



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:39 AM GMT

PDB ID : 2C2X  
Title : THREE DIMENSIONAL STRUCTURE OF BIFUNCTIONAL METHYLE  
NETETRAHYDROFOLATEDEHYDROGENASE-CYCLOHYDROLAS  
EFROM MYCOBACTERIUM TUBERCULOSIS  
Authors : Javid-Majd, F.; Sacchettini, J.C.; Tb Structural Genomics Consortium (Tb-  
sgc)  
Deposited on : 2005-09-30  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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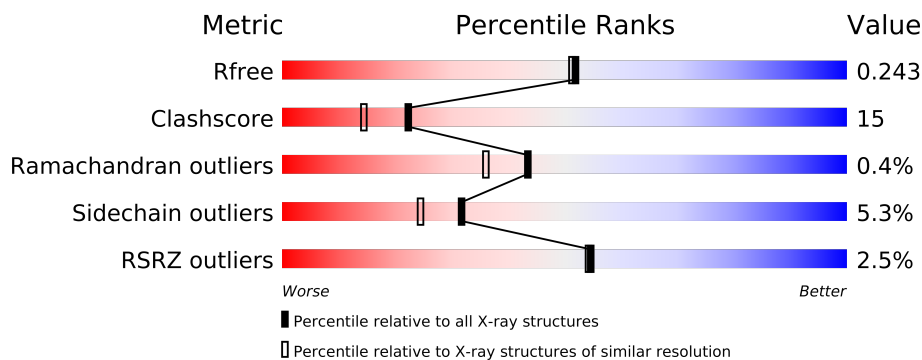
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4384 atoms, of which 0 are hydrogen and 0 are deuterium.

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 METHYLENETETRAHYDROFOLATEDEHYDROGENASE-METHENYLTETRAHYDROFOLATECYCLOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2062	1283	383	390	6			
1	B	280	Total	C	N	O	S	0	0	0
			2062	1283	383	390	6			

- Molecule 2 is water.

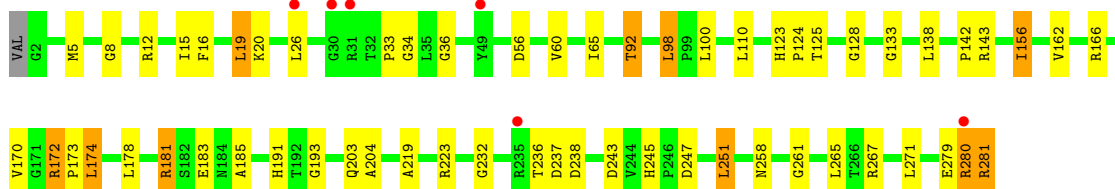
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	121	Total	O	0	0
			121	121		

### 3 Residue-property plots

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.

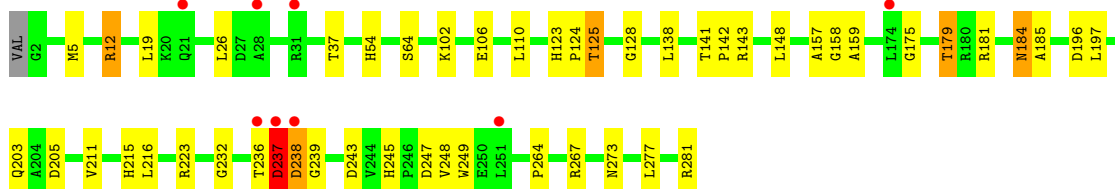
- Molecule 1: METHYLENETETRAHYDROFOLATEDEHYDROGENASE-METHENYLTETRAHYDROFOLATECYCLOHYDROLASE

Chain A: 



