



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1QZR  
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF SACCHAROMYCES CEREVISIAE TOPOISOMERASE II BOUND TO ICRF-187 (DEXRAZOXANE)  
Authors : Classen, S.; Olland, S.; Berger, J.M.  
Deposited on : 2003-09-17  
Resolution : 1.90 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](mailto: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.

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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

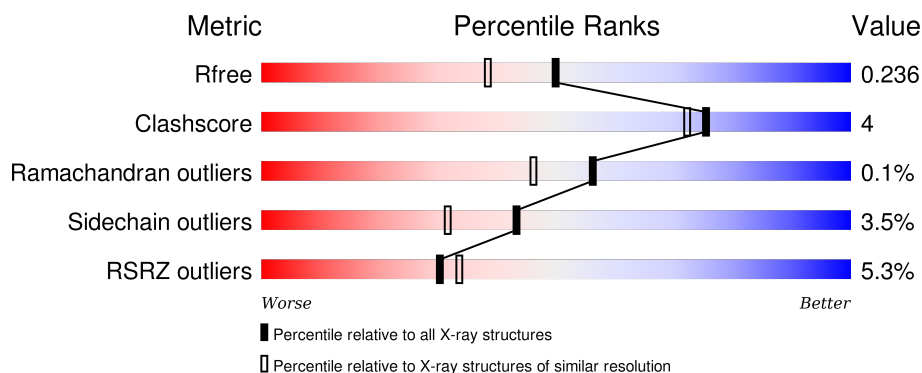
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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>4%</div> <div>80% 11% 9%</div> </div>
1	B	418	<div> <div>6%</div> <div>80% 9% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CDX	B	901[A]	X	-	-	X
3	CDX	B	901[B]	X	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6978 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	382	Total	C	N	O	S	0	0	0
			3069	1954	520	580	15			
1	B	378	Total	C	N	O	S	0	0	0
			3041	1940	513	573	15			

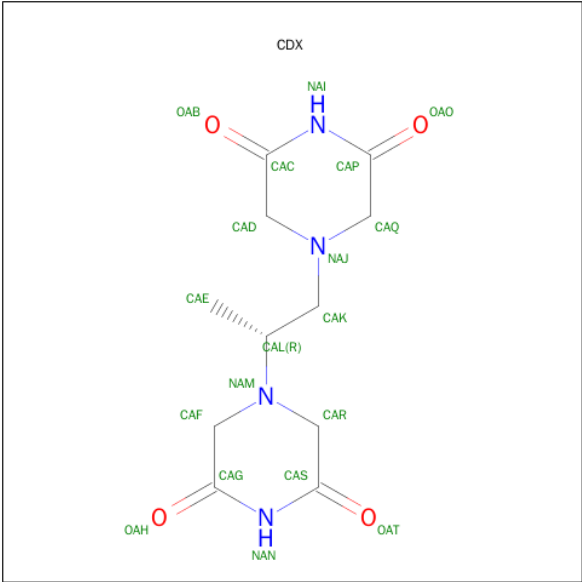
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P06786
A	-3	HIS	-	CLONING ARTIFACT	UNP P06786
A	-2	MET	-	CLONING ARTIFACT	UNP P06786
A	-1	VAL	-	CLONING ARTIFACT	UNP P06786
A	0	THR	-	CLONING ARTIFACT	UNP P06786
B	-4	GLY	-	CLONING ARTIFACT	UNP P06786
B	-3	HIS	-	CLONING ARTIFACT	UNP P06786
B	-2	MET	-	CLONING ARTIFACT	UNP P06786
B	-1	VAL	-	CLONING ARTIFACT	UNP P06786
B	0	THR	-	CLONING ARTIFACT	UNP P06786

