wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 09:53 PM EDT

PDB ID	:	6OY5
Title	:	X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter at 3 min
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2019-05-14
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

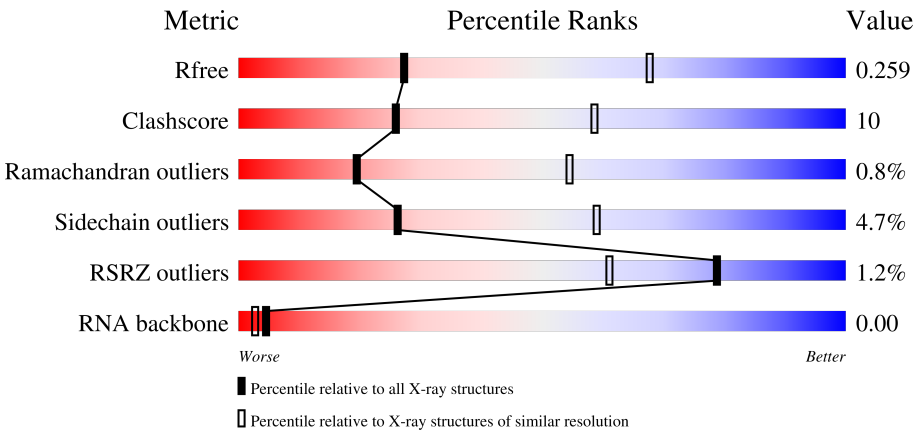
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	54% 17% • 28%
1	B	315	52% 18% • 29%
2	C	1119	.% 71% 27% ••
3	D	1524	.% 70% 25% • •

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Mol	Chain	Length	Quality of chain
4	E	99	74% 20% • 5%
5	F	423	4% 60% 19% • 18%
6	G	22	23% 27% 36% 14%
7	H	27	22% 48% 11% 19%
8	I	2	50% 50%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28534 atoms, of which 0 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1782	1138	310	332	2	0	0	0
1	B	224	1767	1129	307	329	2	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1111	8764	5545	1561	1634	24	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1484	11722	7431	2065	2191	35	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	761	486	132	139	4	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2807	1770	509	524	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*CP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	19	386	183	75	109	19	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP*GP*AP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	22	453	216	87	129	21	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	2	55	20	10	21	4	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

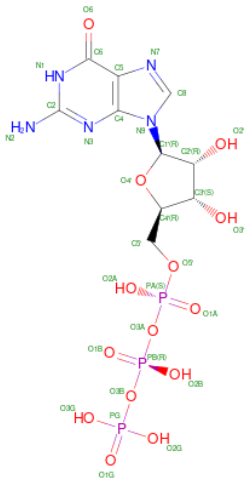
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0
9	D	2	2	2	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
10	D	2	2	2	0	0

- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



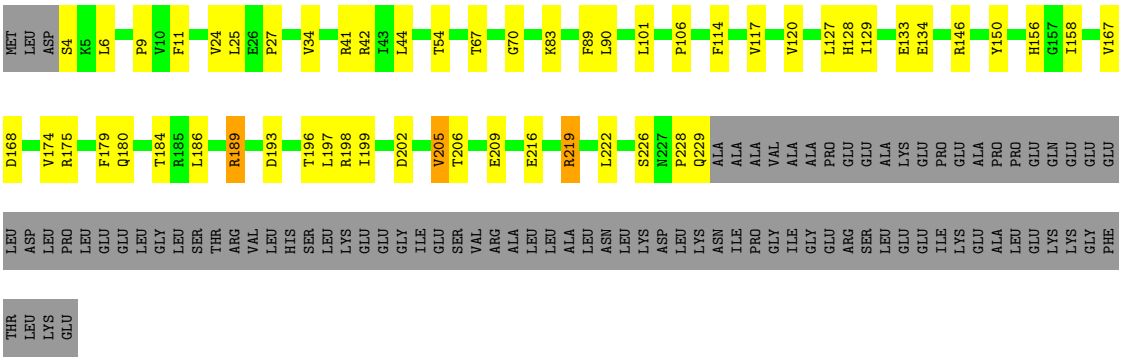
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	D	1	32	10	5	14	3	0	0

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.