- Molecule 1: METHYLENETETRAHYDROFOLATEDEHYDROGENASE-METHENYLTETRAHYDROFOLATECYCLOHYDROLASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.51Å 86.76Å 111.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.80 – 2.00 34.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (111.80-2.00) 99.5 (34.17-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.248 0.204 , 0.243	Depositor DCC
$R_{free}$ test set	1974 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 39466 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.40	0/2096	0.61	0/2864
1	B	0.41	0/2096	0.63	1/2864 (0.0%)
All	All	0.41	0/4192	0.62	1/5728 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	238	ASP	N-CA-C	7.36	130.88	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ASP	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2062	0	2105	68	1
1	B	2062	0	2105	67	1
2	A	139	0	0	24	0
2	B	121	0	0	21	0
All	All	4384	0	4210	124	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:157:ALA:HB1	2:B:2081:HOH:O	1.24	1.34
1:A:124:PRO:CG	2:A:2056:HOH:O	1.65	1.26
1:B:277:LEU:HG	2:B:2119:HOH:O	1.06	1.24
1:B:157:ALA:CB	2:B:2081:HOH:O	1.77	1.24
1:B:159:ALA:HB3	2:B:2082:HOH:O	1.43	1.14
1:A:26:LEU:HD13	2:A:2014:HOH:O	0.99	1.13
1:A:223:ARG:NH2	2:A:2122:HOH:O	1.83	1.10
1:A:124:PRO:HG3	2:A:2056:HOH:O	1.29	1.09
1:B:157:ALA:C	2:B:2081:HOH:O	1.87	1.07
1:B:157:ALA:CA	2:B:2081:HOH:O	1.91	1.05
1:B:159:ALA:O	2:B:2082:HOH:O	1.77	1.02
1:B:159:ALA:CA	2:B:2082:HOH:O	2.09	0.98
1:B:159:ALA:CB	2:B:2082:HOH:O	2.04	0.96
1:B:123:HIS:CD2	1:B:125:THR:HG23	2.01	0.94
1:B:159:ALA:C	2:B:2082:HOH:O	2.08	0.92
1:A:123:HIS:HD2	1:A:125:THR:H	1.16	0.91
1:B:138:LEU:CD2	2:B:2075:HOH:O	2.18	0.91
1:B:138:LEU:HD22	2:B:2075:HOH:O	1.71	0.90
1:B:12:ARG:HH11	1:B:12:ARG:HG3	1.35	0.90
1:B:277:LEU:CG	2:B:2119:HOH:O	1.78	0.88
1:A:281:ARG:NH1	1:A:281:ARG:HB3	1.89	0.88
1:B:102:LYS:H	1:B:102:LYS:HD2	1.38	0.87
1:B:237:ASP:HA	1:B:239:GLY:H	1.40	0.86
1:A:26:LEU:CD1	2:A:2014:HOH:O	1.68	0.85
1:A:34:GLY:H	1:A:92:THR:CG2	1.88	0.84
1:A:251:LEU:HD22	2:A:2130:HOH:O	1.77	0.83
1:B:125:THR:HG21	2:B:2068:HOH:O	1.78	0.81
2:A:2093:HOH:O	1:B:179:THR:HG21	1.81	0.79
1:A:34:GLY:H	1:A:92:THR:HG23	1.45	0.79
1:B:277:LEU:CD2	2:B:2119:HOH:O	2.16	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:HIS:HD2	1:A:193:GLY:H	1.30	0.78
1:A:281:ARG:HH11	1:A:281:ARG:HB3	1.48	0.75
1:B:245:HIS:O	1:B:248:VAL:HG13	1.87	0.73
1:A:245:HIS:HD2	2:A:2129:HOH:O	1.72	0.72
1:A:245:HIS:HD2	1:A:247:ASP:H	1.37	0.72
1:B:245:HIS:HD2	1:B:247:ASP:H	1.36	0.72
1:A:203:GLN:HE22	1:B:203:GLN:HE22	1.35	0.71
1:A:125:THR:C	2:A:2066:HOH:O	2.27	0.71
1:B:102:LYS:HD2	1:B:102:LYS:N	2.05	0.71
1:B:37:THR:OG1	1:B:54:HIS:HE1	1.75	0.69
1:B:196:ASP:HB3	2:B:2101:HOH:O	1.92	0.68
1:B:138:LEU:HB2	1:B:143:ARG:HD2	1.76	0.68
1:B:12:ARG:NH1	1:B:264:PRO:O	2.28	0.67
1:A:166:ARG:HH12	1:B:184:ASN:HD22	1.43	0.66
1:B:236:THR:HG22	1:B:237:ASP:H	1.61	0.66
1:A:5:MET:CE	2:A:2134:HOH:O	2.44	0.66
1:B:123:HIS:HD2	1:B:125:THR:HG23	1.58	0.65
1:A:123:HIS:CD2	1:A:125:THR:H	2.07	0.63
1:B:158:GLY:N	2:B:2081:HOH:O	2.16	0.63
1:A:16:PHE:O	1:A:20:LYS:HG3	1.99	0.63
1:A:181:ARG:HH21	1:A:181:ARG:CG	2.11	0.63
1:B:123:HIS:HD2	1:B:125:THR:H	1.47	0.62
