



wwPDB X-ray Structure Validation Summary Report

Oct 29, 2014 – 10:56 AM EDT

PDB ID : 4R1F
Title : Re-refined Human DNA topoisomerase IIa (ATPase and transducer domains)
in complex with ADP and SO₄
Authors : Stanger, F.V.; Schirmer, T.
Deposited on : 2014-08-05
Resolution : 2.51 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

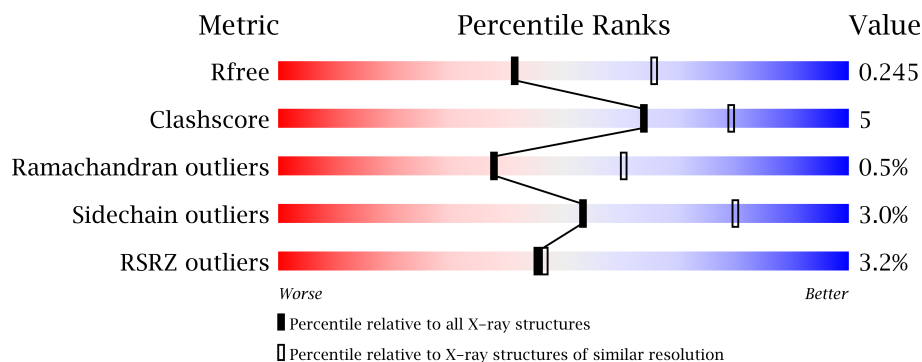
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.51 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	400	
1	B	400	
1	C	400	
1	D	400	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	501	-	X
4	GOL	A	503	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12360 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

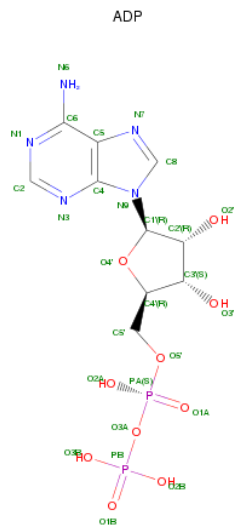
- Molecule 1 is a protein called DNA topoisomerase 2-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2955	1890	499	548	18			
1	B	379	Total	C	N	O	S	0	0	0
			3053	1952	518	564	19			
1	C	384	Total	C	N	O	S	0	0	0
			3080	1970	525	566	19			
1	D	373	Total	C	N	O	S	0	0	0
			3005	1922	510	554	19			

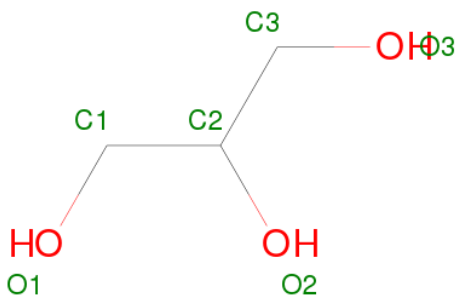
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