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

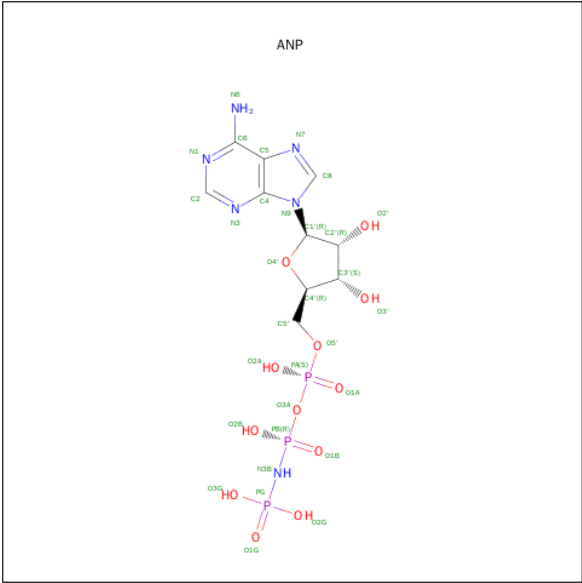
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (S)-4,4'-(1-METHYL-1,2-ETHANEDIYL)BIS-2,6-PIPERAZINEDIONE (three-letter code: CDX) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	1
			38	22	8	8		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

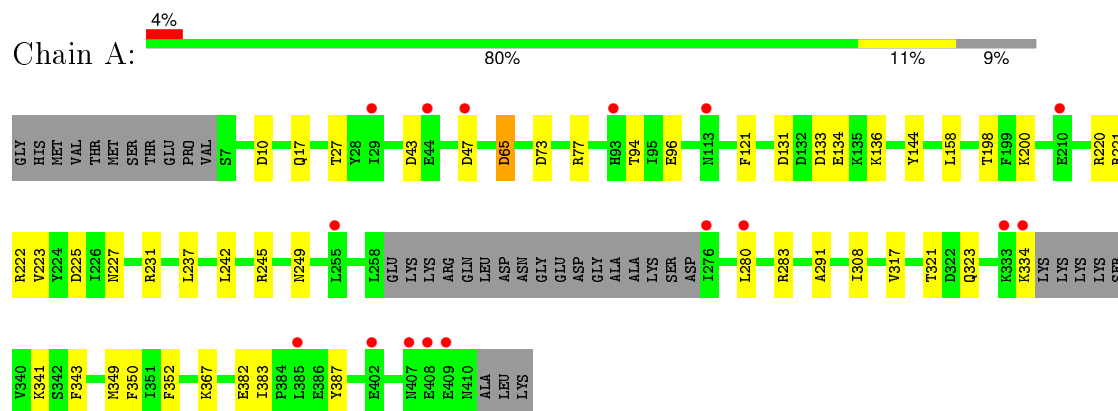
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	419	Total 419	O 419	0	0
5	B	347	Total 347	O 347	0	0

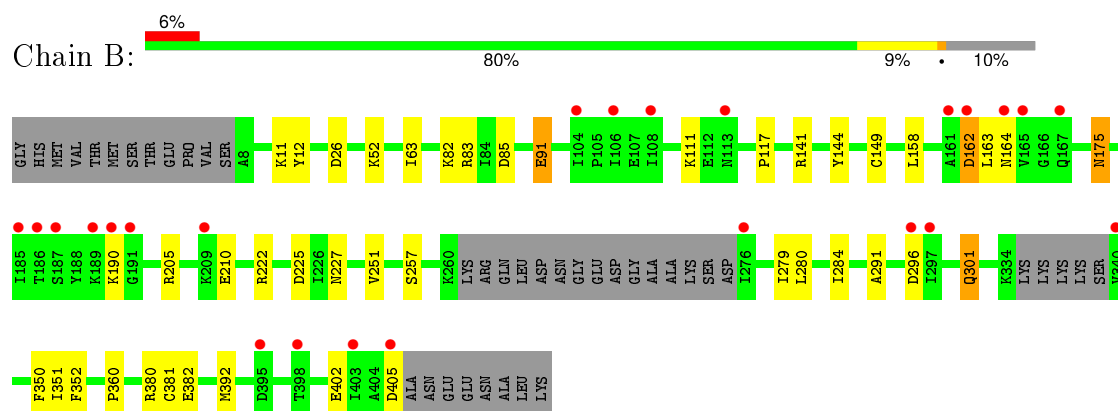
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	58.55Å 71.44Å 215.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 1.90 45.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.8 (45.18-1.90) 90.8 (45.40-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.196 , 0.237 0.194 , 0.236	Depositor DCC
$R_{free}$ test set	5512 reflections (9.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65579 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CDX, 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	0.49	0/3124	0.66	5/4216 (0.1%)
1	B	0.46	0/3096	0.66	5/4179 (0.1%)
All	All	0.48	0/6220	0.66	10/8395 (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	73	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	85	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	43	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	65	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	296	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	26	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	47	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	405	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	133	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	162	ASP	CB-CG-OD2	5.06	122.85	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	3069	0	3059	22	0
1	B	3041	0	3035	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	38	0	32	8	0
4	A	31	0	13	0	0
4	B	31	0	13	0	0
5	A	419	0	0	0	0
5	B	347	0	0	4	0
All	All	6978	0	6152	48	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 4.