1:A:166:ARG:HH12	1:B:184:ASN:ND2	1.97	0.62
1:B:12:ARG:NH1	1:B:12:ARG:HG3	2.10	0.61
1:A:267:ARG:HB2	2:A:2022:HOH:O	2.00	0.61
1:A:267:ARG:CB	2:A:2022:HOH:O	2.48	0.61
1:B:159:ALA:N	2:B:2082:HOH:O	2.28	0.60
1:A:124:PRO:O	1:B:128:GLY:HA3	2.01	0.60
1:A:267:ARG:HB3	2:A:2021:HOH:O	2.01	0.60
1:B:138:LEU:H	1:B:273:ASN:HD21	1.50	0.59
1:A:166:ARG:HH22	1:B:184:ASN:HD21	1.51	0.59
1:A:156:ILE:HD11	1:A:183:GLU:HB3	1.84	0.59
1:A:142:PRO:HG2	2:A:2090:HOH:O	2.02	0.59
1:A:33:PRO:HG3	2:A:2014:HOH:O	2.02	0.58
1:B:12:ARG:HH12	1:B:267:ARG:HB2	1.69	0.58
1:A:181:ARG:HH21	1:A:181:ARG:HG2	1.69	0.57
1:B:123:HIS:NE2	1:B:125:THR:HG23	2.19	0.57
1:A:181:ARG:HG2	1:A:181:ARG:NH2	2.21	0.56
1:B:143:ARG:HD3	2:B:2076:HOH:O	2.05	0.56
1:B:205:ASP:HA	1:B:223:ARG:HH11	1.72	0.55
1:A:172:ARG:HB3	1:A:173:PRO:HD3	1.88	0.55
1:B:123:HIS:CD2	1:B:125:THR:H	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:PRO:HG2	2:A:2056:HOH:O	1.61	0.54
1:A:36:GLY:HA2	1:A:65:ILE:O	2.08	0.54
1:B:232:GLY:HA3	1:B:243:ASP:OD2	2.08	0.54
1:A:236:THR:HG22	1:A:238:ASP:H	1.72	0.53
1:A:280:ARG:O	1:A:281:ARG:HG2	2.08	0.53
1:A:156:ILE:HD12	1:A:185:ALA:HB2	1.90	0.53
1:A:128:GLY:HA3	1:B:124:PRO:O	2.08	0.53
1:A:172:ARG:HH12	1:B:179:THR:HG22	1.73	0.53
1:A:172:ARG:HB3	1:A:173:PRO:CD	2.39	0.53
1:A:143:ARG:N	2:A:2074:HOH:O	2.39	0.52
1:A:5:MET:HE1	2:A:2134:HOH:O	2.09	0.51
1:B:141:THR:HB	1:B:142:PRO:HD3	1.93	0.51
1:A:203:GLN:NE2	1:B:203:GLN:HE22	2.07	0.51
1:B:54:HIS:CD2	1:B:64:SER:CB	2.95	0.50
1:A:236:THR:HG22	1:A:237:ASP:N	2.26	0.50
1:A:191:HIS:HE1	1:B:185:ALA:O	1.94	0.50
1:A:124:PRO:CB	2:A:2056:HOH:O	2.26	0.50
1:A:33:PRO:HA	1:A:92:THR:HG21	1.94	0.49
1:A:162:VAL:HG23	1:A:204:ALA:HB2	1.93	0.49
1:B:54:HIS:HD2	1:B:64:SER:OG	1.95	0.49
1:A:125:THR:CA	2:A:2066:HOH:O	2.38	0.49
1:A:279:GLU:O	1:A:281:ARG:NH1	2.46	0.48
1:B:197:LEU:HD23	1:B:216:LEU:HD11	1.96	0.48
1:A:33:PRO:HD3	2:A:2014:HOH:O	2.14	0.48
1:A:170:VAL:O	1:A:174:LEU:HB2	2.14	0.48
1:A:281:ARG:CZ	1:A:281:ARG:HB3	2.45	0.47
1:A:172:ARG:NH1	1:B:179:THR:CG2	2.77	0.47
1:B:54:HIS:CD2	1:B:64:SER:HB3	2.48	0.47
1:B:54:HIS:CD2	1:B:64:SER:OG	2.67	0.47
1:A:56:ASP:HB3	1:A:271:LEU:HD11	1.97	0.47
1:B:237:ASP:HA	1:B:239:GLY:N	2.20	0.46
1:A:191:HIS:HD2	1:A:193:GLY:N	2.07	0.46
1:B:5:MET:HG3	1:B:249:TRP:CH2	2.53	0.44
1:A:33:PRO:CG	2:A:2014:HOH:O	2.63	0.44
1:A:172:ARG:NH1	1:B:179:THR:HG22	2.32	0.44
1:B:106:GLU:O	1:B:110:LEU:HG	2.17	0.44
1:A:20:LYS:HG2	1:A:60:VAL:HA	2.00	0.44
1:A:133:GLY:HA2	2:A:2069:HOH:O	2.17	0.44
1:A:219:ALA:O	1:A:251:LEU:HD11	2.17	0.43
1:B:37:THR:OG1	1:B:54:HIS:CE1	2.65	0.43
1:B:277:LEU:HD23	2:B:2119:HOH:O	2.02	0.43
1:A:98:LEU:HD21	1:A:110:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:GLY:HA3	1:A:261:GLY:O	2.19	0.42
1:B:237:ASP:CA	1:B:239:GLY:H	2.22	0.42
2:A:2093:HOH:O	1:B:179:THR:CG2	2.54	0.42
1:A:15:ILE:HG22	1:A:19:LEU:HD22	2.02	0.42
1:B:175:GLY:O	1:B:179:THR:HB	2.20	0.41
1:A:174:LEU:HD22	1:A:178:LEU:CD1	2.49	0.41
1:B:12:ARG:NH1	1:B:12:ARG:CG	2.81	0.41
1:B:181:ARG:NH2	2:B:2092:HOH:O	2.53	0.41
1:A:232:GLY:HA3	1:A:243:ASP:OD2	2.21	0.40
1:A:12:ARG:HH11	1:A:12:ARG:HD3	1.76	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:ASP:OD2	1:B:215:HIS:NE2[2_555]	2.17	0.03

