



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:54 AM GMT

PDB ID : 3NI7  
Title : Crystal structure of the TetR transcriptional regulator from *Nitrosomonas europaea* ATCC 19718  
Authors : Knapik, A.; Chruszcz, M.; Cymborowski, M.; Xu, X.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Minor, W.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-06-15  
Resolution : 2.78 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

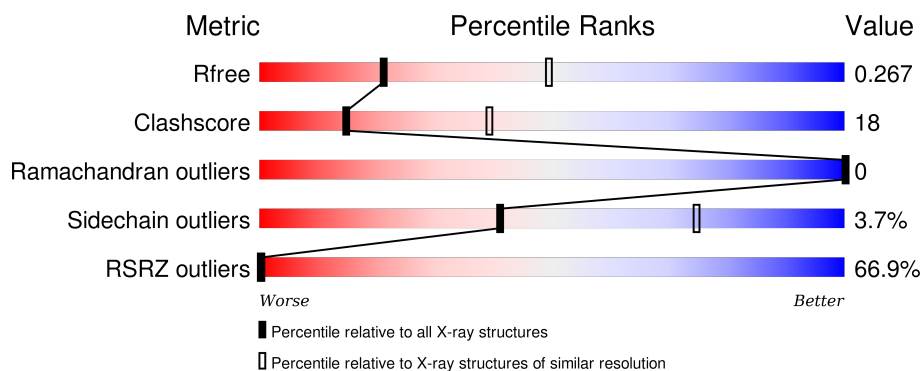
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	213	<div> <div>55%</div> <div> <div>56%</div> <div>22%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	213	<div> <div>48%</div> <div> <div>62%</div> <div>18%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2735 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 Bacterial regulatory proteins, TetR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	Se	0	1	0
			1383	880	241	252	10			
1	B	173	Total	C	N	O	Se	0	0	0
			1352	869	233	241	9			

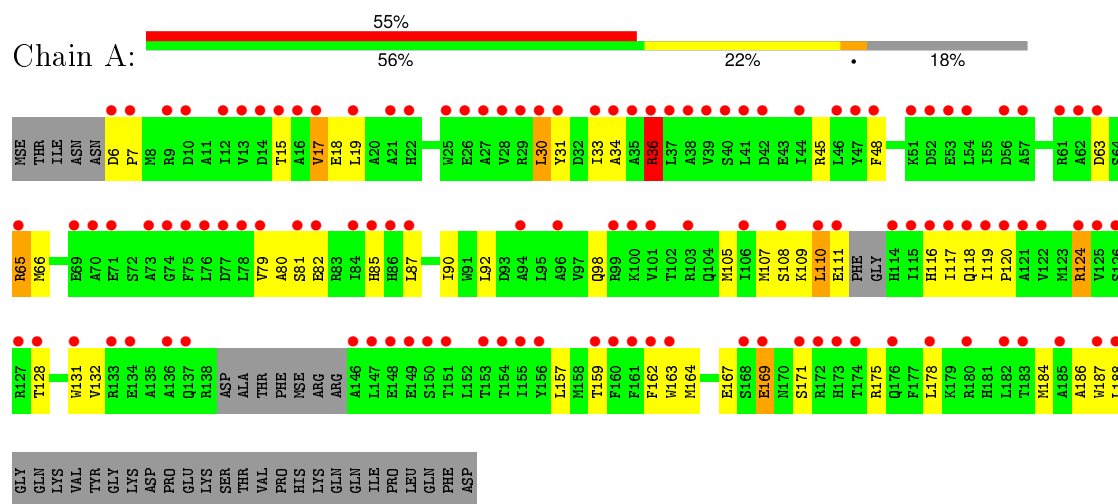
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	INITIATING METHIONINE	UNP Q82XH4
B	1	MSE	-	INITIATING METHIONINE	UNP Q82XH4

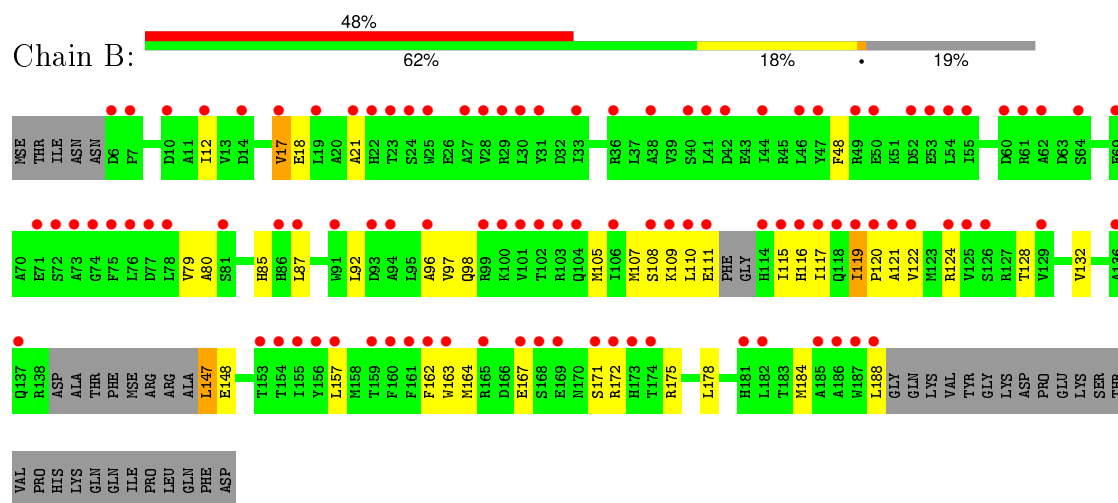
### 3 Residue-property plots [i](#)

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: Bacterial regulatory proteins, TetR family



- Molecule 1: Bacterial regulatory proteins, TetR family



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.22Å 75.38Å 98.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.78 34.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.78) 99.7 (34.62-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109, COOT	Depositor
R, $R_{free}$	0.249 , 0.279 0.255 , 0.267	Depositor DCC
$R_{free}$ test set	583 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.991	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 138.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 12224 reflections (0.025%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.96	2/1399 (0.1%)	0.90	2/1881 (0.1%)
1	B	0.91	2/1369 (0.1%)	0.85	1/1843 (0.1%)
All	All	0.94	4/2768 (0.1%)	0.88	3/3724 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLU	CB-CG	-5.84	1.41	1.52
1	B	148	GLU	CG-CD	5.71	1.60	1.51
1	B	167	GLU	CB-CG	-5.67	1.41	1.52
1	A	167	GLU	CB-CG	-5.36	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	65	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	36	ARG	NE-CZ-NH2	-5.39	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1383	0	1325	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1352	0	1297	39	0
All	All	2735	0	2622	95	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 18.