All (48) 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:149:CYS:SG	5:B:1226:HOH:O	2.28	0.85
1:A:245:ARG:H	1:A:249:ASN:HD22	1.30	0.79
1:B:91:GLU:CD	1:B:91:GLU:H	1.94	0.69
1:A:134:GLU:HG3	1:A:136:LYS:HE2	1.83	0.59
1:A:17:GLN:NE2	1:A:144:TYR:OH	2.38	0.56
3:B:901[B]:CDX:HAE2	3:B:901[B]:CDX:HAQ2	1.88	0.55
1:A:131:ASP:O	1:A:134:GLU:HG3	2.06	0.55
1:A:94:THR:HG22	1:A:200:LYS:HE2	1.89	0.54
1:A:121:PHE:CD2	1:A:158:LEU:HD22	2.43	0.53
1:B:392:MET:HA	1:B:392:MET:CE	2.38	0.52
3:B:901[B]:CDX:HAE2	3:B:901[B]:CDX:CAQ	2.39	0.52
1:B:251:VAL:CG1	1:B:279:ILE:HG21	2.39	0.52
1:A:323:GLN:HE22	1:A:383:ILE:H	1.58	0.51
1:B:11:LYS:HE3	1:B:12:TYR:CE2	2.46	0.50
1:B:222:ARG:O	1:B:225:ASP:HB2	2.11	0.49
1:B:63:ILE:O	5:B:1226:HOH:O	2.20	0.49
1:A:223:VAL:HG12	1:A:242:LEU:HD11	1.94	0.48
1:B:210:GLU:HG3	5:B:1162:HOH:O	2.14	0.48
1:A:220:ARG:HG2	1:A:237:LEU:HD21	1.95	0.47
1:B:291:ALA:HB3	1:B:352:PHE:HB2	1.97	0.46
1:B:284:ILE:HG13	1:B:381:CYS:SG	2.55	0.46
1:A:280:LEU:HG	1:A:387:TYR:CE1	2.51	0.46
1:A:323:GLN:NE2	1:A:383:ILE:H	2.13	0.45
1:A:96:GLU:HG2	1:A:198:THR:HG23	1.98	0.45
1:A:323:GLN:HE22	1:A:382:GLU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLN:HB2	1:B:301:GLN:HE21	1.61	0.45
3:B:901[B]:CDX:HAK1	3:B:901[B]:CDX:HAF1	1.72	0.45
1:A:291:ALA:HB3	1:A:352:PHE:HB2	1.98	0.45
1:A:341:LYS:HD2	1:A:343:PHE:CE2	2.52	0.44
3:B:901[B]:CDX:HAK2	5:B:1252:HOH:O	2.17	0.44
1:A:317:VAL:O	1:A:321:THR:HG23	2.18	0.43
3:B:901[A]:CDX:HAF1	3:B:901[A]:CDX:HAK1	1.69	0.43
1:B:251:VAL:HG12	1:B:279:ILE:HG21	2.00	0.42
1:A:94:THR:CG2	1:A:200:LYS:HE2	2.49	0.42
1:A:231:ARG:HD3	1:A:283:ARG:NH2	2.35	0.42
1:B:144:TYR:CZ	3:B:901[A]:CDX:HAQ1	2.55	0.41
1:A:308:ILE:HD13	1:A:367:LYS:HD3	2.01	0.41
1:B:251:VAL:HG11	1:B:279:ILE:HG21	2.02	0.41
1:A:222:ARG:O	1:A:225:ASP:HB2	2.21	0.41
1:B:91:GLU:CD	1:B:91:GLU:N	2.70	0.41
1:A:65:ASP:OD1	1:A:222:ARG:NE	2.49	0.41
1:B:117:PRO:HB3	1:B:158:LEU:CD2	2.50	0.40
1:A:27:THR:OG1	3:B:901[B]:CDX:HAE1	2.22	0.40
1:B:280:LEU:O	1:B:291:ALA:HA	2.21	0.40
1:B:141:ARG:HD3	1:B:360:PRO:HD2	2.03	0.40
1:B:175:ASN:N	1:B:175:ASN:HD22	2.20	0.40
3:B:901[A]:CDX:CAQ	3:B:901[A]:CDX:HAE2	2.51	0.40
1:B:82:LYS:HD2	1:B:82:LYS:HA	1.97	0.40

