



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PVG
Title : Crystal Structure of the ATPase region of *Saccharomyces Cerevisiae* topoisomerase II
Authors : Classen, S.; Olland, S.; Berger, J.M.
Deposited on : 2003-06-27
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

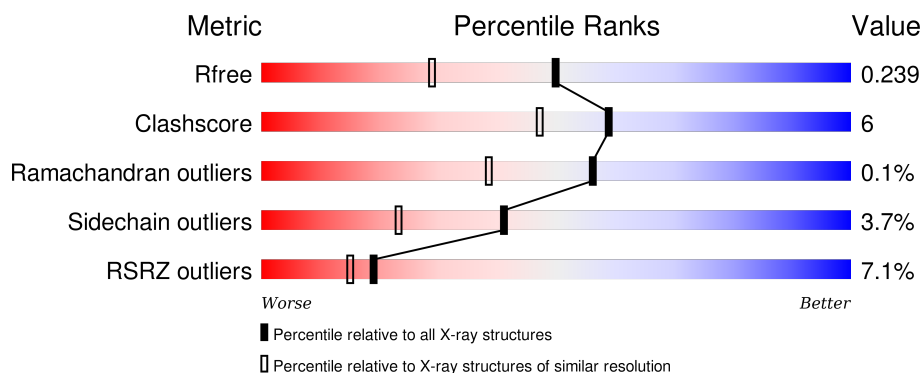
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	418	<div> <div>5%</div> <div>77%</div> <div>12%</div> <div>10%</div> </div>
1	B	418	<div> <div>8%</div> <div>76%</div> <div>14%</div> <div>10%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6892 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 topoisomerase II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	Se	0	0	0
			3038	1937	514	572	5	10			
1	B	378	Total	C	N	O	S	Se	0	0	0
			3045	1943	514	573	5	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	GLY	CLONING ARTIFACT	UNP P06786
A	-3	HIS	HIS	CLONING ARTIFACT	UNP P06786
A	-2	MET	MET	CLONING ARTIFACT	UNP P06786
A	-1	VAL	VAL	CLONING ARTIFACT	UNP P06786
A	0	THR	THR	CLONING ARTIFACT	UNP P06786
A	49	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	81	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	119	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	177	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	208	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	219	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	312	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	349	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	392	MSE	MET	MODIFIED RESIDUE	UNP P06786
A	400	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	-4	GLY	GLY	CLONING ARTIFACT	UNP P06786
B	-3	HIS	HIS	CLONING ARTIFACT	UNP P06786
B	-2	MET	MET	CLONING ARTIFACT	UNP P06786
B	-1	VAL	VAL	CLONING ARTIFACT	UNP P06786
B	0	THR	THR	CLONING ARTIFACT	UNP P06786
B	49	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	81	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	119	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	177	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	208	MSE	MET	MODIFIED RESIDUE	UNP P06786

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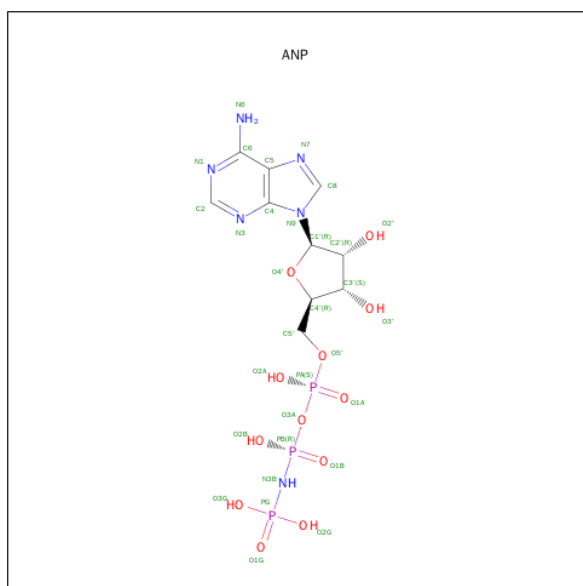
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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	312	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	349	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	392	MSE	MET	MODIFIED RESIDUE	UNP P06786
B	400	MSE	MET	MODIFIED RESIDUE	UNP P06786