All (95) 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:A:110:LEU:HD23	1:A:111:GLU:N	1.52	1.25
1:A:110:LEU:C	1:A:110:LEU:HD23	1.76	1.06
1:A:116:HIS:O	1:A:120:PRO:HD3	1.54	1.06
1:A:110:LEU:CD2	1:A:110:LEU:C	2.30	0.98
1:B:115:ILE:O	1:B:119:ILE:HG22	1.63	0.98
1:A:117:ILE:O	1:A:120:PRO:HG2	1.69	0.93
1:A:119:ILE:HG23	1:A:120:PRO:HD3	1.52	0.89
1:A:85:HIS:CD2	1:A:178:LEU:HD23	2.16	0.80
1:A:119:ILE:N	1:A:120:PRO:HD2	1.97	0.79
1:A:116:HIS:O	1:A:120:PRO:CD	2.30	0.78
1:A:117:ILE:O	1:A:120:PRO:CG	2.30	0.78
1:A:19:LEU:HD21	1:A:36:ARG:HG3	1.68	0.75
1:B:119:ILE:HG23	1:B:120:PRO:HD3	1.67	0.75
1:A:107:MSE:O	1:A:110:LEU:HB3	1.88	0.73
1:B:119:ILE:HG23	1:B:120:PRO:CD	2.19	0.73
1:A:117:ILE:C	1:A:120:PRO:HD2	2.11	0.71
1:B:105:MSE:O	1:B:108:SER:HB3	1.90	0.71
1:A:110:LEU:HD23	1:A:111:GLU:CB	2.20	0.70
1:A:110:LEU:HD23	1:A:111:GLU:CA	2.20	0.69
1:A:157:LEU:HD12	1:B:157:LEU:HD12	1.72	0.69
1:A:119:ILE:CG2	1:A:120:PRO:HD3	2.21	0.69
1:A:117:ILE:O	1:A:120:PRO:HD2	1.94	0.67
1:A:110:LEU:CD2	1:A:111:GLU:CB	2.73	0.67
1:A:17:VAL:HG13	1:A:98:GLN:HG3	1.77	0.66
1:A:162:PHE:CE1	1:B:111:GLU:HA	2.31	0.65
1:A:119:ILE:N	1:A:120:PRO:CD	2.59	0.65
1:A:119:ILE:HG23	1:A:120:PRO:CD	2.27	0.64
1:B:110:LEU:HG	1:B:111:GLU:N	2.12	0.63
1:B:92:LEU:HD22	1:B:163:TRP:CD2	2.33	0.62
1:A:105:MSE:O	1:A:108:SER:HB3	1.99	0.62
1:B:17:VAL:HG13	1:B:98:GLN:HG3	1.81	0.62
1:A:117:ILE:O	1:A:120:PRO:CD	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HB	1:B:184:MSE:CE	2.32	0.60
1:A:162:PHE:HE1	1:B:111:GLU:HA	1.67	0.59
1:A:107:MSE:CE	1:A:164:MSE:HE1	2.32	0.59
1:B:119:ILE:N	1:B:120:PRO:HD2	2.17	0.59
1:B:171:SER:O	1:B:175:ARG:HG3	2.03	0.59
1:B:128:THR:O	1:B:132:VAL:HG23	2.03	0.58
1:A:92:LEU:HD22	1:A:163:TRP:CD2	2.38	0.58
1:A:171:SER:O	1:A:175:ARG:HG3	2.03	0.58
1:B:117:ILE:O	1:B:120:PRO:HG2	2.04	0.57
1:A:63:ASP:OD2	1:A:124:ARG:NH2	2.37	0.57
1:A:119:ILE:O	1:A:119:ILE:HD12	2.05	0.56
1:B:116:HIS:O	1:B:120:PRO:HG3	2.05	0.56
1:A:110:LEU:HD22	1:A:110:LEU:C	2.22	0.55
1:B:85:HIS:CD2	1:B:178:LEU:HD23	2.41	0.55
1:A:116:HIS:O	1:A:119:ILE:CG2	2.55	0.55
1:A:118:GLN:C	1:A:120:PRO:HD2	2.26	0.55
1:B:110:LEU:O	1:B:111:GLU:C	2.43	0.55
1:A:107:MSE:HE2	1:A:164:MSE:HE1	1.89	0.54