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	376/418 (90%)	368 (98%)	8 (2%)	0	100	100
1	B	372/418 (89%)	362 (97%)	9 (2%)	1 (0%)	46	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	748/836 (90%)	730 (98%)	17 (2%)	1 (0%)	56 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	LYS

### 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	342/381 (90%)	335 (98%)	7 (2%)	63 57
1	B	339/381 (89%)	322 (95%)	17 (5%)	30 18
All	All	681/762 (89%)	657 (96%)	24 (4%)	43 31

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	77	ARG
1	A	221	ARG
1	A	227	ASN
1	A	334	LYS
1	A	349	MET
1	A	350	PHE
1	B	52	LYS
1	B	83	ARG
1	B	91	GLU
1	B	111	LYS
1	B	162	ASP
1	B	163	LEU
1	B	164	ASN
1	B	175	ASN
1	B	205	ARG
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	257	SER
1	B	301	GLN
1	B	350	PHE
1	B	351	ILE
1	B	380	ARG
1	B	382	GLU
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	35	GLN
1	A	93	HIS
1	A	129	ASN
1	A	249	ASN
1	A	323	GLN
1	A	389	ASN
1	B	175	ASN
1	B	234	ASN
1	B	249	ASN
1	B	301	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	ANP	A	902	2	27,33,33	1.78	8 (29%)	30,52,52	1.87	3 (10%)
3	CDX	B	901[A]	-	20,20,20	0.97	0	23,28,28	2.10	6 (26%)
3	CDX	B	901[B]	-	20,20,20	0.91	0	23,28,28	2.04	6 (26%)
4	ANP	B	903	2	27,33,33	1.98	7 (25%)	30,52,52	1.88	3 (10%)

