



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:05 am GMT

PDB ID : 1VDK  
Title : Crystal structure of fumarase from thermus thermophilus HB8  
Authors : Mizutani, H.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-03-23  
Resolution : 1.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

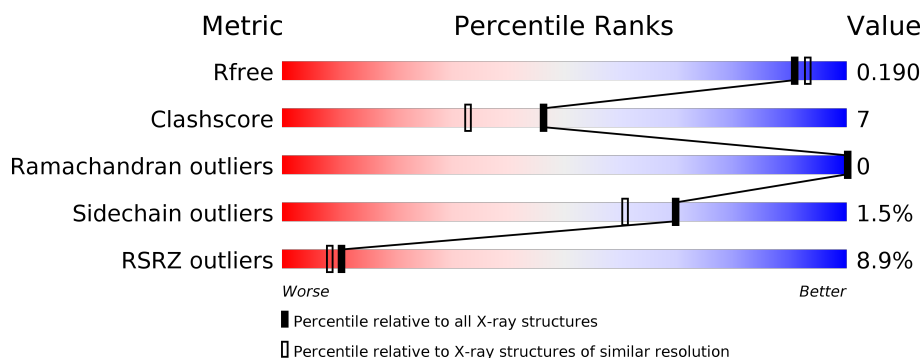
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	466	<div> <div>11%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	B	466	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7680 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 Fumarate hydratase class II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3515	2231	617	653	14			
1	B	457	Total	C	N	O	S	0	0	0
			3517	2234	617	652	14			

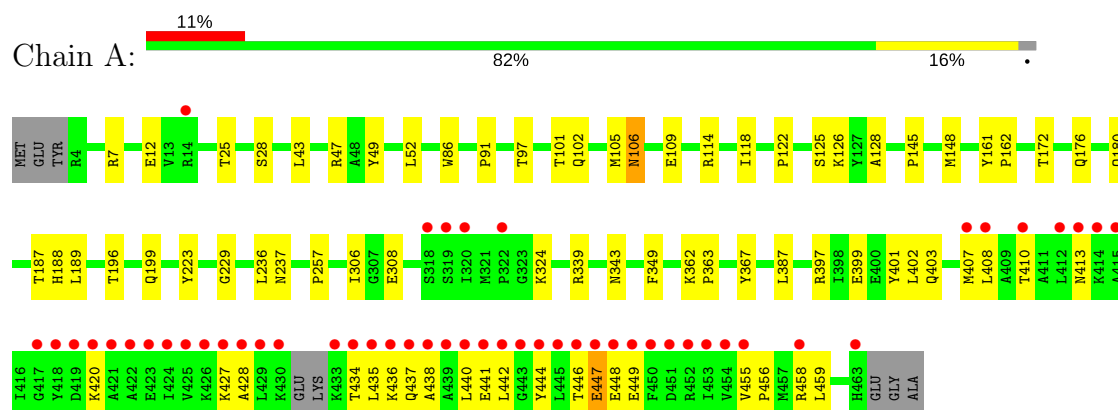
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	357	Total	O	0	0
			357	357		
2	B	291	Total	O	0	0
			291	291		

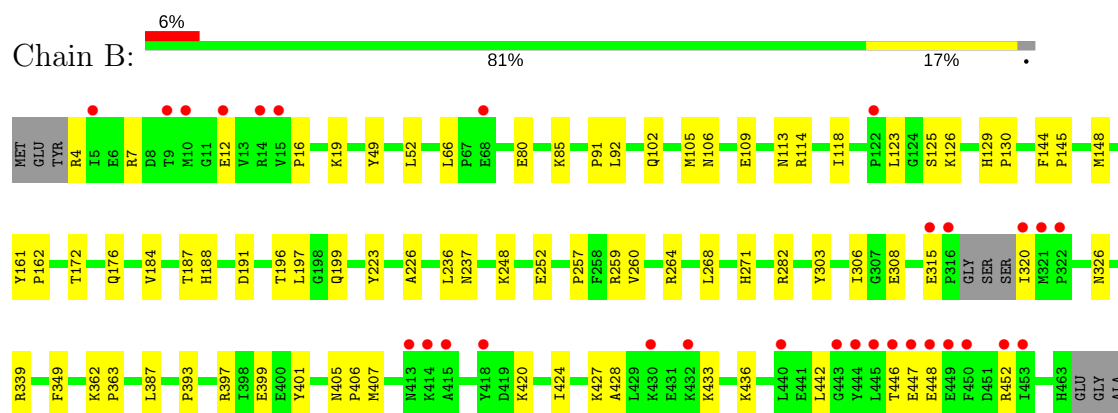
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Fumarate hydratase class II



