



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 03:43 PM EST

PDB ID : 1X7O  
Title : Crystal structure of the SpoU Methyltransferase AviRb from *Streptomyces viridochromogenes*  
Authors : Mosbacher, T.G.; Bechthold, A.; Schulz, G.E.  
Deposited on : 2004-08-16  
Resolution : 2.37 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

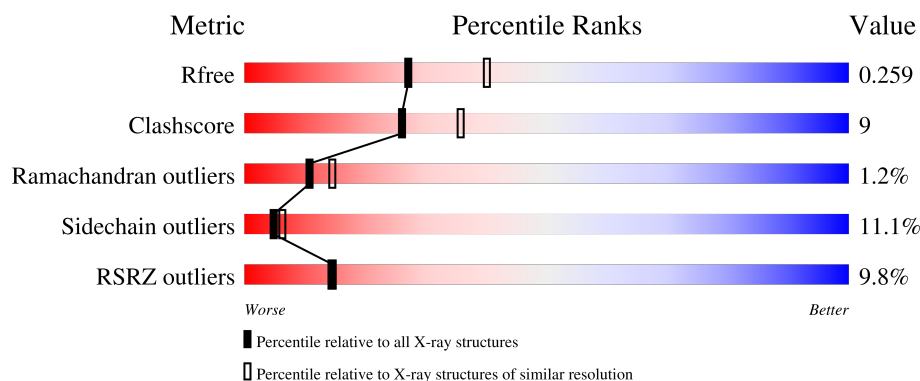
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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))
$R_{free}$	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	287	<div> <div>4%</div> <div>74%</div> <div>15%</div> <div>7%</div> </div>
1	B	287	<div> <div>13%</div> <div>64%</div> <div>22%</div> <div>10%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4127 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 rRNA methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	Se	0	0	0
			2041	1279	369	385	2	6			
1	B	257	Total	C	N	O	S	Se	0	0	0
			1957	1232	350	367	2	6			

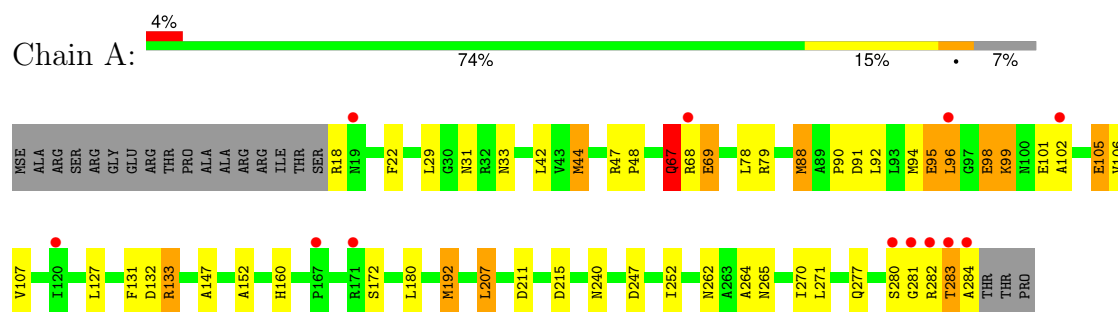
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	39	Total	O	0	0
			39	39		

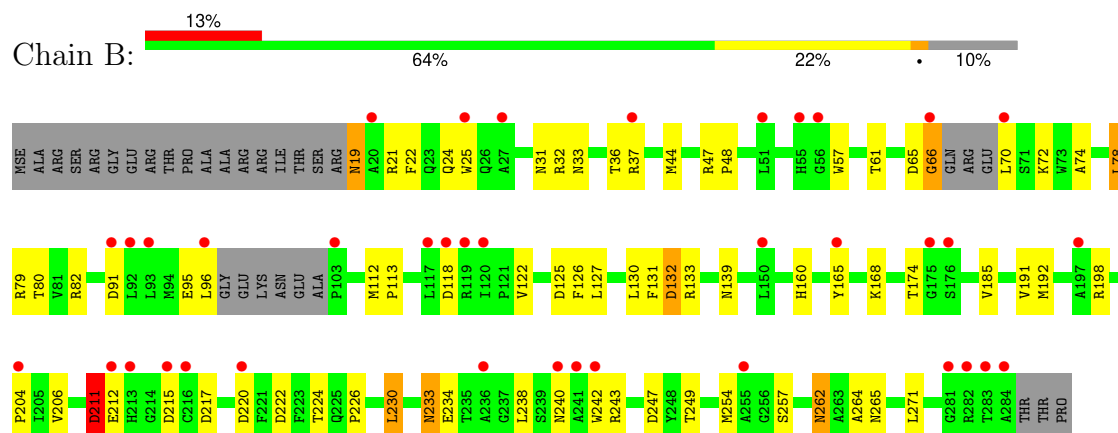
### 3 Residue-property plots [i](#)

