles
1	В	189/190~(100%)	185~(98%)	4 (2%)	0	100	100
1	D	192/190~(101%)	189~(98%)	3~(2%)	0	100	100
2	А	483/482~(100%)	470 (97%)	12 (2%)	1 (0%)	47	68
2	С	490/482~(102%)	470 (96%)	19 (4%)	1 (0%)	47	68
All	All	1354/1344~(101%)	1314 (97%)	38 (3%)	2 (0%)	47	73



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	33	ARG
2	А	33	ARG

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	155/158~(98%)	149~(96%)	6 (4%)	32 57
1	D	156/158~(99%)	146 (94%)	10 (6%)	17 33
2	А	412/416~(99%)	394~(96%)	18 (4%)	28 52
2	С	421/416~(101%)	404 (96%)	17 (4%)	31 56
All	All	1144/1148 (100%)	1093 (96%)	51 (4%)	28 51

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	422	SER
1	В	424	LYS
1	В	442	SER
1	В	447	ARG
1	В	581	LYS
1	В	600	HIS
2	А	84	SER
2	А	88	GLU
2	А	112	SER
2	А	113	MET
2	А	116	ASP
2	А	121	MET
2	А	143	THR
2	А	191	LEU
2	А	238	ARG
2	А	284	LYS
2	А	299	ARG
2	А	391	ILE



Mol	Chain	Res	Type
2	А	393	GLU
2	А	414	ARG
2	А	436	LEU
2	А	438	ARG
2	А	489	GLN
2	А	490	LEU
1	D	418	LEU
1	D	420	ASP
1	D	430	GLU
1	D	442	SER
1	D	445	SER
1	D	457	LEU
1	D	589	ASP
1	D	590	GLN
1	D	595	THR
1	D	615	ASP
2	С	62	LYS
2	С	63	SER
2	С	66	LYS
2	С	69	ARG
2	С	85	SER
2	С	122	ARG
2	С	139	ILE
2	С	244	ARG
2	С	252	ARG
2	С	285	LYS
2	С	295	GLU
2	С	319	ASN
2	С	342[A]	ARG
2	С	342[B]	ARG
2	С	423	GLN
2	С	431[A]	ARG
2	С	431[B]	ARG

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

Mol	Chain	Res	Type
1	В	501	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)

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

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

Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	B	ond ang	gles
MOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	PTR	С	123	2,4	15,16,17	1.31	1 (6%)	19,22,24	1.02	1 (5%)
2	PTR	А	123	2,4	15,16,17	1.21	1 (6%)	19,22,24	0.64	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
2	PTR	С	123	2,4	-	1/10/11/13	0/1/1/1
2	PTR	А	123	2,4	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	123	PTR	OH-CZ	-4.33	1.30	1.40
2	А	123	PTR	OH-CZ	-4.25	1.31	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	123	PTR	CB-CA-C	-3.79	104.36	111.47
2	А	123	PTR	CB-CA-C	-2.12	107.49	111.47

There are no chirality outliers.



All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	123	PTR	CZ-OH-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	123	PTR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	GOL	А	503	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.84	0
9	54Q	Ι	2101	-	29,30,30	0.62	0	39,47,47	0.76	1 (2%)
6	GOL	В	1002	-	$5,\!5,\!5$	1.04	1 (20%)	$5,\!5,\!5$	1.11	0
10	DT	N	2101[B]	-	0,3,22	-	-	0,3,33	-	-
7	SO4	А	501	-	4,4,4	0.39	0	6,6,6	0.29	0
10	DT	N	2101[A]	-	0,3,22	-	-	0,3,33	-	-
9	54Q	N	2102	-	29,30,30	0.78	1 (3%)	39,47,47	0.75	1 (2%)

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	В	1002	-	-	2/4/4/4	-
6	GOL	А	503	-	-	4/4/4/4	-
9	54Q	N	2102	-	-	0/2/55/55	0/4/4/4
9	54Q	Ι	2101	-	-	0/2/55/55	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
6	В	1002	GOL	O2-C2	-2.31	1.36	1.43
9	N	2102	54Q	C-N	2.30	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
9	N	2102	54Q	C5-N-C6	2.93	124.49	118.69
9	Ι	2101	54Q	C5-N-C6	2.82	124.28	118.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	1002	GOL	C1-C2-C3-O3
6	В	1002	GOL	O2-C2-C3-O3
6	А	503	GOL	O1-C1-C2-C3
6	А	503	GOL	C1-C2-C3-O3
6	А	503	GOL	O1-C1-C2-O2
6	А	503	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Ι	2101	54Q	3	0
6	В	1002	GOL	2	0
10	Ν	2101[B]	DT	1	0
10	Ν	2101[A]	DT	2	0
9	N	2102	54Q	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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	В	189/190~(99%)	-0.01	0 100 100	35, 55, 76, 103	0
1	D	190/190~(100%)	0.07	1 (0%) 91 91	38, 59, 83, 97	0
2	А	481/482~(99%)	-0.10	2 (0%) 92 93	30, 46, 71, 95	0
2	С	480/482~(99%)	-0.18	0 100 100	26, 45, 66, 82	0
3	Ε	8/8~(100%)	-0.32	0 100 100	34, 39, 48, 59	0
3	F	7/8~(87%)	-0.28	0 100 100	35, 37, 54, 83	0
4	Ι	12/12~(100%)	-0.33	0 100 100	39, 45, 76, 98	0
4	Ν	11/12~(91%)	-0.30	0 100 100	35, 39, 51, 52	0
All	All	1378/1384 (99%)	-0.10	3 (0%) 95 95	26, 48, 74, 103	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	А	9	ILE	3.0
1	D	580	TYR	3.0
2	А	490	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	PTR	А	123	16/17	0.98	0.17	31,38,43,44	0
2	PTR	С	123	16/17	0.99	0.17	36,46,56,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q < 0.9
6	GOL	В	1002	6/6	0.89	0.16	40,48,53,54	0
10	DT	N	2101[A]	4/21	0.91	0.19	23,29,33,42	4
10	DT	N	2101[B]	4/21	0.91	0.19	26,31,33,38	4
7	SO4	А	501	5/5	0.92	0.16	$61,\!61,\!67,\!74$	0
6	GOL	А	503	6/6	0.96	0.15	29,48,67,70	0
9	54Q	Ι	2101	27/27	0.96	0.14	$29,\!36,\!43,\!50$	0
8	NA	А	502	1/1	0.98	0.08	41,41,41,41	0
9	54Q	N	2102	27/27	0.98	0.12	27,35,43,50	0
5	MN	В	1001	1/1	0.99	0.17	43,43,43,43	0
5	MN	D	701	1/1	0.99	0.17	38,38,38,38	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.

6.5 Other polymers (i)

There are no such residues in this entry.

