

wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2023 – 02:24 AM EDT

PDB ID : 40IP

Title: Crystal structure of Thermus thermophilus transcription initiation complex

soaked with GE23077, ATP, and CMPcPP

Authors: Zhang, Y.; Ebright, R.H.; Arnold, E.

Deposited on : 2014-01-20

Resolution : 3.40 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 (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

buster-report

EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

 $CCP4 : 7.0.044 ext{ (Gargrove)}$

1.1.7 (2018)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

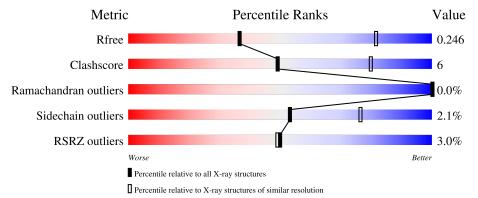
Validation Pipeline (wwPDB-VP) : 2.35.1

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 3.40 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	.%	120/	270/								
1	А	910	60% 2 <u>%</u>	13%	27%								
1	В	315	57%	14% •	28%								
2	С	1119	2%										
	C	1119	83%		16%								
3	D	1524	80%	•	17% •								
	П	0.0	2%										
4	Е	99	84%		10% • 5%								

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Mol	Chain	Length	Quality of chain								
5	F	443	67%	11%	22%						
6	G	21	71%	5%	24%						
7	Н	27	44%	44%	11%						
8	I	7	43%	57%							



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 28603 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		Ato	oms		ZeroOcc	AltConf	Trace	
1	Λ	231	Total	С	N	О	S	0	0	0
1	Λ	231	1809	1155	315	337	2	U	U	
1	D	227	Total	С	N	О	S	0	0	0
1	Ъ	221	1789	1143	310	334	2	0	U	0

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

:	Mol	Chain	Residues		\mathbf{A}	toms		ZeroOcc	AltConf	Trace	
	2	С	1112	Total 8774	C 5550	N 1565	O 1635	S 24	0	0	0

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

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
3	D	1486	Total 11746	C 7446	N 2070	O 2195	S 35	0	1	0

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

\mathbf{Mol}	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	E	94	Total 758	C 483	N 132	O 139	S 4	0	0	0

• Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

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

There are 20 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

• Molecule 6 is a DNA chain called 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*G P*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total 331	C 156	N 63	O 96	P 16	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Н	24	Total 495	C 236	N 94	O 142	P 23	0	0	0

• Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
8	I	7	Total 50	C 26	N 9	O 15	0	0	0

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

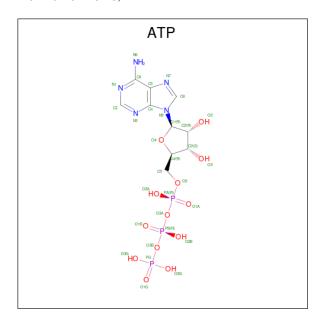


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Mg 1 1	0	0
9	D	4	Total Mg 4 4	0	0
9	F	1	Total Mg 1 1	0	0

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

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

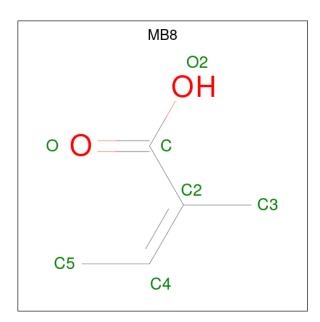
• Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
11	D	1	Total 31		N 5		P 3	10	0

 \bullet Molecule 12 is (2Z)-2-methylbut-2-enoic acid (three-letter code: MB8) (formula: $\mathrm{C}_5\mathrm{H}_8\mathrm{O}_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	I	1	Total C O 2 1 1	0	0

• Molecule 13 is water.