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. 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. 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: rRNA methyltransferase



#### • Molecule 1: rRNA methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.62Å 76.62Å 208.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.37 25.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.37) 99.5 (25.00-2.37)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.86 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.206 , 0.249 0.227 , 0.259	Depositor DCC
$R_{free}$ test set	1259 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	0.69	2/2076 (0.1%)	0.88	5/2817 (0.2%)
1	B	0.66	1/1990 (0.1%)	0.83	10/2700 (0.4%)
All	All	0.68	3/4066 (0.1%)	0.86	15/5517 (0.3%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLN	CD-OE1	8.53	1.42	1.24
1	A	192	MSE	SE-CE	-7.88	1.49	1.95
1	B	66	GLY	C-O	7.67	1.35	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	211	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	211	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	118	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	215	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	133	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	217	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	98	GLU	N-CA-C	-5.68	95.67	111.00
1	B	247	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	247	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	125	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	132	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	220	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	91	ASP	CB-CG-OD2	5.13	122.91	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLN	Peptide
1	A	68	ARG	Peptide
1	A	94	MSE	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	2041	0	2030	32	0
1	B	1957	0	1950	43	0
2	A	90	0	0	5	0
2	B	39	0	0	2	0
All	All	4127	0	3980	74	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 (74) 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:130:LEU:HD11	1:B:242:TRP:CZ2	2.19	0.78
1:A:192:MSE:HE1	1:A:207:LEU:HD11	1.66	0.76
1:A:31:ASN:HD22	1:A:33:ASN:H	1.34	0.76
1:A:67:GLN:OE1	1:A:90:PRO:HG3	1.85	0.76
1:A:160:HIS:ND1	2:A:298:HOH:O	2.20	0.73
1:B:130:LEU:HD11	1:B:242:TRP:CH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:O	2:B:307:HOH:O	2.10	0.69
1:A:132:ASP:OD1	1:A:133:ARG:HD3	1.93	0.69
1:B:112:MSE:HE2	1:B:165:TYR:CD2	2.29	0.67
1:A:262:ASN:HD22	1:A:265:ASN:H	1.39	0.67
1:A:29:LEU:HD22	1:A:96:LEU:HG	1.76	0.67
1:A:277:GLN:O	1:A:281:GLY:HA2	1.94	0.67
1:B:204:PRO:HD2	1:B:226:PRO:HG3	1.78	0.66
1:B:130:LEU:CD1	1:B:242:TRP:CH2	2.79	0.66
1:B:204:PRO:HD2	1:B:226:PRO:CG	2.26	0.66
1:A:265:ASN:ND2	1:B:265:ASN:OD1	2.29	0.66
1:B:21:ARG:NH2	1:B:25:TRP:CZ2	2.65	0.65
1:A:92:LEU:O	1:A:95:GLU:HB2	1.97	0.65
1:A:96:LEU:HD11	2:A:353:HOH:O	2.01	0.61
1:B:238:LEU:HD22	1:B:242:TRP:CB	2.31	0.60
1:A:47:ARG:HB3	1:A:48:PRO:HD3	1.83	0.60
1:B:262:ASN:HD22	1:B:265:ASN:H	1.48	0.59
1:B:230:LEU:CD1	1:B:242:TRP:CE3	2.85	0.59
1:B:185:VAL:O	1:B:185:VAL:HG23	2.04	0.58
1:A:67:GLN:OE1	1:A:90:PRO:CG	2.52	0.56
1:A:44:MSE:HG3	1:A:107:VAL:HG22	1.86	0.56
1:A:262:ASN:HD21	1:A:264:ALA:HB3	1.71	0.56