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

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

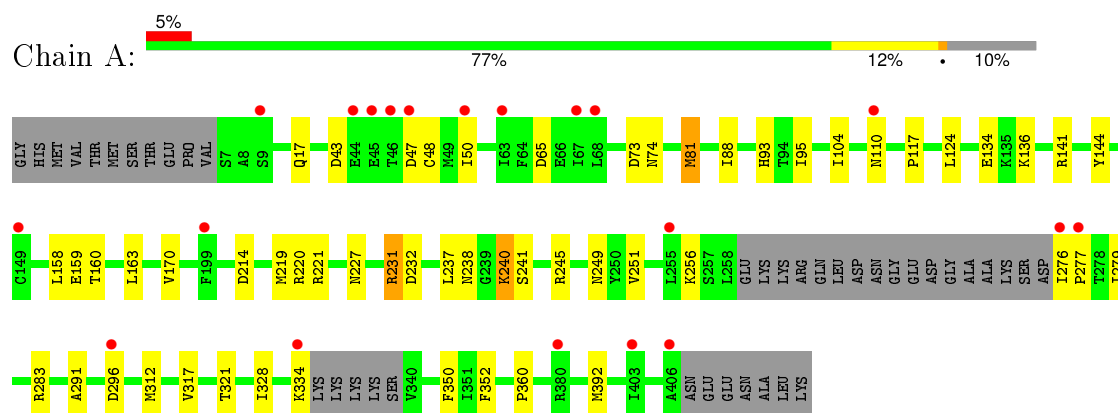


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	399	Total 399	O 399	0	0
4	B	346	Total 346	O 346	0	0

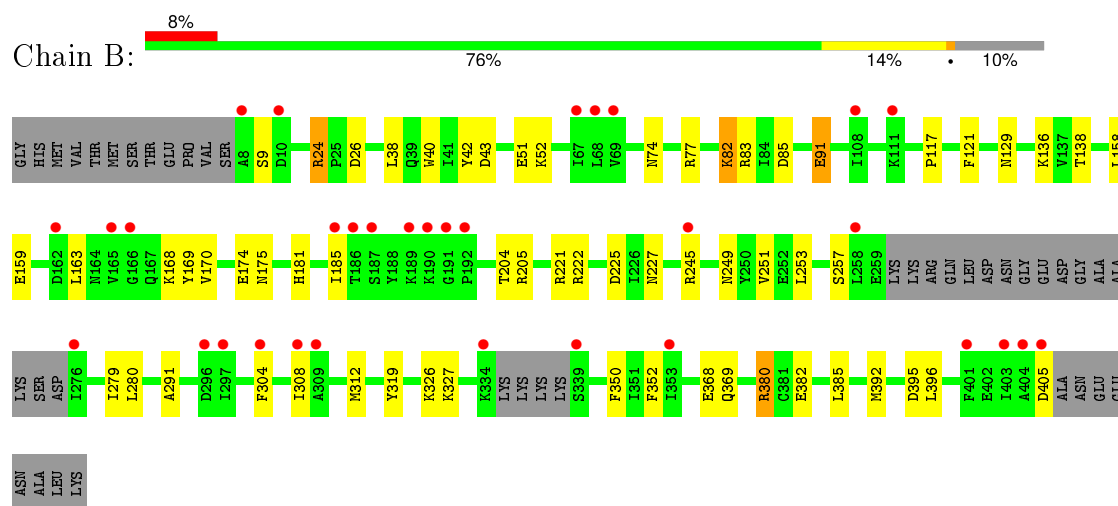
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 topoisomerase II



• Molecule 1: DNA topoisomerase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.46 Å 71.08 Å 216.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 1.80 29.24 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.7 (29.75-1.80) 89.6 (29.24-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.206 , 0.241 0.206 , 0.239	Depositor DCC
R_{free} test set	6385 reflections (9.21%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 75706 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/3083	0.66	5/4144 (0.1%)
1	B	0.40	0/3090	0.64	5/4153 (0.1%)
All	All	0.41	0/6173	0.65	10/8297 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	296	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	405	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	43	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	73	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	85	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	214	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	26	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	43	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	395	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3038	0	3037	39	0
1	B	3045	0	3046	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
4	A	399	0	0	0	0
4	B	346	0	0	2	0
All	All	6892	0	6109	71	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.