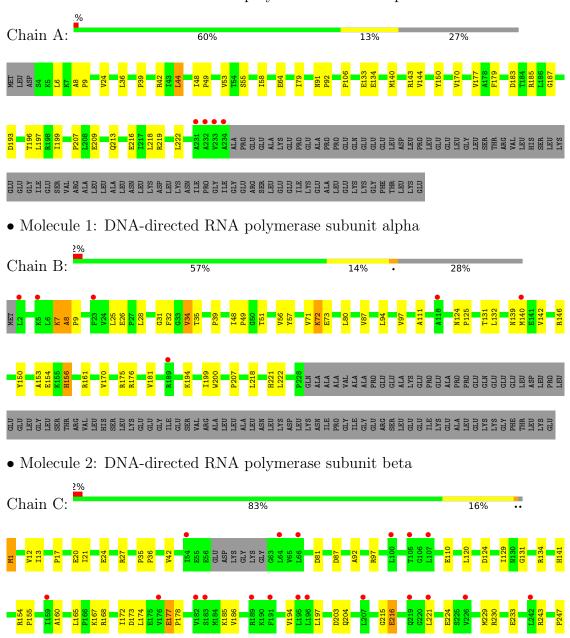
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	3	Total O 3 3	0	0



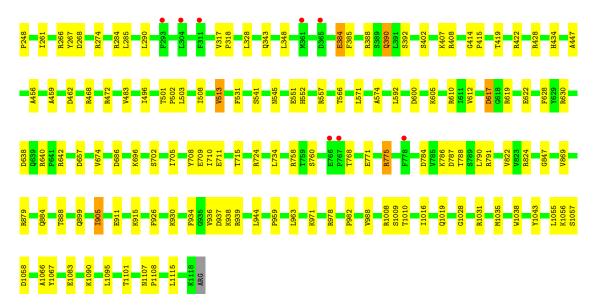
3 Residue-property plots (i)

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.

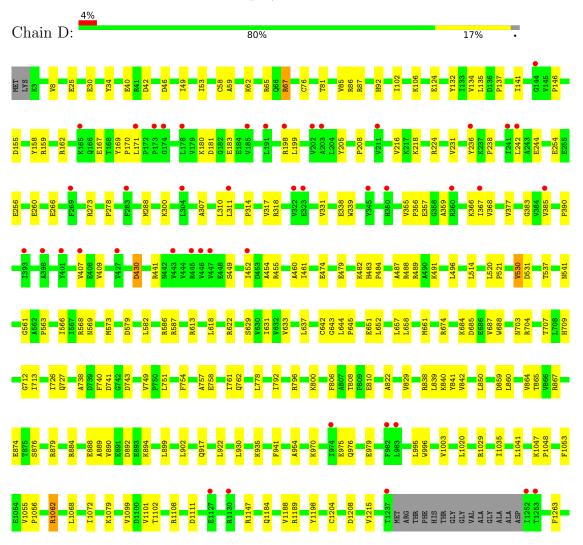
• Molecule 1: DNA-directed RNA polymerase subunit alpha