1:A:98:GLU:O	1:A:101:GLU:HB2	2.06	0.55
1:B:133:ARG:O	1:B:233:ASN:ND2	2.39	0.55
1:A:44:MSE:CG	1:A:107:VAL:HG22	2.36	0.55
1:B:21:ARG:NH2	1:B:25:TRP:CH2	2.75	0.55
1:B:113:PRO:HD2	1:B:165:TYR:OH	2.07	0.54
1:B:222:ASP:OD1	1:B:224:THR:OG1	2.22	0.54
1:B:130:LEU:CD1	1:B:242:TRP:CZ2	2.92	0.53
1:B:238:LEU:HD22	1:B:242:TRP:HB3	1.91	0.53
1:B:47:ARG:HB3	1:B:48:PRO:HD3	1.91	0.52
1:A:22:PHE:HD2	1:A:88:MSE:HE1	1.75	0.51
1:A:95:GLU:CG	1:A:96:LEU:N	2.74	0.51
1:B:174:THR:HG22	1:B:174:THR:O	2.11	0.51
1:B:230:LEU:HD11	1:B:242:TRP:CE3	2.45	0.51
1:B:204:PRO:HD2	1:B:226:PRO:HG2	1.94	0.50
1:B:185:VAL:HG21	1:B:191:VAL:HG22	1.92	0.50
1:A:92:LEU:O	1:A:95:GLU:CB	2.59	0.50
1:A:105:GLU:HG2	1:A:106:VAL:HG23	1.95	0.49
1:A:96:LEU:HD21	2:A:353:HOH:O	2.11	0.49
1:B:212:GLU:O	2:B:323:HOH:O	2.20	0.49
1:A:31:ASN:ND2	1:A:33:ASN:H	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:O	1:B:78:LEU:HD22	2.14	0.47
1:A:98:GLU:O	1:A:99:LYS:C	2.53	0.47
1:B:130:LEU:HD13	1:B:242:TRP:CH2	2.48	0.47
1:B:130:LEU:HD21	1:B:242:TRP:CZ2	2.50	0.46
1:B:19:ASN:HB2	1:B:22:PHE:HB3	1.99	0.45
1:B:132:ASP:HB2	1:B:242:TRP:CD1	2.51	0.45
1:B:139:ASN:ND2	1:B:234:GLU:HG2	2.32	0.44
1:B:122:VAL:HG22	1:B:126:PHE:CD1	2.54	0.43
1:B:262:ASN:ND2	1:B:265:ASN:H	2.13	0.43
1:B:262:ASN:HD21	1:B:264:ALA:HB3	1.83	0.43
1:B:130:LEU:HD21	1:B:242:TRP:CE2	2.53	0.42
1:B:122:VAL:HG21	1:B:198:ARG:HG3	2.00	0.42
1:B:122:VAL:HG22	1:B:126:PHE:CE1	2.55	0.42
1:A:240:ASN:HD22	1:A:240:ASN:HA	1.69	0.42
1:A:252:ILE:HD11	1:A:270:ILE:HG13	2.02	0.41
1:A:192:MSE:HA	1:A:192:MSE:HE2	2.01	0.41
1:B:238:LEU:HD22	1:B:242:TRP:HB2	2.00	0.41
1:B:112:MSE:HG3	1:B:165:TYR:CE2	2.54	0.41
1:A:96:LEU:HD22	1:A:96:LEU:HA	1.87	0.41
1:A:277:GLN:HG2	1:A:283:THR:O	2.20	0.41
1:B:192:MSE:N	1:B:192:MSE:HE2	2.35	0.41
1:A:95:GLU:HA	2:A:306:HOH:O	2.20	0.41
1:A:147:ALA:HB1	1:A:152:ALA:HB3	2.02	0.41
1:A:284:ALA:C	2:A:352:HOH:O	2.59	0.41
1:B:211:ASP:HB2	1:B:249:THR:CG2	2.51	0.41
1:B:33:ASN:N	1:B:33:ASN:HD22	2.20	0.40
1:B:57:TRP:CZ3	1:B:113:PRO:HD3	2.56	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	265/287 (92%)	251 (95%)	11 (4%)	3 (1%)	12	16
1	B	251/287 (88%)	241 (96%)	7 (3%)	3 (1%)	11	14
All	All	516/574 (90%)	492 (95%)	18 (4%)	6 (1%)	11	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	B	160	HIS
1	B	233	ASN
1	A	69	GLU
1	B	257	SER
1	A	102	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	215/224 (96%)	195 (91%)	20 (9%)	7	10
1	B	207/224 (92%)	180 (87%)	27 (13%)	3	4
All	All	422/448 (94%)	375 (89%)	47 (11%)	5	6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	42	LEU
1	A	44	MSE
1	A	69	GLU
1	A	78	LEU
1	A	79	ARG
1	A	88	MSE
1	A	91	ASP
1	A	96	LEU
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	105	GLU
1	A	127	LEU
1	A	131	PHE
1	A	172	SER
1	A	180	LEU
1	A	207	LEU
1	A	271	LEU
1	A	280	SER
1	A	282	ARG
1	A	283	THR
1	B	19	ASN
1	B	24	GLN
1	B	31	ASN
1	B	32	ARG
1	B	36	THR
1	B	37	ARG
1	B	44	MSE
1	B	61	THR
1	B	70	LEU
1	B	72	LYS
1	B	78	LEU
1	B	79	ARG
1	B	80	THR
1	B	82	ARG
1	B	95	GLU
1	B	96	LEU
1	B	127	LEU
1	B	131	PHE
1	B	168	LYS
1	B	206	VAL
1	B	211	ASP
1	B	230	LEU
1	B	240	ASN
1	B	243	ARG
1	B	254	MSE
1	B	262	ASN
1	B	271	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	ASN
1	A	240	ASN
1	A	262	ASN
1	A	265	ASN
1	B	33	ASN
1	B	262	ASN
1	B	265	ASN