#### • Molecule 1: Fumarate hydratase class II



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.34Å 140.12Å 135.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.80) 100.0 (29.95-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.201 0.185 , 0.190	Depositor DCC
$R_{free}$ test set	5490 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.7	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	0.96	EDS
Total number of atoms	7680	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 4.90% 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	0.30	0/3580	0.57	1/4853 (0.0%)
1	B	0.28	0/3582	0.54	0/4855
All	All	0.29	0/7162	0.55	1/9708 (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	A	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	A	128	ALA	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	TYR	Sidechain

### 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	3515	0	3557	55	0
1	B	3517	0	3563	48	2
2	A	357	0	0	2	0
2	B	291	0	0	7	0
All	All	7680	0	7120	102	2

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 7.

All (102) 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:7:ARG:HG2	1:B:12:GLU:HG2	1.45	0.94
1:A:428:ALA:HB3	1:A:435:LEU:HD23	1.64	0.79
1:B:436:LYS:HD3	1:B:447:GLU:HG3	1.65	0.79
1:A:440:LEU:HD21	1:A:447:GLU:N	2.03	0.73
1:A:446:THR:HG23	1:A:449:GLU:H	1.55	0.72
1:B:113:ASN:HB3	1:B:123:LEU:HD22	1.72	0.71
1:B:145:PRO:HA	1:B:148:MET:HG2	1.73	0.70
1:A:145:PRO:HA	1:A:148:MET:HG2	1.75	0.68
1:A:105:MET:O	1:A:109:GLU:HG3	1.99	0.62
1:A:196:THR:OG1	1:A:199:GLN:HG3	2.00	0.61
1:A:402:LEU:HG	1:A:408:LEU:HD11	1.81	0.61
1:A:434:THR:HG23	1:A:437:GLN:HB2	1.81	0.61
1:A:122:PRO:HG2	1:A:125:SER:HB3	1.81	0.61
1:A:420:LYS:HD2	1:A:420:LYS:N	2.15	0.61
1:B:248:LYS:O	1:B:252:GLU:HG3	2.01	0.60
1:A:440:LEU:HD21	1:A:447:GLU:H	1.70	0.56
1:A:7:ARG:HB3	1:A:12:GLU:HG2	1.87	0.56
1:B:260:VAL:HG11	1:B:264:ARG:HE	1.70	0.56
1:B:303:TYR:HA	1:B:397:ARG:NH2	2.20	0.56
1:B:320:ILE:HD12	1:B:320:ILE:N	2.21	0.56
1:B:16:PRO:HB2	1:B:19:LYS:HG2	1.88	0.55
1:A:408:LEU:HD22	1:A:456:PRO:HG3	1.89	0.55
1:A:172:THR:O	1:A:176:GLN:HG3	2.07	0.54
1:B:172:THR:O	1:B:176:GLN:HG3	2.07	0.54
1:A:229:GLY:HA3	2:A:696:HOH:O	2.08	0.54
1:B:264:ARG:O	1:B:268:LEU:HD13	2.08	0.53
1:B:105:MET:O	1:B:109:GLU:HG3	2.09	0.53
1:A:436:LYS:HE2	1:A:447:GLU:HB2	1.90	0.53
1:A:407:MET:HB3	1:A:459:LEU:HD13	1.91	0.52
1:B:387:LEU:C	1:B:387:LEU:HD23	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD23	1:A:387:LEU:C	2.29	0.52
1:B:282:ARG:HD2	2:B:583:HOH:O	2.10	0.52
1:A:114:ARG:O	1:A:118:ILE:HG13	2.10	0.52
1:A:236:LEU:O	1:A:237:ASN:HB2	2.10	0.52
1:B:446:THR:C	1:B:448:GLU:H	2.13	0.52
1:B:260:VAL:CG1	1:B:264:ARG:HE	2.22	0.51
1:A:428:ALA:HB2	1:A:438:ALA:HB2	1.93	0.51
1:A:362:LYS:HB2	1:A:363:PRO:HD3	1.93	0.50
1:A:410:THR:HA	1:A:413:ASN:HD22	1.77	0.50