1:A:128:THR:O	1:A:132:VAL:HG23	2.09	0.53
1:A:116:HIS:O	1:A:119:ILE:HG22	2.10	0.52
1:A:111:GLU:HA	1:B:162:PHE:CE1	2.46	0.51
1:B:87:LEU:HD12	1:B:132:VAL:HG13	1.92	0.51
1:B:116:HIS:O	1:B:120:PRO:CG	2.59	0.51
1:A:119:ILE:HB	1:B:184:MSE:HE3	1.94	0.50
1:A:117:ILE:C	1:A:120:PRO:CD	2.80	0.49
1:A:45:ARG:HA	1:A:48:PHE:O	2.13	0.48
1:B:124:ARG:O	1:B:128:THR:OG1	2.26	0.47
1:A:30:LEU:HD12	1:A:33:ILE:HD12	1.97	0.47
1:A:6:ASP:N	1:A:7:PRO:CD	2.78	0.47
1:B:12:ILE:HG21	1:B:48:PHE:CD1	2.50	0.47
1:A:66:MSE:HE3	1:A:131:TRP:CE3	2.49	0.46
1:B:107:MSE:O	1:B:110:LEU:HB2	2.16	0.46
1:A:79:VAL:HG12	1:A:80:ALA:N	2.31	0.46
1:B:116:HIS:O	1:B:120:PRO:CD	2.64	0.46
1:B:119:ILE:HD12	1:B:119:ILE:O	2.16	0.45
1:B:171:SER:O	1:B:172:ARG:C	2.56	0.44
1:A:111:GLU:HA	1:B:162:PHE:HE1	1.83	0.44
1:B:92:LEU:HD22	1:B:163:TRP:CG	2.53	0.44
1:A:119:ILE:CG2	1:A:120:PRO:CD	2.91	0.43
1:A:15:THR:HG23	1:A:36:ARG:HD2	2.00	0.43
1:B:119:ILE:HG23	1:B:120:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:NH1	1:A:90:ILE:HD12	2.33	0.43
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.75	0.43
1:B:188:LEU:HD12	1:B:188:LEU:N	2.33	0.43
1:B:18:GLU:O	1:B:21:ALA:HB3	2.19	0.43
1:A:31:TYR:O	1:A:34:ALA:HB3	2.19	0.43
1:A:92:LEU:HD22	1:A:163:TRP:CG	2.54	0.43
1:A:18:GLU:HB3	1:A:36:ARG:HH22	1.85	0.42
1:B:119:ILE:N	1:B:120:PRO:CD	2.82	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.70	0.42
1:A:169:GLU:O	1:A:169:GLU:HG2	2.18	0.42
1:A:110:LEU:HD22	1:A:110:LEU:O	2.19	0.42
1:B:79:VAL:HG12	1:B:80:ALA:N	2.34	0.41
1:A:159:THR:HG21	1:A:178:LEU:HD13	2.02	0.41
1:A:110:LEU:CD2	1:A:111:GLU:N	2.44	0.41
1:A:15:THR:CG2	1:A:33:ILE:HG23	2.50	0.41
1:A:188:LEU:N	1:A:188:LEU:HD12	2.35	0.41
1:B:121:ALA:O	1:B:122:VAL:C	2.56	0.41
1:A:87:LEU:HD12	1:A:132:VAL:HG13	2.03	0.41
1:A:186:ALA:O	1:A:187:TRP:C	2.59	0.41
1:B:107:MSE:CE	1:B:164:MSE:HE1	2.51	0.40
1:B:96:ALA:O	1:B:97:VAL:C	2.59	0.40
1:A:81:SER:OG	1:A:82:GLU:N	2.53	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	169/213 (79%)	165 (98%)	4 (2%)	0	100	100
1	B	167/213 (78%)	159 (95%)	8 (5%)	0	100	100
All	All	336/426 (79%)	324 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	137/176 (78%)	129 (94%)	8 (6%)	25	55