### 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 oligosaccharides 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 ⓘ

**Warning:** The R factor obtained from EDS is 0.2731, which does not match the depositor's R factor of 0.20561. Please interpret the results in this section carefully.

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	261/287 (90%)	0.37	12 (4%) 38 38	26, 33, 44, 56	0
1	B	251/287 (87%)	1.04	38 (15%) 6 7	24, 34, 43, 53	0
All	All	512/574 (89%)	0.70	50 (9%) 14 14	24, 33, 44, 56	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	HIS	6.1
1	B	212	GLU	5.8
1	B	242	TRP	5.5
1	B	215	ASP	5.3
1	A	282	ARG	4.5
1	B	240	ASN	4.5
1	A	283	THR	4.2
1	B	284	ALA	4.2
1	B	282	ARG	4.0
1	B	216	CYS	4.0
1	A	281	GLY	3.9
1	B	283	THR	3.9
1	A	96	LEU	3.6
1	B	56	GLY	3.6
1	B	236	ALA	3.3
1	B	51	LEU	3.3
1	A	102	ALA	3.3
1	B	165	TYR	3.2
1	B	241	ALA	3.2
1	B	120	ILE	3.1
1	A	280	SER	2.9
1	A	68	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	93	LEU	2.9
1	B	220	ASP	2.9
1	B	117	LEU	2.8
1	B	66	GLY	2.8
1	B	103	PRO	2.8
1	B	70	LEU	2.7
1	B	92	LEU	2.7
1	B	96	LEU	2.6
1	B	20	ALA	2.6
1	B	55	HIS	2.6
1	A	167	PRO	2.5
1	B	176	SER	2.5
1	B	175	GLY	2.5
1	B	281	GLY	2.5
1	B	27	ALA	2.5
1	B	91	ASP	2.5
1	A	284	ALA	2.4
1	B	204	PRO	2.3
1	B	255	ALA	2.3
1	B	25	TRP	2.2
1	B	150	LEU	2.2
1	A	120	ILE	2.2
1	B	197	ALA	2.2
1	A	171	ARG	2.1
1	B	118	ASP	2.1
1	B	119	ARG	2.1
1	B	37	ARG	2.1
1	A	19	ASN	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 monosaccharides 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.