## 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	278/281 (99%)	272 (98%)	6 (2%)	0	100	100
1	B	278/281 (99%)	268 (96%)	8 (3%)	2 (1%)	30	20
All	All	556/562 (99%)	540 (97%)	14 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ASP
1	B	237	ASP

### 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	219/220 (100%)	205 (94%)	14 (6%)	25	17
1	B	219/220 (100%)	210 (96%)	9 (4%)	41	35
All	All	438/440 (100%)	415 (95%)	23 (5%)	32	24

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	92	THR
1	A	98	LEU
1	A	100	LEU
1	A	138	LEU
1	A	156	ILE
1	A	172	ARG
1	A	174	LEU
1	A	181	ARG
1	A	251	LEU
1	A	258	ASN
1	A	265	LEU
1	A	280	ARG
1	A	281	ARG
1	B	12	ARG
1	B	19	LEU
1	B	26	LEU
1	B	125	THR
1	B	148	LEU
1	B	179	THR
1	B	184	ASN
1	B	211	VAL
1	B	281	ARG

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	123	HIS

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Mol	Chain	Res	Type
1	A	126	ASN
1	A	191	HIS
1	A	203	GLN
1	A	245	HIS
1	A	258	ASN
1	B	21	GLN
1	B	54	HIS
1	B	123	HIS
1	B	184	ASN
1	B	245	HIS
1	B	273	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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, 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	280/281 (99%)	0.20	6 (2%) 60 61	26, 30, 39, 47	0
1	B	280/281 (99%)	0.27	8 (2%) 49 49	26, 30, 39, 50	0
All	All	560/562 (99%)	0.24	14 (2%) 54 54	26, 30, 39, 50	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	ASP	4.7
1	B	238	ASP	3.9
1	A	31	ARG	2.9
1	A	235	ARG	2.9
1	A	30	GLY	2.8
1	B	31	ARG	2.7
1	B	251	LEU	2.6
1	B	28	ALA	2.6
1	B	174	LEU	2.5
1	B	236	THR	2.4
1	A	49	TYR	2.4
1	B	21	GLN	2.3
1	A	26	LEU	2.2
1	A	280	ARG	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.