1	B	131/176 (74%)	128 (98%)	3 (2%)	58	87
All	All	268/352 (76%)	257 (96%)	11 (4%)	41	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	30	LEU
1	A	36	ARG
1	A	109	LYS
1	A	110	LEU
1	A	124	ARG
1	A	184[A]	MSE
1	A	184[B]	MSE
1	B	17	VAL
1	B	109	LYS
1	B	119	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [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	165/213 (77%)	2.79	118 (71%) 0 0	75, 95, 126, 159	0
1	B	164/213 (76%)	2.94	102 (62%) 0 0	78, 99, 133, 172	0
All	All	329/426 (77%)	2.86	220 (66%) 0 0	75, 97, 133, 172	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	HIS	11.4
1	B	77	ASP	8.4
1	A	117	ILE	8.2
1	A	136	ALA	7.9
1	B	94	ALA	7.7
1	B	117	ILE	7.7
1	B	108	SER	7.4
1	B	50	GLU	7.4
1	B	7	PRO	7.3
1	A	74	GLY	7.3
1	B	73	ALA	6.8
1	B	38	ALA	6.8
1	A	73	ALA	6.8
1	B	19	LEU	6.8
1	A	7	PRO	6.7
1	A	76	LEU	6.6
1	B	21	ALA	6.6
1	A	162	PHE	6.4
1	B	12	ILE	6.2
1	A	69	GLU	5.9
1	A	30	LEU	5.7
1	A	101	VAL	5.7
1	B	93	ASP	5.6
1	B	169	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	28	VAL	5.4
1	A	34	ALA	5.4
1	A	40	SER	5.4
1	B	81	SER	5.4
1	B	168	SER	5.3
1	B	17	VAL	5.3
1	B	162	PHE	5.3
1	A	114	HIS	5.2
1	A	108	SER	5.1
1	B	153	THR	5.1
1	A	81	SER	5.1
1	B	122	VAL	5.1
1	A	173	HIS	5.1
1	B	125	VAL	5.1
1	B	100	LYS	5.0
1	A	16	ALA	5.0
1	A	27	ALA	4.9
1	B	186	ALA	4.8
1	A	42	ASP	4.7
1	B	27	ALA	4.7
1	B	172	ARG	4.6
1	B	121	ALA	4.6
1	B	110	LEU	4.6
1	B	120	PRO	4.5
1	A	6	ASP	4.4
1	B	76	LEU	4.4
1	A	96	ALA	4.4
1	A	100	LYS	4.4
1	A	168	SER	4.3
1	B	174	THR	4.3
1	B	165	ARG	4.3
1	B	167	GLU	4.3
1	B	74	GLY	4.2
1	A	82	GLU	4.2
1	B	62	ALA	4.2
1	B	188	LEU	4.2
1	B	96	ALA	4.2
1	B	101	VAL	4.2
1	A	120	PRO	4.1
1	B	36	ARG	4.1
1	A	176	GLN	4.1
1	A	116	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	174	THR	4.1
1	B	136	ALA	4.0
1	A	87	LEU	4.0
1	A	171	SER	4.0
1	A	103	ARG	4.0
1	A	94	ALA	4.0
1	B	87	LEU	4.0
1	A	99	ARG	3.9
1	A	28	VAL	3.9
1	B	115	ILE	3.9
1	A	172	ARG	3.8
1	B	137	GLN	3.8
1	B	23	THR	3.8
1	B	109	LYS	3.8
1	A	75	PHE	3.8
1	A	131	TRP	3.7
1	A	10	ASP	3.7
1	A	163	TRP	3.7
1	A	17	VAL	3.7
1	B	14	ASP	3.7
1	B	10	ASP	3.6
1	B	154	THR	3.6
1	A	38	ALA	3.6
1	B	6	ASP	3.6
1	A	159	THR	3.5
1	A	148	GLU	3.5
1	A	110	LEU	3.5