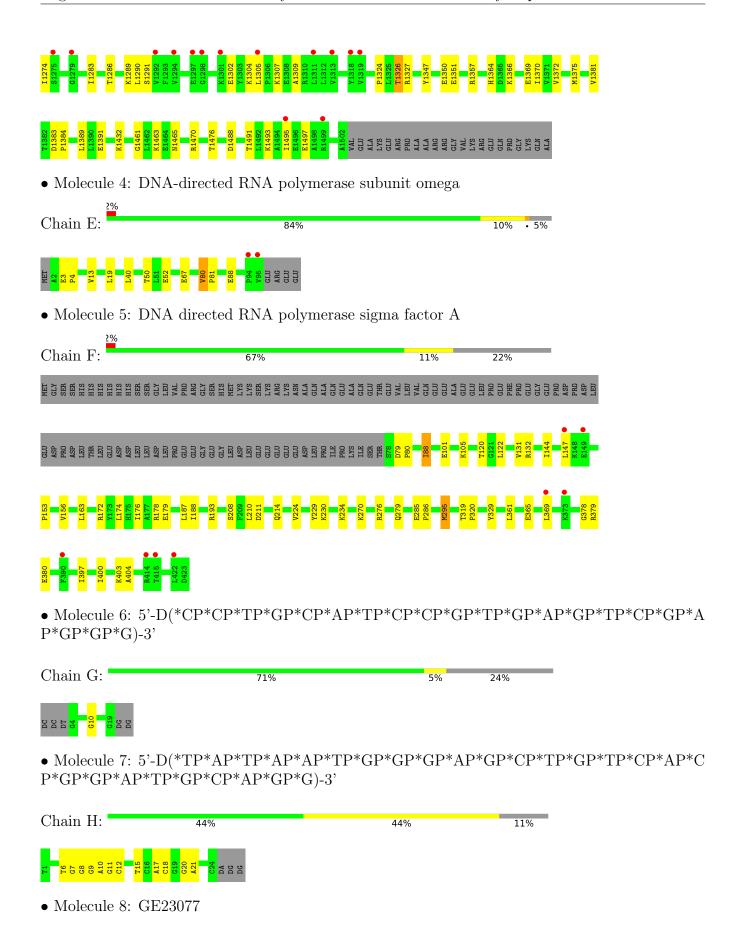




• Molecule 3: DNA-directed RNA polymerase subunit beta'









Chain I: 43% 57%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	182.92Å 104.39Å 294.21Å	Denesites
a, b, c, α , β , γ	90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.12 - 3.40	Depositor
Resolution (A)	49.12 - 3.40	EDS
% Data completeness	81.5 (49.12-3.40)	Depositor
(in resolution range)	81.5 (49.12-3.40)	EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) > 1$	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
D D	0.208 , 0.246	Depositor
R, R_{free}	0.211 , 0.246	DCC
R_{free} test set	1643 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28, 26.7	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.30$	Xtriage
	0.018 for 1/2 *h-3/2 *k,-1/2 *h-1/2 *k,-1/2 *h	
Estimated twinning fraction	+1/2*k-l 0.014 for $1/2*$ h $+3/2*$ k, $1/2*$ h- $1/2*$ k,- $1/2*$ h-	Xtriage
220111111111111111111111111111111111111		110110.80
E E completion	1/2*k-l	EDC
F_o, F_c correlation	0.93	EDS
Total number of atoms	28603	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: MB8, MG, ZN, DVA, FGL, R2T, 2TL, 0QZ, DSN, ATP, 2RA

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
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.22	0/1841	0.44	0/2504
1	В	0.22	0/1821	0.45	0/2476
2	С	0.22	0/8941	0.42	0/12092
3	D	0.22	0/11955	0.42	0/16163
4	Е	0.23	0/772	0.39	0/1040
5	F	0.21	0/2852	0.38	0/3837
6	G	0.44	0/371	0.93	0/571
7	Н	0.46	0/556	1.02	0/858
All	All	0.23	0/29109	0.45	0/39541

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.

\mathbf{Mol}	Chain	#Chirality outliers	#Planarity outliers
8	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	5	2TL	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	1809	0	1863	29	0
1	В	1789	0	1841	32	0
2	С	8774	0	8877	110	0
3	D	11746	0	11984	154	0
4	Ε	758	0	770	6	0
5	F	2807	0	2882	31	0
6	G	331	0	180	2	0
7	Н	495	0	272	12	0
8	I	50	0	37	0	0
9	В	1	0	0	0	0
9	D	4	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	31	0	12	1	0
12	I	2	0	0	0	0
13	D	3	0	0	0	0
All	All	28603	0	28718	337	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 6.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:42:ARG:NH2	1:B:31:GLY:O	2.18	0.77
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
1:A:44:LEU:HA	1:A:48:ILE:HG12	1.70	0.73
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.71	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.23	0.72

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	Perce	ntiles
1	A	$229/315 \ (73\%)$	227 (99%)	2 (1%)	0	100	100
1	В	225/315 (71%)	221 (98%)	3 (1%)	1 (0%)	34	67
2	С	1108/1119 (99%)	1088 (98%)	20 (2%)	0	100	100
3	D	1483/1524 (97%)	1463 (99%)	20 (1%)	0	100	100
4	E	92/99~(93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3481/3815 (91%)	3429 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type		
1	В	8	ALA		

