



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:53 am BST

PDB ID : 5YEJ  
Title : Crystal structure of BioQ with its naturel double-stranded DNA operator  
Authors : Yan, L.; Guan, Z.Y.; Zou, T.T.  
Deposited on : 2017-09-17  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

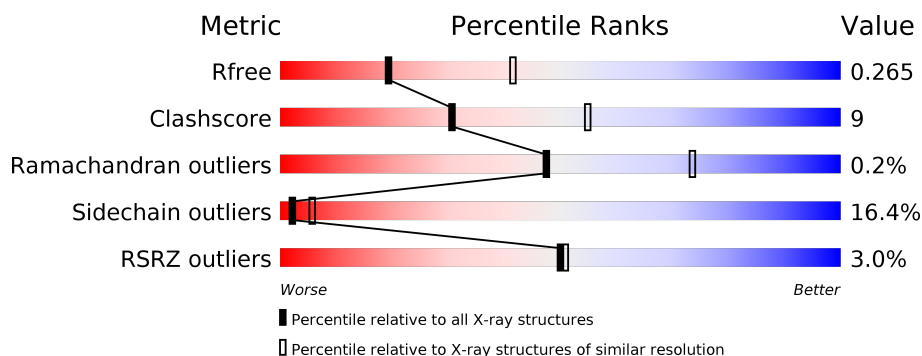
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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  $\leq 5\%$ . 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	232	<div> <div>57%</div> <div>13%</div> <div>•</div> <div>27%</div> </div>
1	B	232	<div>5%</div> <div>51%</div> <div>17%</div> <div>•</div> <div>29%</div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5011 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 TetR family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1298	813	241	242	2			
1	B	165	Total	C	N	O	S	0	0	0
			1253	785	228	238	2			
1	C	169	Total	C	N	O	S	0	0	0
			1301	814	240	245	2			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP I7FDJ0
A	-25	GLY	-	expression tag	UNP I7FDJ0
A	-24	SER	-	expression tag	UNP I7FDJ0
A	-23	HIS	-	expression tag	UNP I7FDJ0
A	-22	HIS	-	expression tag	UNP I7FDJ0
A	-21	HIS	-	expression tag	UNP I7FDJ0
A	-20	HIS	-	expression tag	UNP I7FDJ0
A	-19	HIS	-	expression tag	UNP I7FDJ0
A	-18	HIS	-	expression tag	UNP I7FDJ0
A	-17	SER	-	expression tag	UNP I7FDJ0
A	-16	SER	-	expression tag	UNP I7FDJ0
A	-15	GLY	-	expression tag	UNP I7FDJ0
A	-14	LEU	-	expression tag	UNP I7FDJ0
A	-13	VAL	-	expression tag	UNP I7FDJ0
A	-12	PRO	-	expression tag	UNP I7FDJ0
A	-11	ARG	-	expression tag	UNP I7FDJ0
A	-10	GLY	-	expression tag	UNP I7FDJ0
A	-9	SER	-	expression tag	UNP I7FDJ0
A	-8	HIS	-	expression tag	UNP I7FDJ0
A	-7	SER	-	expression tag	UNP I7FDJ0
A	-6	ASP	-	expression tag	UNP I7FDJ0
A	-5	GLU	-	expression tag	UNP I7FDJ0
A	-4	VAL	-	expression tag	UNP I7FDJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ASP	-	expression tag	UNP I7FDJ0
A	-2	ALA	-	expression tag	UNP I7FDJ0
A	-1	HIS	-	expression tag	UNP I7FDJ0
A	0	MET	-	expression tag	UNP I7FDJ0
A	1	VAL	-	expression tag	UNP I7FDJ0
B	-26	MET	-	expression tag	UNP I7FDJ0
B	-25	GLY	-	expression tag	UNP I7FDJ0
B	-24	SER	-	expression tag	UNP I7FDJ0
B	-23	HIS	-	expression tag	UNP I7FDJ0
B	-22	HIS	-	expression tag	UNP I7FDJ0
B	-21	HIS	-	expression tag	UNP I7FDJ0
B	-20	HIS	-	expression tag	UNP I7FDJ0
B	-19	HIS	-	expression tag	UNP I7FDJ0
B	-18	HIS	-	expression tag	UNP I7FDJ0
B	-17	SER	-	expression tag	UNP I7FDJ0
B	-16	SER	-	expression tag	UNP I7FDJ0
B	-15	GLY	-	expression tag	UNP I7FDJ0
B	-14	LEU	-	expression tag	UNP I7FDJ0
B	-13	VAL	-	expression tag	UNP I7FDJ0
B	-12	PRO	-	expression tag	UNP I7FDJ0
B	-11	ARG	-	expression tag	UNP I7FDJ0
B	-10	GLY	-	expression tag	UNP I7FDJ0
B	-9	SER	-	expression tag	UNP I7FDJ0
B	-8	HIS	-	expression tag	UNP I7FDJ0
B	-7	SER	-	expression tag	UNP I7FDJ0
B	-6	ASP	-	expression tag	UNP I7FDJ0
B	-5	GLU	-	expression tag	UNP I7FDJ0
B	-4	VAL	-	expression tag	UNP I7FDJ0
B	-3	ASP	-	expression tag	UNP I7FDJ0
B	-2	ALA	-	expression tag	UNP I7FDJ0
B	-1	HIS	-	expression tag	UNP I7FDJ0
B	0	MET	-	expression tag	UNP I7FDJ0
B	1	VAL	-	expression tag	UNP I7FDJ0
C	-26	MET	-	expression tag	UNP I7FDJ0
C	-25	GLY	-	expression tag	UNP I7FDJ0
C	-24	SER	-	expression tag	UNP I7FDJ0
C	-23	HIS	-	expression tag	UNP I7FDJ0
C	-22	HIS	-	expression tag	UNP I7FDJ0
C	-21	HIS	-	expression tag	UNP I7FDJ0
C	-20	HIS	-	expression tag	UNP I7FDJ0
C	-19	HIS	-	expression tag	UNP I7FDJ0
C	-18	HIS	-	expression tag	UNP I7FDJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP I7FDJ0
C	-16	SER	-	expression tag	UNP I7FDJ0
C	-15	GLY	-	expression tag	UNP I7FDJ0
C	-14	LEU	-	expression tag	UNP I7FDJ0
C	-13	VAL	-	expression tag	UNP I7FDJ0
C	-12	PRO	-	expression tag	UNP I7FDJ0
C	-11	ARG	-	expression tag	UNP I7FDJ0
C	-10	GLY	-	expression tag	UNP I7FDJ0
C	-9	SER	-	expression tag	UNP I7FDJ0
C	-8	HIS	-	expression tag	UNP I7FDJ0
C	-7	SER	-	expression tag	UNP I7FDJ0
C	-6	ASP	-	expression tag	UNP I7FDJ0
C	-5	GLU	-	expression tag	UNP I7FDJ0
C	-4	VAL	-	expression tag	UNP I7FDJ0
C	-3	ASP	-	expression tag	UNP I7FDJ0
C	-2	ALA	-	expression tag	UNP I7FDJ0
C	-1	HIS	-	expression tag	UNP I7FDJ0
C	0	MET	-	expression tag	UNP I7FDJ0
C	1	VAL	-	expression tag	UNP I7FDJ0