All (71) 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:392:MSE:HE2	1:B:392:MSE:HA	1.56	0.88
1:B:74:ASN:HD21	1:B:77:ARG:HH11	1.23	0.85
1:A:74:ASN:HB3	1:A:81:MSE:HE1	1.60	0.84
1:B:245:ARG:HB2	1:B:249:ASN:ND2	1.97	0.79
1:A:245:ARG:H	1:A:249:ASN:HD22	1.31	0.78
1:A:74:ASN:CB	1:A:81:MSE:HE1	2.17	0.73
1:B:245:ARG:HB2	1:B:249:ASN:HD22	1.57	0.69
1:B:129:ASN:HD21	1:B:138:THR:HG21	1.57	0.69
1:A:74:ASN:HD22	1:A:81:MSE:CE	2.07	0.68
1:B:136:LYS:HE2	4:B:933:HOH:O	1.93	0.67
1:B:91:GLU:CD	1:B:91:GLU:H	1.98	0.67
1:B:129:ASN:ND2	1:B:138:THR:HG21	2.09	0.67
1:A:312:MSE:HE1	1:B:369:GLN:OE1	1.94	0.66
1:A:74:ASN:ND2	1:A:81:MSE:HE1	2.10	0.66
1:A:220:ARG:HG2	1:A:237:LEU:HD21	1.80	0.64
1:A:328:ILE:HA	1:A:392:MSE:HE1	1.79	0.64
1:A:88:ILE:H	1:A:238:ASN:HD21	1.46	0.63
1:B:74:ASN:ND2	1:B:77:ARG:HH11	1.94	0.63
1:A:95:ILE:HD13	1:A:219:MSE:HE1	1.80	0.63
1:A:74:ASN:HD22	1:A:81:MSE:HE1	1.65	0.61
1:B:40:TRP:O	1:B:221:ARG:HD3	2.02	0.59
1:B:291:ALA:HB3	1:B:352:PHE:HB2	1.85	0.59
1:A:134:GLU:O	1:A:136:LYS:HE2	2.03	0.58
1:A:95:ILE:CD1	1:A:219:MSE:HE1	2.34	0.57
1:B:74:ASN:HD21	1:B:77:ARG:NH1	1.99	0.57
1:A:74:ASN:ND2	1:A:81:MSE:CE	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:NE2	1:A:144:TYR:OH	2.40	0.55
1:A:117:PRO:HB3	1:A:158:LEU:HD22	1.88	0.55
1:B:312:MSE:HG3	1:B:368:GLU:HB3	1.89	0.55
1:A:231:ARG:CZ	1:A:232:ASP:H	2.20	0.54
1:B:392:MSE:HA	1:B:392:MSE:CE	2.35	0.54
1:B:159:GLU:HG3	1:B:170:VAL:HG22	1.90	0.53
1:A:48:CYS:HB3	1:A:256:LYS:HE3	1.91	0.53
1:B:319:TYR:OH	1:B:380:ARG:NH1	2.42	0.52
1:B:121:PHE:CD2	1:B:158:LEU:HD22	2.46	0.51
1:A:74:ASN:HD22	1:A:81:MSE:HE2	1.78	0.48
1:B:74:ASN:ND2	1:B:77:ARG:HD3	2.29	0.47
1:A:159:GLU:HG3	1:A:170:VAL:HG22	1.94	0.47
1:B:222:ARG:O	1:B:225:ASP:HB2	2.14	0.47
1:A:158:LEU:HG	1:A:159:GLU:N	2.30	0.46
1:A:104:ILE:HB	1:A:160:THR:HG21	1.97	0.46
1:A:17:GLN:HG2	1:A:124:LEU:HD13	1.98	0.46
1:B:312:MSE:HG2	4:B:1161:HOH:O	2.15	0.45
1:A:88:ILE:HD13	1:A:95:ILE:HG23	1.97	0.45
1:A:141:ARG:HD3	1:A:360:PRO:HD2	1.97	0.44
1:A:117:PRO:HB3	1:A:158:LEU:CD2	2.46	0.44
1:A:291:ALA:HB3	1:A:352:PHE:HB2	1.99	0.44
1:B:168:LYS:O	1:B:185:ILE:HA	2.18	0.44
1:A:251:VAL:HG12	1:A:279:ILE:HG21	2.00	0.43
1:B:82:LYS:HA	1:B:82:LYS:HD2	1.73	0.43
1:A:317:VAL:O	1:A:321:THR:HG23	2.18	0.43
1:B:251:VAL:HG12	1:B:279:ILE:HD13	1.98	0.43
1:B:42:TYR:HE1	1:B:253:LEU:HD22	1.83	0.43
1:B:117:PRO:HB2	1:B:169:TYR:CE2	2.54	0.42
1:B:38:LEU:HG	1:B:51:GLU:HG2	2.01	0.42
1:A:110:ASN:OD1	1:B:9:SER:HB3	2.19	0.42
1:A:74:ASN:CG	1:A:81:MSE:HE1	2.38	0.42
1:A:276:ILE:HA	1:A:277:PRO:HD3	1.82	0.42
1:B:392:MSE:HE1	1:B:396:LEU:HD22	2.02	0.42
1:A:251:VAL:CG1	1:A:279:ILE:HG21	2.50	0.42
1:A:240:LYS:HE2	1:A:240:LYS:HB3	1.57	0.41
1:A:240:LYS:HD2	1:A:241:SER:O	2.21	0.41
1:B:174:GLU:OE1	1:B:181:HIS:HE1	2.03	0.41
1:B:24:ARG:HG2	1:B:24:ARG:HH11	1.86	0.41
1:A:283:ARG:HH11	1:A:283:ARG:HG3	1.85	0.41
1:B:280:LEU:O	1:B:291:ALA:HA	2.21	0.41
1:A:231:ARG:HA	1:A:231:ARG:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:MSE:HB3	1:A:312:MSE:HE2	1.91	0.40
1:B:304:PHE:HA	1:B:308:ILE:O	2.20	0.40
1:A:283:ARG:HG3	1:A:283:ARG:NH1	2.37	0.40
1:B:327:LYS:HE2	1:B:385:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/418 (89%)	365 (98%)	6 (2%)	1 (0%)	46	29
1	B	372/418 (89%)	361 (97%)	11 (3%)	0	100	100
All	All	744/836 (89%)	726 (98%)	17 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	HIS