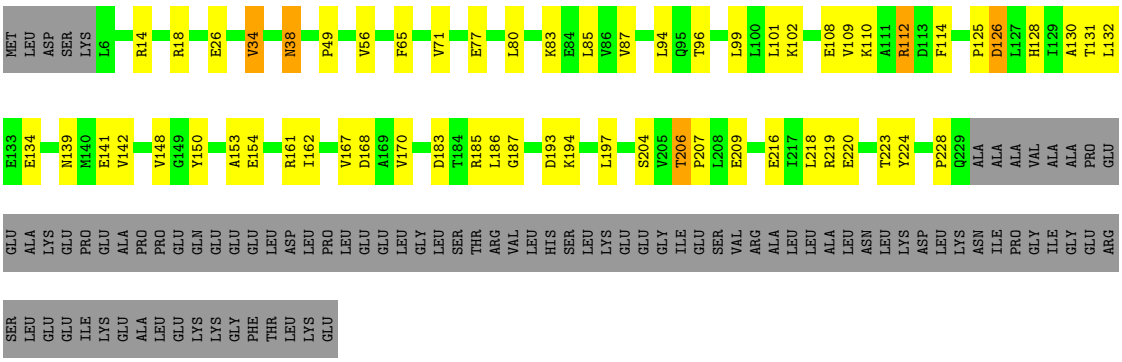
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



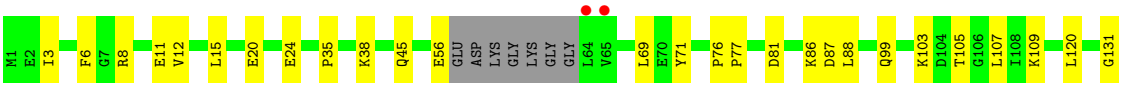
• Molecule 1: DNA-directed RNA polymerase subunit alpha

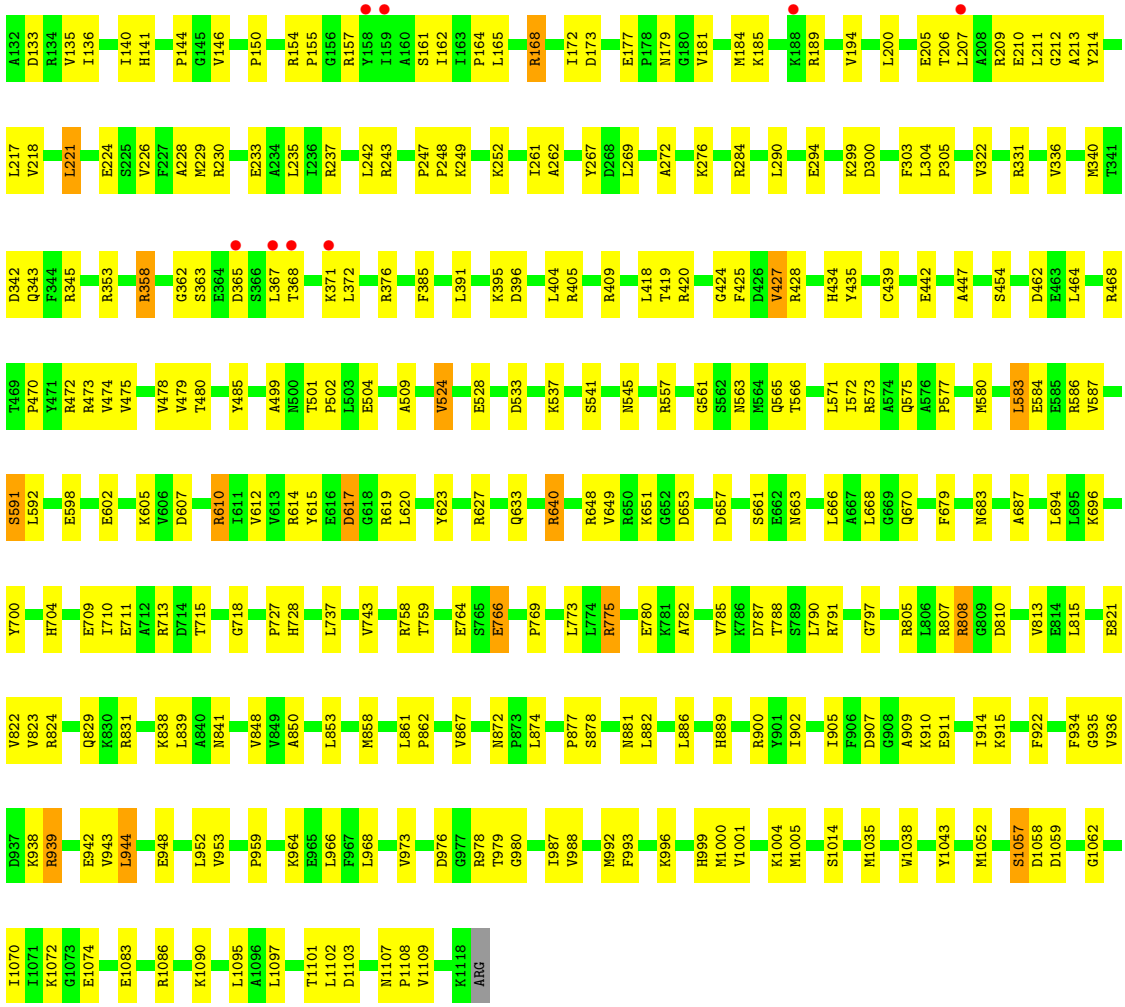
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