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*CP\*CP\*TP\*GP\*AP\*AP\*CP\*AP\*CP\*CP\*GP\*TP\*TP\*CP\*AP\*AP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			382	184	71	109	18			
2	G	19	Total	C	N	O	P	0	0	0
			383	184	71	110	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	19	Total	C	N	O	P	0	0	0
			390	187	71	114	18			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total	O	0	0
			2	2		

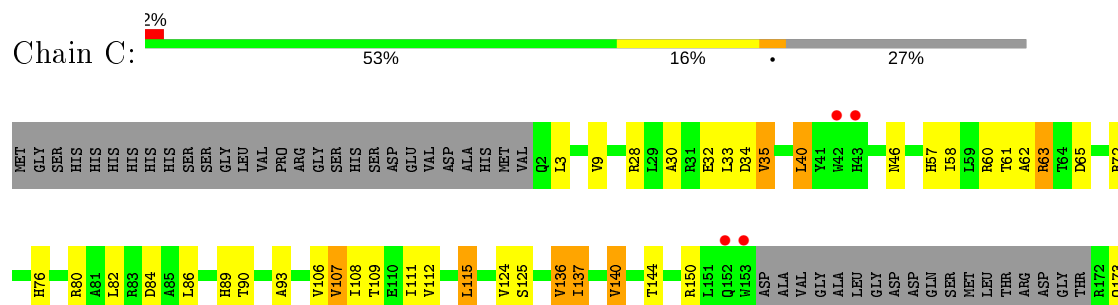
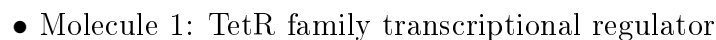
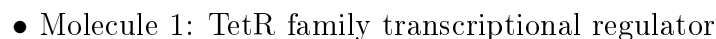
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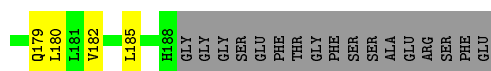
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		