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	200/273 (73%)	198 (99%)	2 (1%)	76 88
1	В	200/273 (73%)	194 (97%)	6 (3%)	41 68
2	\mathbf{C}	936/941 (100%)	913 (98%)	23 (2%)	47 72
3	D	1254/1279 (98%)	1231 (98%)	23 (2%)	59 79
4	E	82/88 (93%)	80 (98%)	2 (2%)	49 74
5	F	301/388 (78%)	296 (98%)	5 (2%)	60 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2973/3242 (92%)	2912 (98%)	61 (2%)	53 76

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	905	ILE
4	Е	80	VAL
3	D	135	LEU
4	Е	50	THR
5	F	369	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type	
2	2 C 834		GLN	
3	D	696	HIS	
3	D	724	GLN	
3	D	762	GLN	

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	В	Bond lengths			Bond angles		
MIOI			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
8	0QZ	I	6	8	4,5,6	1.56	1 (25%)	2,5,7	0.63	0	
8	FGL	I	7	8	5,6,7	1.43	1 (20%)	1,7,9	1.72	0	
8	2RA	I	1	12,8	3,5,6	0.62	0	1,5,7	0.29	0	



Mol	Trunc	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	R2T	I	4	8	8,10,11	1.87	2 (25%)	6,13,15	1.04	0
8	2TL	I	5	8	5,6,7	1.02	0	6,7,9	0.86	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
8	0QZ	I	6	8	-	1/3/4/6	-
8	FGL	I	7	8	-	0/4/6/8	-
8	2RA	I	1	12,8	-	0/2/4/6	-
8	R2T	I	4	8	-	2/13/14/16	-
8	2TL	I	5	8	-	1/5/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.19	1.43	1.32
8	I	6	0QZ	OB-CA	-2.95	1.38	1.43
8	I	4	R2T	OB1-CB	-2.24	1.37	1.43
8	I	7	FGL	OG2-CB	2.02	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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).

Mo	1 Trees	Chain	Res	Link	Bo	Bond lengths			Bond angles		
IVIC	l Type	Chain			Counts	RMSZ	# Z > 2	Counts	$\mid \text{RMSZ} \mid \# Z > 2$		
12	MB8	I	101	8	0,1,6	-	-	-			
11	ATP	D	2007	9	26,33,33	0.93	1 (3%)	31,52,52	1.59 5 (16%)		

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	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	D	2007	9	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
11	D	2007	ATP	C5-C4	2.50	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
11	D	2007	ATP	PA-O3A-PB	-3.58	120.53	132.83
11	D	2007	ATP	PB-O3B-PG	-3.39	121.19	132.83
11	D	2007	ATP	C3'-C2'-C1'	3.32	105.97	100.98
11	D	2007	ATP	N3-C2-N1	-3.23	123.63	128.68
11	D	2007	ATP	C4-C5-N7	-2.69	106.59	109.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2007	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	D	2007	ATP	C5'-O5'-PA-O2A
11	D	2007	ATP	C3'-C4'-C5'-O5'
11	D	2007	ATP	O4'-C4'-C5'-O5'
11	D	2007	ATP	PB-O3B-PG-O1G

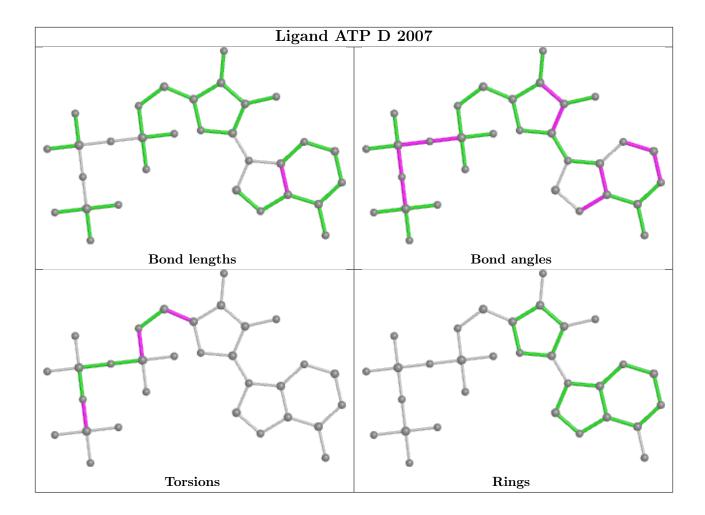
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2007	ATP	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.