1:A:447:GLU:OE2	1:A:448:GLU:HG3	2.11	0.50
1:B:236:LEU:O	1:B:237:ASN:HB2	2.10	0.50
1:B:92:LEU:HD13	1:B:102:GLN:HB3	1.94	0.50
1:A:440:LEU:HD11	1:A:447:GLU:HB3	1.93	0.50
1:A:427:LYS:HE2	1:A:441:GLU:HB2	1.94	0.49
1:B:161:TYR:HB2	1:B:162:PRO:HD3	1.94	0.49
1:B:196:THR:OG1	1:B:199:GLN:HG3	2.11	0.49
1:A:126:LYS:HA	2:A:693:HOH:O	2.13	0.48
1:B:362:LYS:HB2	1:B:363:PRO:HD3	1.94	0.48
1:B:427:LYS:HD2	1:B:442:LEU:HD21	1.95	0.48
1:A:324:LYS:HE2	1:B:191:ASP:O	2.14	0.48
1:B:306:ILE:HG22	1:B:308:GLU:HG3	1.96	0.48
1:B:420:LYS:HG3	2:B:694:HOH:O	2.14	0.48
1:A:180:GLN:HE21	1:A:180:GLN:HA	1.79	0.48
1:A:188:HIS:O	1:A:189:LEU:HB2	2.14	0.47
1:B:197:LEU:CD2	1:B:393:PRO:HB3	2.45	0.47
1:B:184:VAL:HG13	1:B:407:MET:CE	2.45	0.47
1:B:223:TYR:CD1	1:B:257:PRO:HG2	2.49	0.47
1:B:52:LEU:HD23	1:B:52:LEU:C	2.34	0.47
1:B:80:GLU:HG2	1:B:85:LYS:HD2	1.95	0.47
1:A:434:THR:CG2	1:A:437:GLN:HB2	2.46	0.46
1:A:436:LYS:CE	1:A:447:GLU:HB2	2.46	0.46
1:A:427:LYS:HD3	1:A:438:ALA:HB1	1.97	0.46
1:B:420:LYS:O	1:B:424:ILE:HG13	2.15	0.46
1:A:180:GLN:NE2	1:A:180:GLN:HA	2.30	0.46
1:A:52:LEU:C	1:A:52:LEU:HD23	2.36	0.46
1:B:105:MET:HG3	2:B:723:HOH:O	2.16	0.46
1:B:187:THR:O	1:B:188:HIS:HB2	2.16	0.46
1:B:114:ARG:O	1:B:118:ILE:HG13	2.16	0.45
1:A:25:THR:OG1	1:A:106:ASN:HA	2.16	0.45
1:A:223:TYR:CD1	1:A:257:PRO:HG2	2.51	0.45
1:B:446:THR:C	1:B:448:GLU:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLU:HG3	2:B:612:HOH:O	2.18	0.44
1:A:306:ILE:HG22	1:A:308:GLU:HG3	2.00	0.44
1:A:455:VAL:HB	1:A:458:ARG:HD2	1.99	0.44
1:A:97:THR:HG21	1:A:101:THR:HB	1.99	0.44
1:A:161:TYR:HB2	1:A:162:PRO:HD3	2.00	0.43
1:A:339:ARG:NH1	1:A:343:ASN:OD1	2.51	0.43
1:B:326:ASN:HB3	2:B:591:HOH:O	2.17	0.43
1:A:28:SER:HB2	1:A:102:GLN:HG2	2.01	0.43
1:B:428:ALA:HB1	1:B:433:LYS:O	2.19	0.43
1:A:446:THR:HG22	1:A:449:GLU:OE1	2.18	0.43
1:A:43:LEU:O	1:A:47:ARG:HG2	2.19	0.42
1:B:129:HIS:HA	1:B:130:PRO:HD3	1.91	0.42
1:B:145:PRO:HB3	1:B:271:HIS:CE1	2.55	0.42
1:B:66:LEU:HD11	2:B:531:HOH:O	2.19	0.42
1:A:434:THR:HG23	1:A:437:GLN:CB	2.49	0.42
1:A:125:SER:O	1:A:126:LYS:HB2	2.20	0.42
1:A:86:TRP:CZ2	1:A:114:ARG:HD3	2.54	0.42
1:B:125:SER:O	1:B:126:LYS:HB2	2.19	0.42
1:A:397:ARG:HD2	1:A:401:TYR:CZ	2.55	0.42
1:A:427:LYS:HE3	1:A:441:GLU:OE1	2.20	0.42
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.85	0.41
1:A:442:LEU:HB3	1:A:444:TYR:CD1	2.55	0.41
1:B:144:PHE:N	1:B:145:PRO:HD2	2.35	0.41
1:A:420:LYS:CD	1:A:420:LYS:N	2.84	0.41
1:A:187:THR:O	1:A:188:HIS:HB2	2.21	0.41
1:B:405:ASN:HA	1:B:406:PRO:HD3	1.86	0.41
1:A:399:GLU:OE2	1:A:403:GLN:NE2	2.53	0.41
1:B:126:LYS:HA	2:B:751:HOH:O	2.21	0.41
1:A:455:VAL:HB	1:A:458:ARG:CD	2.51	0.40
1:B:226:ALA:HB1	1:B:268:LEU:HD12	2.02	0.40
1:B:401:TYR:O	1:B:405:ASN:HB2	2.21	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:NH2	1:B:339:ARG:NH2[3_655]	1.75	0.45
1:B:452:ARG:NH1	1:B:452:ARG:NH1[4_555]	1.83	0.37