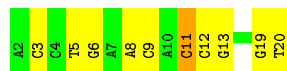


- Molecule 1: TetR family transcriptional regulator

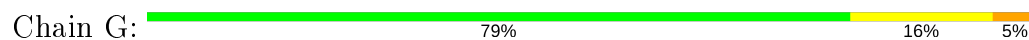




- Molecule 2: DNA (5'-D(\*AP\*CP\*CP\*TP\*GP\*AP\*AP\*CP\*AP\*CP\*CP\*GP\*TP\*TP\*CP\*AP\*AP\*GP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*CP\*CP\*TP\*GP\*AP\*AP\*CP\*AP\*CP\*CP\*GP\*TP\*TP\*CP\*AP\*AP\*GP\*T)-3')



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.69 Å   212.47 Å   88.13 Å 90.00°   99.43°   90.00°	Depositor
Resolution (Å)	37.68 – 2.70 37.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.68-2.70) 97.7 (37.68-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155)	Depositor
R, $R_{free}$	0.212   ,   0.265 0.212   ,   0.265	Depositor DCC
$R_{free}$ test set	1399 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 76.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.47	0/1319	0.65	0/1791
1	B	0.35	0/1271	0.51	0/1725
1	C	0.47	0/1322	0.59	0/1795
2	D	1.00	0/428	1.11	2/658 (0.3%)
2	G	1.00	0/429	1.09	1/659 (0.2%)
3	F	0.99	0/437	1.17	0/674
All	All	0.62	0/5206	0.77	3/7302 (0.0%)

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	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	11	DC	O4'-C4'-C3'	-7.42	101.53	104.50
2	G	26	DA	O4'-C1'-N9	6.70	112.69	108.00
2	D	3	DC	C1'-O4'-C4'	-5.08	105.02	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	173	GLN	Peptide

## 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	1298	0	1278	17	0
1	B	1253	0	1228	30	0
1	C	1301	0	1278	22	0
2	D	382	0	212	12	0
2	G	383	0	215	2	0
3	F	390	0	217	9	0
4	C	1	0	0	0	0
4	F	2	0	0	1	0
4	G	1	0	0	0	0
All	All	5011	0	4428	85	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 9.