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>	$\# \mathrm{RSRZ}{>}2$	$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	231/315 (73%)	-0.08	4 (1%) 70 68	38, 57, 83, 133	0
1	В	$227/315 \ (72\%)$	-0.03	6 (2%) 56 54	39, 69, 97, 117	0
2	C	1112/1119 (99%)	0.08	27 (2%) 59 57	19, 52, 116, 143	0
3	D	1486/1524 (97%)	0.16	58 (3%) 39 38	21, 56, 116, 157	0
4	E	94/99 (94%)	-0.20	2 (2%) 63 62	32, 60, 98, 101	0
5	F	346/443 (78%)	0.04	8 (2%) 60 59	31, 73, 124, 144	0
6	G	16/21~(76%)	-0.26	0 100 100	65, 94, 203, 205	0
7	Н	24/27 (88%)	-0.29	0 100 100	65, 123, 198, 228	0
8	I	0/7	-	-	-	-
All	All	3536/3870 (91%)	0.08	105 (2%) 50 49	19, 59, 117, 228	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1237	THR	8.8
5	F	422	LEU	5.5
2	С	64	LEU	5.5
5	F	414	ARG	5.1
2	С	221	LEU	5.0

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, 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.

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Mol Type Chain Res Atoms	$oxed{RSCC \mid RSR \mid B\text{-factors}(\mathring{\mathrm{A}}^2) \mid Q{<}0.9}$
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
8	FGL	I	7	7/8	0.90	0.23	33,36,38,39	0
8	R2T	I	4	11/12	0.92	0.21	34,36,45,46	0
8	2RA	I	1	6/7	0.94	0.15	33,35,41,50	0
8	DSN	I	2	6/7	0.95	0.20	34,37,50,56	0
8	2TL	I	5	7/8	0.97	0.22	37,41,43,44	0
8	0QZ	I	6	6/7	0.97	0.22	33,33,37,38	0
8	DVA	I	3	7/8	0.98	0.18	33,36,41,47	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

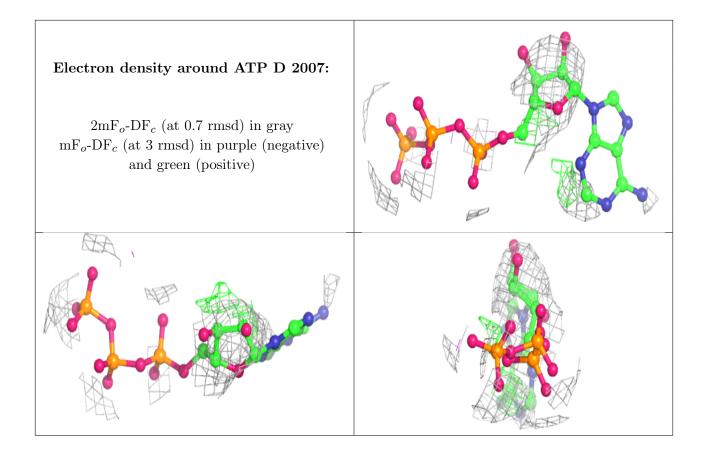
6.4 Ligands (i)

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	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
9	MG	F	2001	1/1	0.56	0.18	68,68,68,68	0
9	MG	D	2006	1/1	0.73	0.17	50,50,50,50	0
9	MG	В	2001	1/1	0.78	0.35	93,93,93,93	0
11	ATP	D	2007	31/31	0.91	0.35	53,108,121,122	10
9	MG	D	2004	1/1	0.92	0.41	69,69,69,69	0
12	MB8	I	101	2/7	0.92	0.16	34,34,34,34	0
9	MG	D	2005	1/1	0.96	0.42	33,33,33,33	0
9	MG	D	2003	1/1	0.98	0.20	26,26,26,26	0
10	ZN	D	2002	1/1	0.98	0.10	79,79,79,79	0
10	ZN	D	2001	1/1	1.00	0.19	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.