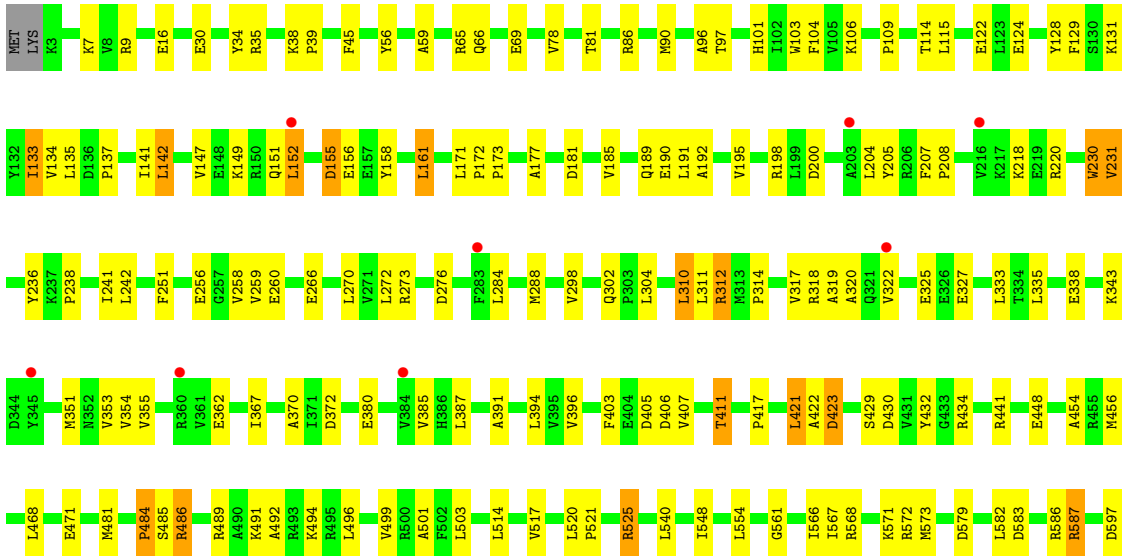
Chain C:





- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



R598 P599 L603 R613 L618 V623 D624 Y625 S629 V630 L639 H640 Q641 C642 G643 L644 P645 M648 A649 L650 E651 L652 P655 F656 L657 L658 M661 K664 N669 R675 E693 V694 I695 H696 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 G712 I713

Q714 A715 P718 G723 Q727 L728 H729 N737 D741 Q744 M745 V749 P750 L751 F754 M763 L764 H767 E776 P777 L778 D784 I792 T793 R796 K797 E798 K799 K800 G803 L804 E805 F806 A807 T808 P809 E817 R818 G819 A822 L823 N824 A825