All (85) 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:58:ILE:CG2	1:B:89:HIS:CD2	1.75	1.63
1:B:58:ILE:HG21	1:B:89:HIS:CD2	1.49	1.31
1:B:58:ILE:CG2	1:B:89:HIS:NE2	2.12	1.11
1:B:58:ILE:HG22	1:B:89:HIS:CD2	1.69	1.09
2:D:5:DT:OP2	1:C:35:VAL:HG22	1.56	1.04
1:B:58:ILE:HG23	1:B:89:HIS:CD2	1.93	1.00
1:B:58:ILE:HG23	1:B:89:HIS:NE2	1.81	0.88
2:D:19:DG:H2'	2:D:20:DT:H71	1.60	0.84
1:B:27:ARG:NH2	2:D:13:DG:N7	2.26	0.83
3:F:33:DA:H2''	3:F:34:DG:H5''	1.58	0.83
1:B:58:ILE:CG2	1:B:89:HIS:HD2	1.47	0.82
1:B:58:ILE:HG22	1:B:89:HIS:NE2	1.84	0.82
3:F:30:DT:OP2	1:C:46:ASN:HB2	1.81	0.81
3:F:19:DC:OP1	4:F:101:HOH:O	2.05	0.73
2:D:5:DT:OP2	1:C:35:VAL:CG2	2.35	0.70
1:B:36:THR:HG22	1:B:38:GLY:H	1.57	0.69
2:D:12:DC:H2'	2:D:13:DG:C8	2.28	0.68
1:B:58:ILE:HG21	1:B:89:HIS:HD2	1.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD23	1:C:40:LEU:N	2.10	0.67
1:B:93:ALA:O	1:B:97:SER:OG	2.09	0.67
1:A:112:VAL:HG22	1:A:137:ILE:HG12	1.78	0.66
1:C:63:ARG:HG3	1:C:63:ARG:O	1.95	0.64
1:C:76:HIS:NE2	1:C:179:GLN:OE1	2.30	0.64
1:A:4:HIS:O	1:A:7:ASP:HB2	2.00	0.62
1:C:57:HIS:O	1:C:60:ARG:NH1	2.32	0.62
1:C:30:ALA:HB1	1:C:35:VAL:O	2.00	0.62
2:D:11:DC:H2'	2:D:12:DC:C6	2.37	0.60
1:B:42:TRP:HZ2	3:F:18:DA:H5''	1.67	0.59
2:D:11:DC:H2'	2:D:12:DC:H6	1.68	0.59
1:B:69:LEU:HB2	1:B:74:GLN:HG3	1.85	0.58
1:B:92:GLY:O	1:B:96:VAL:HG13	2.03	0.57
1:C:62:ALA:HB1	1:C:82:LEU:HA	1.85	0.56
1:B:61:THR:O	1:B:61:THR:OG1	2.16	0.56
1:B:75:ILE:HD11	1:B:182:VAL:HB	1.88	0.55
1:A:115:LEU:HD12	1:A:133:ALA:HA	1.89	0.55
1:C:179:GLN:HA	1:C:182:VAL:HG22	1.89	0.55
1:A:179:GLN:HA	1:A:182:VAL:HG12	1.89	0.54
1:B:16:LEU:HD22	1:B:95:LEU:HD13	1.90	0.54
1:C:86:LEU:HD13	1:C:93:ALA:HA	1.90	0.54
3:F:29:DG:H2''	3:F:30:DT:O5'	2.08	0.53
1:A:120:ARG:C	1:A:122:ALA:H	2.12	0.53
1:B:179:GLN:HA	1:B:182:VAL:HG12	1.90	0.53
1:C:136:VAL:O	1:C:140:VAL:HG12	2.10	0.52
1:B:55:ALA:O	1:B:59:LEU:HG	2.09	0.52
3:F:29:DG:H2''	3:F:30:DT:C5'	2.39	0.52
1:A:132:ALA:O	1:A:135:THR:HB	2.11	0.51
2:D:5:DT:P	1:C:35:VAL:CG2	2.99	0.51
1:A:175:ARG:HB2	1:A:175:ARG:HH21	1.76	0.51
1:B:36:THR:HG22	1:B:38:GLY:N	2.26	0.50
1:C:106:VAL:O	1:C:109:THR:HB	2.12	0.49
1:A:105:SER:HB3	1:A:108:ILE:HG22	1.93	0.49
1:C:112:VAL:HG22	1:C:137:ILE:HG13	1.95	0.48
1:A:50:LEU:O	1:A:54:VAL:HG23	2.12	0.48
1:B:87:LEU:HA	1:B:148:GLN:NE2	2.29	0.48
1:B:66:THR:OG1	1:B:74:GLN:HG2	2.14	0.48
1:C:86:LEU:HB2	1:C:144:THR:HG21	1.96	0.47
3:F:27:DG:H2'	3:F:28:DT:C6	2.50	0.47
1:C:107:VAL:O	1:C:111:ILE:HG13	2.16	0.46
3:F:27:DG:H2'	3:F:28:DT:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:DT:H2''	2:D:6:DG:H5'	1.97	0.46
1:B:59:LEU:CD1	1:B:108:ILE:HG12	2.46	0.45
2:G:26:DA:H2''	2:G:27:DC:O5'	2.16	0.45
2:D:8:DA:OP1	2:D:8:DA:H4'	2.17	0.45
1:A:120:ARG:C	1:A:122:ALA:N	2.71	0.44
1:C:58:ILE:HG23	1:C:89:HIS:ND1	2.32	0.44
1:B:56:ASP:OD1	1:B:107:VAL:HG23	2.18	0.44
1:B:24:LEU:HA	1:B:24:LEU:HD23	1.61	0.43
1:C:111:ILE:O	1:C:115:LEU:HD22	2.18	0.43
1:A:137:ILE:HA	1:A:140:VAL:HG13	2.01	0.43
1:C:182:VAL:HA	1:C:185:LEU:HD12	2.00	0.43
2:D:8:DA:H2'	2:D:9:DC:C6	2.54	0.43
1:B:79:CYS:HB2	1:B:178:LEU:HD11	2.00	0.42
2:D:5:DT:P	1:C:35:VAL:HG23	2.58	0.42
1:A:17:ASP:OD1	1:A:89:HIS:HD2	2.02	0.42
1:C:33:LEU:HD23	1:C:33:LEU:HA	1.79	0.41
1:A:77:GLU:OE2	1:A:80:ARG:NH1	2.53	0.41
1:A:115:LEU:HD12	1:A:133:ALA:CB	2.51	0.41
1:A:73:GLU:O	1:A:77:GLU:HB3	2.20	0.41
1:B:75:ILE:HG13	1:B:76:HIS:N	2.34	0.41
3:F:24:DA:H2''	3:F:25:DC:C6	2.56	0.41
1:A:115:LEU:HD12	1:A:133:ALA:CA	2.50	0.40
1:B:8:VAL:HG23	1:B:29:LEU:HD21	2.02	0.40
1:B:27:ARG:HB2	1:B:27:ARG:HE	1.66	0.40
1:A:137:ILE:HG13	1:A:137:ILE:H	1.64	0.40
2:G:20:DC:H2''	2:G:21:DT:O5'	2.21	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	165/232 (71%)	155 (94%)	9 (6%)	1 (1%)	25	50
1	B	159/232 (68%)	151 (95%)	8 (5%)	0	100	100
1	C	165/232 (71%)	155 (94%)	10 (6%)	0	100	100
All	All	489/696 (70%)	461 (94%)	27 (6%)	1 (0%)	47	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA