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
4	ANP	A	902	2	-	1/12/38/38	0/3/3/3
3	CDX	B	901[A]	-	1/1/7/9	0/8/32/32	0/2/2/2
3	CDX	B	901[B]	-	1/1/7/9	0/8/32/32	0/2/2/2
4	ANP	B	903	2	-	1/12/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	ANP	PB-O3A	-5.65	1.52	1.59
4	A	902	ANP	PB-O3A	-4.24	1.53	1.59
4	A	902	ANP	PG-O2G	-2.56	1.49	1.56
4	A	902	ANP	PB-O2B	-2.46	1.49	1.56
4	A	902	ANP	PG-O3G	-2.24	1.50	1.56
4	B	903	ANP	PB-O2B	-2.24	1.50	1.56
4	B	903	ANP	PG-O2G	-2.18	1.50	1.56
4	B	903	ANP	PG-O3G	-2.08	1.50	1.56
4	A	902	ANP	C2-N3	2.15	1.36	1.32
4	A	902	ANP	C5-C4	2.62	1.46	1.40
4	B	903	ANP	PG-O1G	2.85	1.49	1.46
4	B	903	ANP	C5-C4	2.85	1.46	1.40
4	A	902	ANP	PB-O1B	2.86	1.49	1.46
4	A	902	ANP	PG-O1G	3.69	1.50	1.46
4	B	903	ANP	PB-O1B	4.79	1.51	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	ANP	N3-C2-N1	-7.86	122.88	128.89
4	A	902	ANP	N3-C2-N1	-7.66	123.03	128.89
3	B	901[A]	CDX	CAC-CAD-NAJ	-4.63	106.13	112.48
3	B	901[B]	CDX	CAC-CAD-NAJ	-4.57	106.21	112.48
3	B	901[A]	CDX	CAE-CAL-NAM	-4.44	107.05	114.57
3	B	901[B]	CDX	CAE-CAL-NAM	-4.34	107.21	114.57
3	B	901[B]	CDX	CAP-CAQ-NAJ	-4.19	106.73	112.48
3	B	901[A]	CDX	CAP-CAQ-NAJ	-4.00	107.00	112.48
3	B	901[A]	CDX	CAL-CAK-NAJ	-3.84	108.37	113.48
3	B	901[B]	CDX	CAQ-NAJ-CAD	-2.68	106.87	109.89
3	B	901[B]	CDX	CAL-CAK-NAJ	-2.54	110.10	113.48
4	B	903	ANP	C4-C5-N7	-2.44	107.23	109.48
3	B	901[B]	CDX	CAF-NAM-CAR	-2.28	107.24	109.71
4	A	902	ANP	C4-C5-N7	-2.23	107.42	109.48
3	B	901[A]	CDX	CAF-NAM-CAR	-2.17	107.35	109.71
3	B	901[A]	CDX	CAQ-NAJ-CAD	-2.12	107.51	109.89
4	B	903	ANP	C4'-O4'-C1'	3.56	113.63	109.72
4	A	902	ANP	C4'-O4'-C1'	3.75	113.84	109.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	901[A]	CDX	CAL
3	B	901[B]	CDX	CAL

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	903	ANP	O1G-PG-N3B-PB
4	A	902	ANP	O1G-PG-N3B-PB

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901[A]	CDX	3	0
3	B	901[B]	CDX	5	0

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	382/418 (91%)	0.27	16 (4%) 40 44	13, 20, 32, 79	0
1	B	378/418 (90%)	0.36	24 (6%) 23 26	14, 22, 31, 52	0
All	All	760/836 (90%)	0.32	40 (5%) 30 33	13, 21, 31, 79	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ILE	5.0
1	B	165	VAL	4.6
1	B	405	ASP	4.3
1	B	186	THR	4.2
1	B	162	ASP	4.0
1	A	47	ASP	3.8
1	B	191	GLY	3.8
1	A	276	ILE	3.8
1	B	189	LYS	3.7
1	A	333	LYS	3.6
1	A	385	LEU	3.5
1	B	164	ASN	3.3
1	B	187	SER	3.1
1	A	402	GLU	3.0
1	A	255	LEU	3.0
1	B	161	ALA	2.9
1	A	409	GLU	2.8
1	B	403	ILE	2.8
1	B	106	ILE	2.8
1	A	210	GLU	2.7
1	A	407	ASN	2.7
1	A	44	GLU	2.7
1	A	29	ILE	2.6
1	B	113	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	334	LYS	2.5
1	B	398	THR	2.5
1	B	296	ASP	2.5
1	B	276	ILE	2.5
1	A	408	GLU	2.4
1	B	108	ILE	2.4
1	B	185	ILE	2.4
1	B	190	LYS	2.3
1	B	395	ASP	2.3
1	B	209	LYS	2.2
1	A	113	ASN	2.2
1	A	280	LEU	2.2
1	B	340	VAL	2.2
1	B	167	GLN	2.1
1	A	93	HIS	2.1
1	B	297	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CDX	B	901[A]	19/19	0.87	0.25	3.92	54,55,57,58	19
3	CDX	B	901[B]	19/19	0.87	0.25	3.92	54,56,57,58	19
4	ANP	A	902	31/31	0.98	0.14	0.38	20,23,26,29	0
4	ANP	B	903	31/31	0.97	0.11	-0.26	24,30,38,39	0
2	MG	B	905	1/1	0.94	0.10	-0.48	25,25,25,25	0
2	MG	A	904	1/1	0.98	0.12	-0.60	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.