## 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	454/466 (97%)	431 (95%)	23 (5%)	0	100	100
1	B	453/466 (97%)	439 (97%)	14 (3%)	0	100	100
All	All	907/932 (97%)	870 (96%)	37 (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	361/367 (98%)	356 (99%)	5 (1%)	71	64
1	B	361/367 (98%)	355 (98%)	6 (2%)	66	55
All	All	722/734 (98%)	711 (98%)	11 (2%)	70	61

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

Mol	Chain	Res	Type
1	A	49	TYR
1	A	91	PRO
1	A	106	ASN
1	A	349	PHE
1	A	447	GLU
1	B	49	TYR
1	B	91	PRO
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	259	ARG
1	B	315	GLU
1	B	349	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	131	ASN
1	A	180	GLN
1	A	437	GLN
1	B	31	ASN
1	B	326	ASN
1	B	329	GLN

### 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 ⓘ

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	458/466 (98%)	0.42	51 (11%) 6 4	13, 23, 76, 80	0
1	B	457/466 (98%)	0.21	30 (6%) 19 16	15, 28, 58, 72	0
All	All	915/932 (98%)	0.32	81 (8%) 10 8	13, 26, 68, 80	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	LEU	12.2
1	A	445	LEU	10.0
1	A	428	ALA	9.8
1	A	444	TYR	9.2
1	A	429	LEU	8.5
1	A	440	LEU	8.3
1	A	453	ILE	7.8
1	A	439	ALA	7.7
1	A	421	ALA	7.5
1	A	319	SER	7.4
1	B	316	PRO	7.2
1	A	426	LYS	7.0
1	A	430	LYS	6.6
1	B	321	MET	6.5
1	A	447	GLU	6.4
1	A	438	ALA	6.4
1	A	425	VAL	6.1
1	A	422	ALA	5.9
1	A	414	LYS	5.8
1	A	442	LEU	5.5
1	A	427	LYS	5.5
1	B	5	ILE	5.4
1	A	441	GLU	5.3
1	A	419	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	SER	5.2
1	A	423	GLU	5.1
1	A	420	LYS	5.0
1	A	424	ILE	4.9
1	A	450	PHE	4.9
1	A	437	GLN	4.9
1	A	413	ASN	4.8
1	A	443	GLY	4.7
1	B	9	THR	4.7
1	B	446	THR	4.5
1	A	433	LYS	4.5
1	B	448	GLU	4.4
1	B	430	LYS	4.3
1	A	418	TYR	4.3
1	A	446	THR	4.3
1	A	448	GLU	4.1
1	B	10	MET	4.1
1	A	434	THR	4.0
1	A	451	ASP	3.9
1	A	449	GLU	3.7
1	A	410	THR	3.7
1	A	458	ARG	3.6
1	B	14	ARG	3.6
1	B	453	ILE	3.5
1	B	440	LEU	3.5
1	B	414	LYS	3.5
1	A	322	PRO	3.4
1	A	14	ARG	3.4
1	B	322	PRO	3.0
1	B	413	ASN	3.0
1	B	447	GLU	3.0
1	B	320	ILE	3.0
1	A	407	MET	2.9
1	A	452	ARG	2.8
1	A	436	LYS	2.8
1	B	443	GLY	2.8
1	B	122	PRO	2.7
1	A	320	ILE	2.7
1	B	315	GLU	2.7
1	B	418	TYR	2.6
1	A	417	GLY	2.5
1	B	444	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLU	2.5
1	A	408	LEU	2.4
1	B	449	GLU	2.4
1	A	463	HIS	2.4
1	A	412	LEU	2.4
1	B	445	LEU	2.4
1	A	415	ALA	2.3
1	B	450	PHE	2.3
1	A	455	VAL	2.3
1	B	15	VAL	2.2
1	A	454	VAL	2.2
1	B	432	LYS	2.2
1	B	452	ARG	2.2
1	B	415	ALA	2.1
1	B	68	GLU	2.1

## 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.