### 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	129/181 (71%)	111 (86%)	18 (14%)	3	8
1	B	125/181 (69%)	104 (83%)	21 (17%)	2	5
1	C	130/181 (72%)	106 (82%)	24 (18%)	1	4
All	All	384/543 (71%)	321 (84%)	63 (16%)	2	6

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	21	ILE
1	A	28	ARG
1	A	32	GLU
1	A	35	VAL
1	A	63	ARG
1	A	78	SER
1	A	80	ARG
1	A	84	ASP
1	A	94	GLU
1	A	115	LEU
1	A	124	VAL

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Mol	Chain	Res	Type
1	A	126	ASP
1	A	137	ILE
1	A	140	VAL
1	A	144	THR
1	A	172	ARG
1	A	175	ARG
1	B	3	LEU
1	B	8	VAL
1	B	14	LYS
1	B	17	ASP
1	B	21	ILE
1	B	24	LEU
1	B	27	ARG
1	B	58	ILE
1	B	60	ARG
1	B	61	THR
1	B	63	ARG
1	B	64	THR
1	B	66	THR
1	B	72	ARG
1	B	80	ARG
1	B	84	ASP
1	B	102	SER
1	B	112	VAL
1	B	172	ARG
1	B	173	GLN
1	B	178	LEU
1	C	3	LEU
1	C	9	VAL
1	C	28	ARG
1	C	32	GLU
1	C	34	ASP
1	C	35	VAL
1	C	40	LEU
1	C	61	THR
1	C	63	ARG
1	C	65	ASP
1	C	72	ARG
1	C	80	ARG
1	C	84	ASP
1	C	90	THR
1	C	107	VAL

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Mol	Chain	Res	Type
1	C	108	ILE
1	C	115	LEU
1	C	124	VAL
1	C	125	SER
1	C	136	VAL
1	C	137	ILE
1	C	140	VAL
1	C	150	ARG
1	C	180	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS

### 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](#)

There are no ligands in this entry.

## 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	169/232 (72%)	0.14	1 (0%) 89 91	67, 91, 118, 148	0
1	B	165/232 (71%)	0.38	12 (7%) 15 13	79, 110, 146, 159	0
1	C	169/232 (72%)	0.43	4 (2%) 59 60	72, 102, 137, 163	0
2	D	19/19 (100%)	-0.25	0 100 100	82, 109, 128, 141	0
2	G	19/19 (100%)	-0.35	0 100 100	81, 106, 122, 130	0
3	F	19/19 (100%)	-0.30	0 100 100	85, 111, 126, 129	0
All	All	560/753 (74%)	0.26	17 (3%) 50 51	67, 102, 139, 163	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	TRP	4.0
1	B	68	ASP	3.4
1	B	60	ARG	3.2
1	B	65	ASP	3.1
1	B	121	ALA	3.1
1	B	64	THR	2.9
1	C	152	GLN	2.7
1	A	153	TRP	2.7
1	B	73	GLU	2.7
1	B	42	TRP	2.5
1	B	39	ALA	2.5
1	B	3	LEU	2.5
1	C	43	HIS	2.2
1	B	31	ARG	2.1
1	C	42	TRP	2.1
1	B	70	ALA	2.1
1	B	182	VAL	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.