P826 I827 K828 V829 A830 G831 R832 K840 Y841 V842 F843 A844 N845 P846 V853 V858 D859 L860 Q861 D862 T865 R872 T875 S876 R879 F882 V890 K894 L899 V904 P905 Q906 E907 K908 N909 Q917 R921 L922 G923 M924 F939 T943 G946

I951 D952 E959 K960 V963 K970 L971 L972 Q973 I974 A977 Y978 F982 L993 N1014 M1023 A1028 R1029 G1030 N1031 I1035 R1036 Q1037 L1038 C1039 G1040 L1041 R1042 G1043 L1044 K1047 P1048 S1049 G1050 E1051 P1056 V1057 S1060 F1061 R1062 E1063 L1068 K1079

T1084 R1087 T1088 V1099 I1105 R1108 P1125 R1130 S1131 L1132 R1137 E1141 A1142 G1143 L1144 R1147 V1148 L1149 E1152 V1153 E1154 V1155 V1158 E1161 Y1165 L1166 V1188 R1189 S1190 Q1195 Y1198 G1199 K1203 C1204 D1208 L1209 S1210 M1211 A1212 R1213 P1214

E1219 A1220 V1221 L1236 T1237 MET ARG THR PHE HIS THR GLY GLY VAL ALA GLY ALA ALA ASP ILE THR Q1254 G1255 L1256 P1257 R1258 F1263 R1267 K1271 A1272 I1277 D1278 V1281 E1284 L1290 S1291 V1292 F1293 V1294 S1300 K1301 E1302 Y1303 K1304 L1305 P1306 K1307 V1313 K1314

D1317 Y1318 V1319 Q1323 T1326 D1331 L1336 K1339 E1342 A1343 V1344 Y1347 L1348 V1349 E1350 E1351 K1354 Q1359 K1362 L1363 H1364 D1365 K1366 V1371 M1375 M1376 K1377 Y1378 V1379 E1380 D1386 S1387 R1388 V1400 K1412 T1413 L1420 K1426 T1444 T1448

I1452 K1456 I1460 K1463 I1467 R1470 F1480 V1486 L1492 K1493 A1494 I1495 E1496 E1497 A1498 R1499 A1502 VAL GLU ALA LYS GLU ARG PRO ALA ALA ARG ARG GLY VAL LYS ARG GLU GLN PRO GLY LYS GLN ALA

- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 74% 20% • 5%

MET A2 E3 P4 D7 R18 V22 H33 V39 P46 T50 G53 D57 T62 W63 K66 T70 G71 R72 F75 R84 E88 M89 P94 V95 GLU ARG GLU GLU

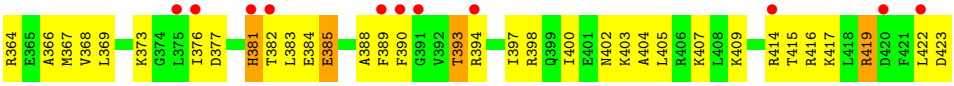
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 4% 60% 19% • 18%

MET LYS LYS SER LYS ARG LYS ASN ALA GLN ALA GLN GLU ALA GLN GLU THR GLU VAL LEU VAL GLN GLU GLU ALA GLU GLU LEU PRO GLU PHE PRO GLU GLY GLU PRO ASP PRO ASP LEU GLU ASP PRO ASP LEU THR LEU GLU ASP ASP LEU LEU ASP LEU PRO GLU GLU GLY GLU GLY

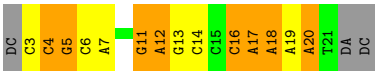
LEU ASP LEU GLU GLU GLU GLU GLU ASP LEU PRO ILE PRO LYS ILE SER THR S78 G89 T95 E98 L122 I127 R128 E129 V130 V131 S138 A139 R140 H143 I144 L147 K148 E149 T150 P153 V156 D160 K164 S165 L166 H170 K171 R172 I176

A177 R178 H186 L187 I188 N191 L192 R193 L194 Y202 R205 L210 I221 V224 F233 T237 N248 T267 K270 T274 Q279 T287 E290 E305 I321 G322 D323 S327 L338 P339 L354 E355 K356 A357 L358 L361 S362 E363