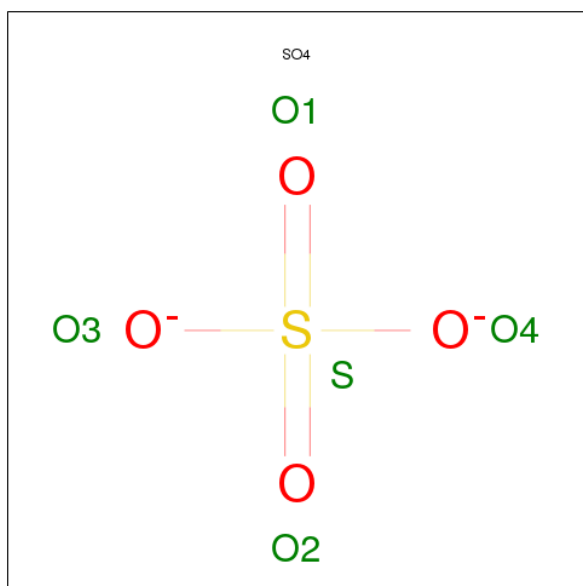


- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

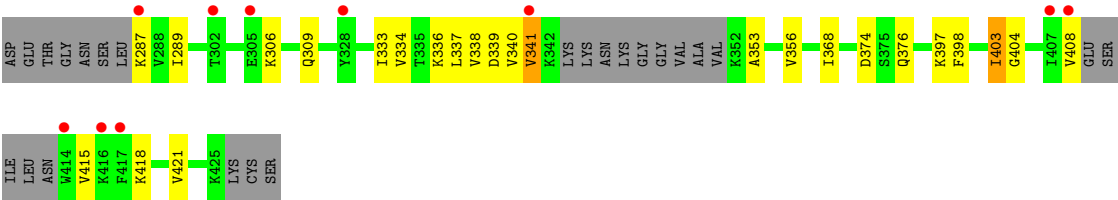
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	46	Total	O	0	0
			46	46		
6	C	40	Total	O	0	0
			40	40		
6	D	11	Total	O	0	0
			11	11		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.02Å 90.49Å 148.29Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	30.00 – 2.51 40.58 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.51) 94.9 (40.58-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.208 , 0.243 0.211 , 0.245	Depositor DCC
R_{free} test set	4648 reflections (8.23%)	DCC
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63748 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SO4, ADP

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	0.65	0/3013	0.74	3/4061 (0.1%)
1	B	0.66	0/3112	0.72	3/4192 (0.1%)
1	C	0.61	0/3139	0.71	2/4228 (0.0%)
1	D	0.57	0/3063	0.71	2/4125 (0.0%)
All	All	0.62	0/12327	0.72	10/16606 (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
1	A	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	ILE	CG1-CB-CG2	-6.17	97.82	111.40
1	D	368	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	A	399	ILE	CG1-CB-CG2	-5.83	98.57	111.40
1	C	374	ASP	CB-CA-C	-5.50	99.40	110.40
1	A	135	MET	CG-SD-CE	5.25	108.60	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	416	LYS	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	2963	38	0
1	B	3053	0	3081	19	0
1	C	3080	0	3119	30	0
1	D	3005	0	3028	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
4	A	6	0	8	0	0
5	B	5	0	0	2	0
5	C	5	0	0	2	0
5	D	5	0	0	0	0
6	A	37	0	0	0	0
6	B	46	0	0	1	0
6	C	40	0	0	0	0
6	D	11	0	0	0	0
All	All	12360	0	12247	131	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 131 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:336:LYS:HD2	1:A:399:ILE:HG22	1.20	1.11
1:A:336:LYS:CD	1:A:399:ILE:HG22	1.81	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:336:LYS:HD2	1:A:399:ILE:CG2	1.83	1.07
1:A:395:SER:O	1:A:399:ILE:HG13	1.59	1.02
1:D:171:ASN:HB3	1:D:198:MET:HE3	1.48	0.95

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	358/400 (90%)	335 (94%)	20 (6%)	3 (1%)	27	46
1	B	373/400 (93%)	352 (94%)	17 (5%)	4 (1%)	21	34
1	C	378/400 (94%)	365 (97%)	13 (3%)	0	100	100
1	D	365/400 (91%)	348 (95%)	16 (4%)	1 (0%)	50	73
All	All	1474/1600 (92%)	1400 (95%)	66 (4%)	8 (0%)	38	60

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	LYS
1	B	353	ALA
1	B	407	ILE
1	A	410	SER
1	A	417	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/358 (92%)	316 (96%)	14 (4%)	40	66
1	B	341/358 (95%)	332 (97%)	9 (3%)	59	84
1	C	343/358 (96%)	339 (99%)	4 (1%)	82	95
1	D	335/358 (94%)	322 (96%)	13 (4%)	43	70
All	All	1349/1432 (94%)	1309 (97%)	40 (3%)	53	80