1	B	163	TRP	3.5
1	B	111	GLU	3.5
1	A	29	ARG	3.4
1	A	57	ALA	3.4
1	B	44	ILE	3.4
1	B	47	TYR	3.4
1	B	53	GLU	3.4
1	B	71	GLU	3.4
1	A	25	TRP	3.4
1	A	133	ARG	3.4
1	B	46	LEU	3.4
1	A	44	ILE	3.4
1	B	114	HIS	3.4
1	A	77	ASP	3.3
1	A	62	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	3.2
1	B	106	ILE	3.2
1	A	48	PHE	3.2
1	A	106	ILE	3.2
1	B	78	LEU	3.2
1	B	157	LEU	3.2
1	B	54	LEU	3.1
1	A	124	ARG	3.1
1	B	55	ILE	3.1
1	A	78	LEU	3.0
1	B	156	TYR	3.0
1	A	169	GLU	3.0
1	B	60	ASP	3.0
1	A	146	ALA	3.0
1	A	119	ILE	3.0
1	A	147	LEU	2.9
1	B	159	THR	2.9
1	A	36	ARG	2.9
1	A	188	LEU	2.9
1	B	160	PHE	2.9
1	A	187	TRP	2.9
1	B	72	SER	2.9
1	A	54	LEU	2.9
1	A	71	GLU	2.9
1	B	185	ALA	2.9
1	A	37	LEU	2.8
1	A	137	GLN	2.8
1	A	61	ARG	2.8
1	B	91	TRP	2.8
1	A	21	ALA	2.8
1	A	65	ARG	2.8
1	B	42	ASP	2.8
1	A	39	VAL	2.8
1	A	183	THR	2.7
1	B	161	PHE	2.7
1	A	155	ILE	2.7
1	A	185	ALA	2.7
1	A	153	THR	2.7
1	A	33	ILE	2.7
1	A	47	TYR	2.7
1	A	128	THR	2.7
1	B	103	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	2.6
1	B	182	LEU	2.6
1	B	30	LEU	2.6
1	B	24	SER	2.6
1	A	160	PHE	2.6
1	B	86	HIS	2.6
1	B	171	SER	2.6
1	B	173	HIS	2.6
1	A	156	TYR	2.5
1	B	99	ARG	2.5
1	A	41	LEU	2.5
1	B	129	VAL	2.5
1	A	178	LEU	2.5
1	B	49	ARG	2.5
1	A	13	VAL	2.5
1	B	64	SER	2.5
1	A	35	ALA	2.4
1	B	22	HIS	2.4
1	A	121	ALA	2.4
1	B	155	ILE	2.4
1	B	40	SER	2.4
1	B	29	ARG	2.4
1	B	187	TRP	2.4
1	A	56	ASP	2.4
1	A	22	HIS	2.4
1	A	86	HIS	2.4
1	B	124	ARG	2.4
1	B	52	ASP	2.3
1	A	125	VAL	2.3
1	B	69	GLU	2.3
1	A	127	ARG	2.3
1	A	63	ASP	2.3
1	B	118	GLN	2.3
1	B	25	TRP	2.3
1	A	111	GLU	2.3
1	A	115	ILE	2.3
1	A	46	LEU	2.3
1	A	118	GLN	2.3
1	A	126	SER	2.3
1	A	150	SER	2.3
1	B	41	LEU	2.2
1	A	14	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	161	PHE	2.2
1	B	33	ILE	2.2
1	A	53	GLU	2.2
1	A	134	GLU	2.2
1	A	182	LEU	2.2
1	A	85	HIS	2.2
1	A	79	VAL	2.2
1	A	154	THR	2.2
1	B	119	ILE	2.2
1	A	12	ILE	2.2
1	A	151	THR	2.2
1	B	75	PHE	2.2
1	B	61	ARG	2.1
1	A	149	GLU	2.1
1	A	52	ASP	2.1
1	B	181	HIS	2.1
1	A	70	ALA	2.1
1	A	31	TYR	2.1
1	A	9	ARG	2.1
1	A	26	GLU	2.1
1	B	104	GLN	2.1
1	A	180	ARG	2.1
1	A	15	THR	2.1
1	B	126	SER	2.1
1	B	102	THR	2.0
1	A	51	LYS	2.0
1	A	84	ILE	2.0
1	B	31	TYR	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.