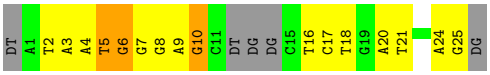
• Molecule 6: DNA (5'-D(P*CP*CP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*AP*AP*T)-3')

Chain G: 23% 27% 36% 14%



• Molecule 7: DNA (5'-D(*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP*GP*AP*TP*GP*CP*AP*G)-3')

Chain H: 22% 48% 11% 19%



• Molecule 8: RNA (5'-D(*(GTP))-R(P*G)-3')

Chain I: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.11Å 102.42Å 297.24Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	43.92 – 3.10 43.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (43.92-3.10) 91.3 (43.92-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.207 , 0.259 0.207 , 0.259	Depositor DCC
R_{free} test set	1837 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	101.2	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28534	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GTP

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	0.54	0/1814	0.81	3/2466 (0.1%)
1	B	0.55	0/1799	0.79	0/2447
2	C	0.51	0/8931	0.80	3/12080 (0.0%)
3	D	0.55	2/11928 (0.0%)	0.82	11/16127 (0.1%)
4	E	0.51	0/775	0.70	0/1045
5	F	0.50	0/2852	0.82	4/3837 (0.1%)
6	G	1.19	2/433 (0.5%)	1.61	12/664 (1.8%)
7	H	1.11	1/508 (0.2%)	1.18	2/781 (0.3%)
8	I	0.51	0/25	1.25	0/37
All	All	0.56	5/29065 (0.0%)	0.84	35/39484 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	12	DA	C3'-O3'	-5.91	1.36	1.44
6	G	14	DC	C3'-O3'	-5.81	1.36	1.44
3	D	1213	ARG	CB-CG	-5.61	1.37	1.52
3	D	16	GLU	CG-CD	5.47	1.60	1.51
7	H	6	DG	N9-C4	-5.17	1.33	1.38

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	16	DC	O5'-P-OP2	-12.56	94.40	105.70
6	G	20	DA	O4'-C1'-N9	9.38	114.57	108.00
6	G	18	DA	O4'-C4'-C3'	-9.33	100.40	106.00
6	G	17	DA	O4'-C1'-N9	9.06	114.34	108.00
6	G	11	DG	O4'-C1'-N9	8.52	113.96	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	766	GLU	Peptide
5	F	389	PHE	Peptide

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	A	1782	0	1834	33	0
1	B	1767	0	1816	42	0
2	C	8764	0	8863	203	0
3	D	11722	0	11950	257	1
4	E	761	0	778	16	0
5	F	2807	0	2882	77	0
6	G	386	0	212	19	0
7	H	453	0	250	35	0
8	I	55	0	22	1	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	D	32	0	12	1	0
All	All	28534	0	28619	596	1

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 10.

The worst 5 of 596 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)
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.44	0.97
6:G:18:DA:H2'	6:G:19:DA:H5'	1.46	0.94
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.56	0.86
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.57	0.85
2:C:211:LEU:O	2:C:213:ALA:N	2.08	0.85

All (1) 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)
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1159]	2.14	0.06

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	224/315 (71%)	220 (98%)	4 (2%)	0	100	100
1	B	222/315 (70%)	211 (95%)	10 (4%)	1 (0%)	29	64
2	C	1107/1119 (99%)	1062 (96%)	38 (3%)	7 (1%)	25	59
3	D	1480/1524 (97%)	1433 (97%)	39 (3%)	8 (0%)	29	64
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	46
5	F	344/423 (81%)	314 (91%)	20 (6%)	10 (3%)	4	24
All	All	3469/3795 (91%)	3329 (96%)	113 (3%)	27 (1%)	19	54

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	GLY
2	C	363	SER
3	D	484	PRO
3	D	486	ARG

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Continued from previous page...