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	339/371 (91%)	329 (97%)	10 (3%)	50	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/371 (92%)	325 (96%)	15 (4%)	35	17
All	All	679/742 (92%)	654 (96%)	25 (4%)	41	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	50	ILE
1	A	81	MSE
1	A	163	LEU
1	A	221	ARG
1	A	227	ASN
1	A	231	ARG
1	A	240	LYS
1	A	334	LYS
1	A	350	PHE
1	B	24	ARG
1	B	52	LYS
1	B	82	LYS
1	B	83	ARG
1	B	91	GLU
1	B	163	LEU
1	B	175	ASN
1	B	204	THR
1	B	205	ARG
1	B	227	ASN
1	B	257	SER
1	B	326	LYS
1	B	350	PHE
1	B	380	ARG
1	B	382	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	238	ASN
1	A	249	ASN
1	A	300	GLN
1	A	344	GLN
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	113	ASN
1	B	129	ASN
1	B	175	ASN
1	B	176	ASN
1	B	181	HIS
1	B	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 4 ligands modelled in this entry, 2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ANP	A	901	2	27,33,33	1.87	6 (22%)	30,52,52	1.91	4 (13%)
3	ANP	B	902	2	27,33,33	2.00	7 (25%)	30,52,52	1.85	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	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	901	2	-	1/12/38/38	0/3/3/3
3	ANP	B	902	2	-	1/12/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ANP	PB-O3A	-5.04	1.52	1.59
3	A	901	ANP	PB-O3A	-4.21	1.53	1.59
3	B	902	ANP	PG-O3G	-2.53	1.49	1.56
3	B	902	ANP	PB-O2B	-2.34	1.50	1.56
3	A	901	ANP	PB-O2B	-2.23	1.50	1.56
3	B	902	ANP	PG-O2G	-2.09	1.50	1.56
3	A	901	ANP	PG-O3G	-2.07	1.50	1.56
3	A	901	ANP	C5-C4	2.75	1.46	1.40
3	B	902	ANP	C5-C4	2.81	1.46	1.40
3	A	901	ANP	PB-O1B	3.59	1.50	1.46
3	B	902	ANP	PG-O1G	4.12	1.50	1.46
3	B	902	ANP	PB-O1B	4.15	1.50	1.46
3	A	901	ANP	PG-O1G	4.47	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ANP	N3-C2-N1	-7.51	123.15	128.89
3	B	902	ANP	N3-C2-N1	-7.51	123.15	128.89
3	B	902	ANP	C4-C5-N7	-2.52	107.16	109.48
3	A	901	ANP	C4-C5-N7	-2.28	107.39	109.48
3	B	902	ANP	C2'-C1'-N9	-2.18	110.96	114.29
3	A	901	ANP	O3G-PG-O1G	-2.09	107.93	113.49
3	B	902	ANP	O3A-PA-O5'	2.01	108.26	102.94
3	B	902	ANP	C4'-O4'-C1'	2.99	113.00	109.72
3	A	901	ANP	C4'-O4'-C1'	3.88	113.98	109.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	ANP	O1G-PG-N3B-PB
3	A	901	ANP	O1G-PG-N3B-PB