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251	LYS
1	B	411	ILE
1	D	397	LYS
1	B	352	LYS
1	C	146	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	ASN
1	D	210	ASN
1	D	59	GLN
1	A	413	ASN
1	D	171	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
3	ADP	A	502	2	29,29,29	1.50	5 (17%)	45,45,45	2.06	9 (20%)
4	GOL	A	503	-	5,5,5	0.57	0	5,5,5	0.93	0
5	SO4	B	502	-	4,4,4	0.81	0	6,6,6	0.27	0
3	ADP	B	503	2	29,29,29	1.44	3 (10%)	45,45,45	2.21	9 (20%)
3	ADP	C	502	2	29,29,29	1.10	2 (6%)	45,45,45	2.29	9 (20%)
5	SO4	C	503	-	4,4,4	0.39	0	6,6,6	0.34	0
5	SO4	D	502	-	4,4,4	0.45	0	6,6,6	0.38	0
3	ADP	D	503	2	29,29,29	1.30	3 (10%)	45,45,45	2.16	11 (24%)

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
3	ADP	A	502	2	-	0/16/32/32	0/3/3/3
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
5	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	ADP	B	503	2	-	0/16/32/32	0/3/3/3
3	ADP	C	502	2	-	0/16/32/32	0/3/3/3
5	SO4	C	503	-	-	0/0/0/0	0/0/0/0
5	SO4	D	502	-	-	0/0/0/0	0/0/0/0
3	ADP	D	503	2	-	0/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	ADP	C4-N9	-5.00	1.30	1.37
3	A	502	ADP	C4-N9	-4.22	1.31	1.37
3	D	503	ADP	C4-N9	-3.60	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	ADP	C5-C4	3.47	1.48	1.40
3	D	503	ADP	C5-C4	3.28	1.47	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ADP	C5-C4-N3	-8.74	117.45	125.98
3	B	503	ADP	N3-C2-N1	-8.03	121.83	128.89
3	A	502	ADP	C5-C4-N3	-6.56	119.58	125.98
3	D	503	ADP	N3-C2-N1	-6.33	123.32	128.89
3	C	502	ADP	N3-C4-N9	6.08	135.82	125.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	366/400 (91%)	0.21	18 (4%)	28 29	37, 64, 95, 117	0
1	B	379/400 (94%)	0.16	10 (2%)	53 55	35, 55, 88, 111	0
1	C	384/400 (96%)	-0.05	2 (0%)	88 90	39, 56, 80, 98	0
1	D	373/400 (93%)	0.38	18 (4%)	29 30	47, 71, 100, 117	0
All	All	1502/1600 (93%)	0.17	48 (3%)	45 47	35, 61, 93, 117	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	VAL	4.6
1	A	414	TRP	4.5
1	A	210	ASN	4.1
1	D	407	ILE	3.5
1	A	420	GLN	3.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	C	501	1/1	0.18	2.24	45,45,45,45	0
4	GOL	A	503	6/6	0.30	2.10	59,66,71,76	0
2	MG	A	501	1/1	0.16	1.30	43,43,43,43	0
2	MG	D	501	1/1	0.25	1.06	50,50,50,50	0
3	ADP	D	503	27/27	0.21	0.39	46,60,73,99	0
2	MG	B	501	1/1	0.20	0.21	40,40,40,40	0
3	ADP	A	502	27/27	0.15	0.14	40,49,57,65	0
3	ADP	B	503	27/27	0.18	-0.02	33,39,47,50	0
3	ADP	C	502	27/27	0.14	-0.30	42,49,55,57	0
5	SO4	D	502	5/5	0.20	-1.11	93,97,112,112	0
5	SO4	C	503	5/5	0.11	-1.25	74,81,82,83	0
5	SO4	B	502	5/5	0.12	-2.08	67,76,82,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.