Mol	Chain	Res	Type
3	D	664	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	189 (95%)	10 (5%)	24	57
1	B	197/273 (72%)	187 (95%)	10 (5%)	24	56
2	C	935/941 (99%)	892 (95%)	43 (5%)	27	59
3	D	1250/1279 (98%)	1184 (95%)	66 (5%)	22	54
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	76
5	F	301/371 (81%)	294 (98%)	7 (2%)	50	77
All	All	2965/3225 (92%)	2827 (95%)	138 (5%)	26	59

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1188	VAL
3	D	1221	VAL
4	E	75	PHE
2	C	610	ARG
2	C	591	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	83	GLN
5	F	269	ASN
5	F	277	GLN
3	D	737	ASN
3	D	744	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	0/2	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
11	GTP	D	2004	9	26,34,34	1.09	2 (7%)	32,54,54	1.58	7 (21%)

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
11	GTP	D	2004	9	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2004	GTP	C5-C6	-3.13	1.41	1.47
11	D	2004	GTP	C2-N3	3.11	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	2004	GTP	C8-N7-C5	3.24	109.17	102.99
11	D	2004	GTP	PA-O3A-PB	-3.18	121.93	132.83
11	D	2004	GTP	C5-C6-N1	3.12	119.46	113.95
11	D	2004	GTP	C2-N1-C6	-3.08	119.42	125.10
11	D	2004	GTP	PB-O3B-PG	-3.08	122.26	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2004	GTP	C5'-O5'-PA-O3A
11	D	2004	GTP	O4'-C4'-C5'-O5'
11	D	2004	GTP	C3'-C4'-C5'-O5'
11	D	2004	GTP	PG-O3B-PB-O1B
11	D	2004	GTP	PA-O3A-PB-O1B

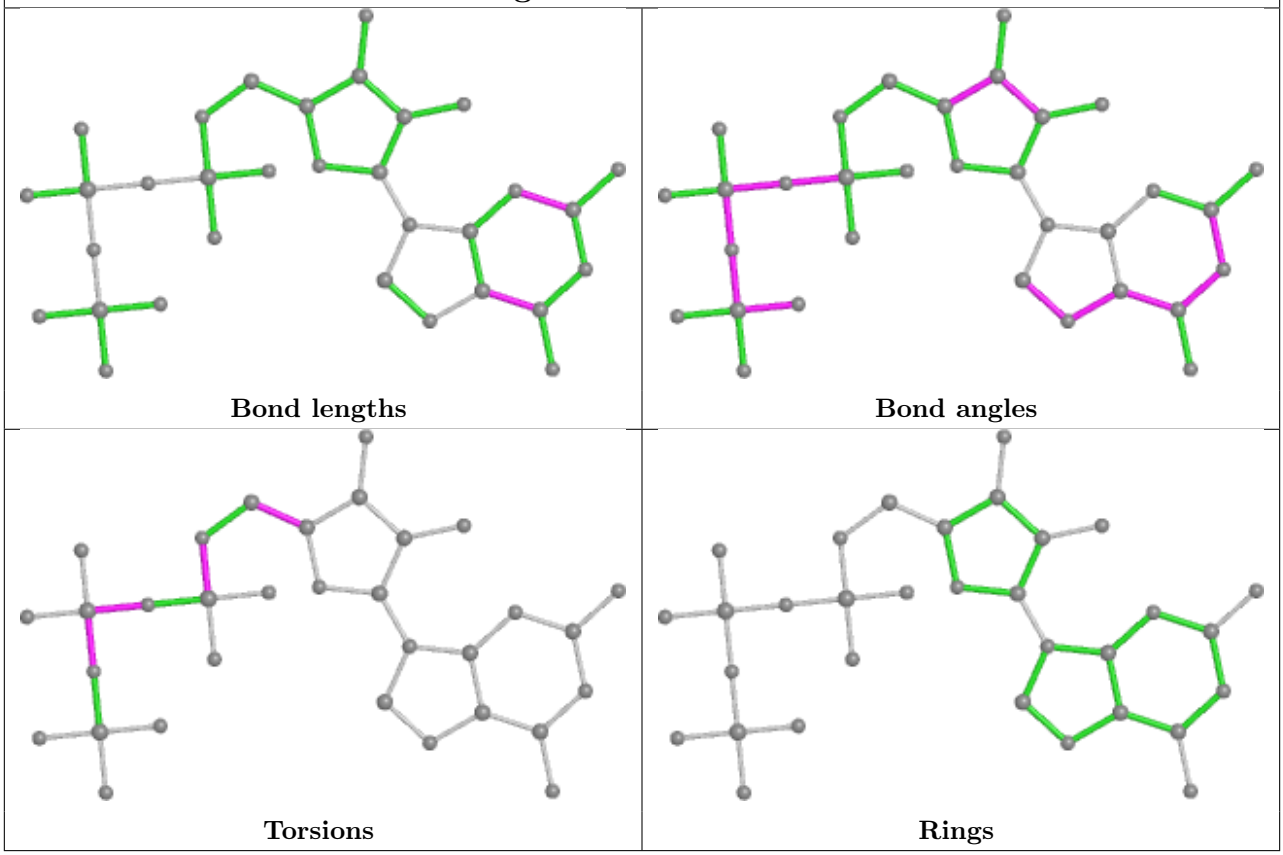
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2004	GTP	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP D 2004