There are no ring outliers.

No monomer is involved in short contacts.

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	368/418 (88%)	0.19	20 (5%) 29 24	12, 17, 27, 39	0
1	B	368/418 (88%)	0.37	32 (8%) 13 10	11, 19, 26, 40	0
All	All	736/836 (88%)	0.28	52 (7%) 19 15	11, 18, 26, 40	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	GLY	6.1
1	A	276	ILE	5.7
1	B	404	ALA	5.4
1	B	165	VAL	5.3
1	B	8	ALA	5.1
1	B	405	ASP	4.9
1	A	406	ALA	4.6
1	B	339	SER	4.1
1	B	10	ASP	3.6
1	A	47	ASP	3.4
1	A	67	ILE	3.3
1	B	297	ILE	3.3
1	B	189	LYS	3.3
1	B	403	ILE	3.3
1	B	190	LYS	3.3
1	B	296	ASP	3.2
1	B	245	ARG	3.2
1	A	45	GLU	3.1
1	B	185	ILE	3.1
1	B	401	PHE	3.0
1	A	44	GLU	2.9
1	B	308	ILE	2.9
1	B	192	PRO	2.8
1	B	166	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	276	ILE	2.7
1	A	149	CYS	2.7
1	B	186	THR	2.7
1	A	46	THR	2.6
1	A	403	ILE	2.6
1	B	309	ALA	2.6
1	A	277	PRO	2.6
1	A	334	LYS	2.5
1	A	68	LEU	2.5
1	A	63	ILE	2.5
1	B	111	LYS	2.5
1	B	67	ILE	2.5
1	B	353	ILE	2.5
1	A	255	LEU	2.5
1	B	304	PHE	2.4
1	A	380	ARG	2.4
1	B	334	LYS	2.4
1	A	296	ASP	2.4
1	B	258	LEU	2.2
1	B	162	ASP	2.2
1	B	69	VAL	2.2
1	A	199	PHE	2.2
1	A	110	ASN	2.2
1	B	68	LEU	2.2
1	B	187	SER	2.1
1	B	108	ILE	2.1
1	A	9	SER	2.0
1	A	50	ILE	2.0

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	903	1/1	0.99	0.15	0.23	22,22,22,22	0
3	ANP	B	902	31/31	0.97	0.12	0.13	21,26,32,33	0
3	ANP	A	901	31/31	0.98	0.12	0.08	19,22,24,27	0
2	MG	B	904	1/1	0.99	0.11	-1.00	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.