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	226/315 (71%)	-0.35	0	100	100	86, 111, 134, 146	0
1	B	224/315 (71%)	-0.39	0	100	100	76, 112, 144, 158	0
2	C	1111/1119 (99%)	-0.19	10 (0%)	84	69	64, 111, 177, 210	0
3	D	1484/1524 (97%)	-0.17	16 (1%)	80	64	63, 102, 170, 219	0
4	E	94/99 (94%)	-0.37	0	100	100	78, 115, 158, 168	0
5	F	346/423 (81%)	-0.07	17 (4%)	29	14	78, 120, 206, 232	0
6	G	19/22 (86%)	-0.34	0	100	100	95, 130, 229, 231	0
7	H	22/27 (81%)	-0.59	0	100	100	102, 146, 235, 245	0
8	I	1/2 (50%)	-0.43	0	100	100	123, 123, 123, 123	0
All	All	3527/3846 (91%)	-0.20	43 (1%)	79	61	63, 110, 179, 245	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	390	PHE	5.9
2	C	207	LEU	4.5
5	F	375	LEU	4.2
5	F	391	GLY	3.9
5	F	382	THR	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

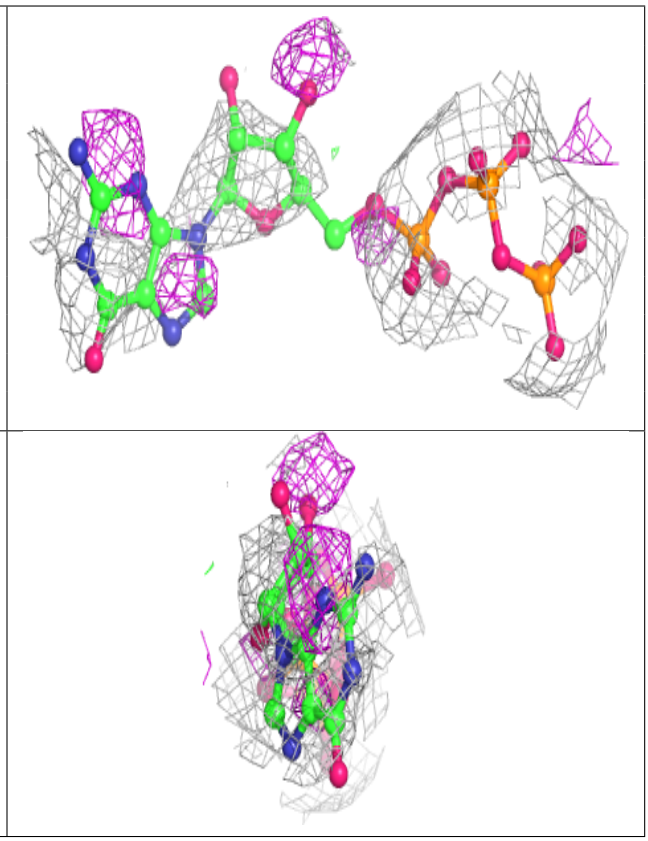
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	GTP	D	2004	32/32	0.82	0.31	93,120,128,141	32
9	MG	D	2005	1/1	0.84	0.30	104,104,104,104	0
9	MG	D	2001	1/1	0.94	0.30	77,77,77,77	0
10	ZN	D	2002	1/1	0.95	0.08	132,132,132,132	0
10	ZN	D	2003	1/1	0.98	0.29	118,118,118,118	0
9	MG	B	1001	1/1	0.98	0.51	81,81,81,81	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 GTP D 2004:

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.