



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:54 pm BST

PDB ID : 1LWD  
Title : CRYSTAL STRUCTURE OF NADP-DEPENDENT ISOCITRATE DEHYDROGENASE FROM PORCINE HEART MITOCHONDRIA  
Authors : Ceccarelli, C.; Bahnson, B.J.  
Deposited on : 2002-05-31  
Resolution : 1.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

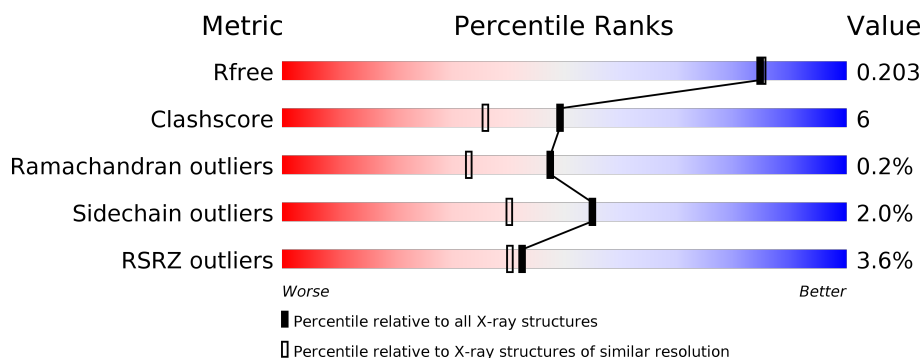
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	413	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	413	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7323 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.

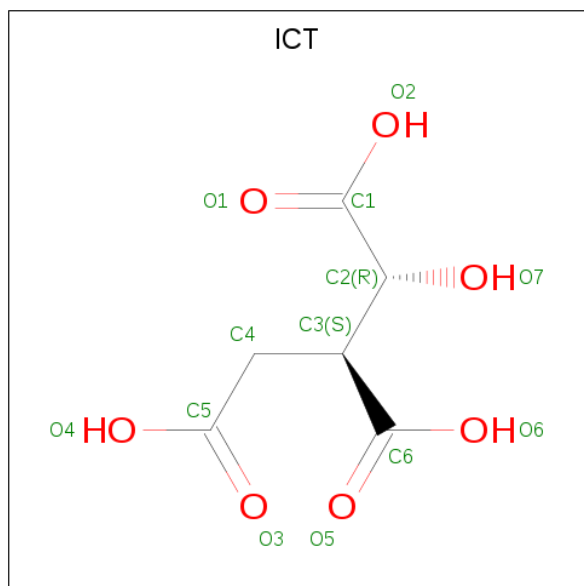
- Molecule 1 is a protein called Isocitrate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3285	2090	570	609	16			
1	B	413	Total	C	N	O	S	0	0	0
			3285	2090	570	609	16			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

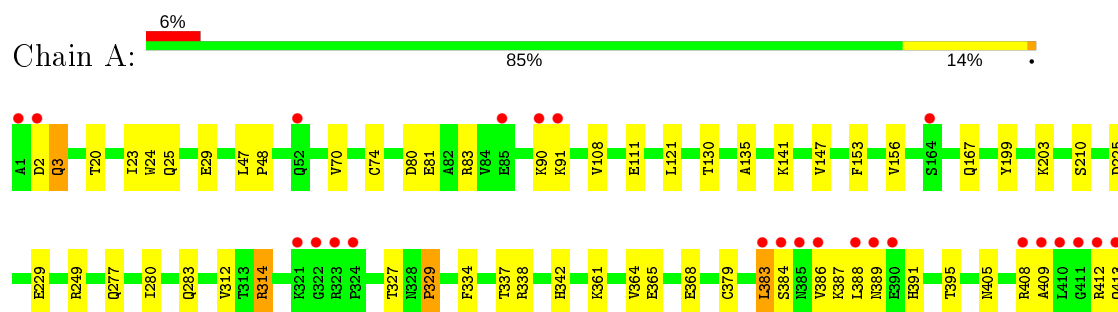
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	295	Total	O	0	0
			295	295		
5	B	420	Total	O	0	0
			420	420		

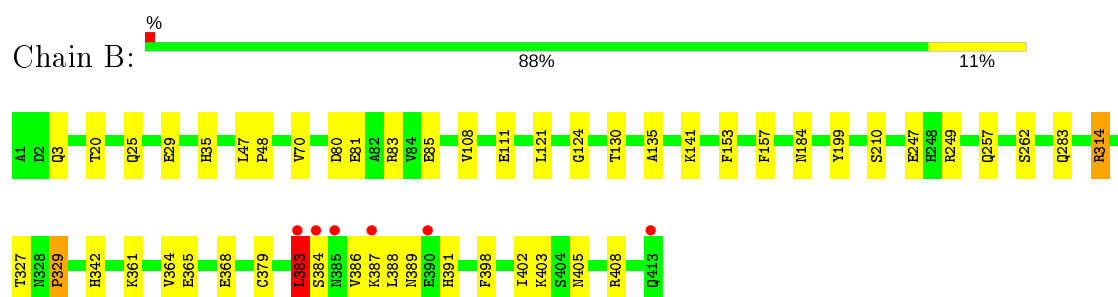
### 3 Residue-property plots

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: Isocitrate Dehydrogenase



#### • Molecule 1: Isocitrate Dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.86 Å   112.57 Å   66.08 Å 90.00°   97.00°   90.00°	Depositor
Resolution (Å)	29.23 – 1.85 29.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.23-1.85) 90.0 (29.93-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.182 , 0.210 0.175 , 0.203	Depositor DCC
$R_{free}$ test set	7728 reflections (8.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.8	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	0.96	EDS
Total number of atoms	7323	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, SO4, ICT

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	0.31	0/3360	0.58	0/4539
1	B	0.31	0/3360	0.60	0/4539
All	All	0.31	0/6720	0.59	0/9078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3285	0	3264	43	0
1	B	3285	0	3264	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	4	0	0
3	B	13	0	4	0	0
4	B	10	0	0	0	0
5	A	295	0	0	2	0
5	B	420	0	0	3	0
All	All	7323	0	6536	77	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 6.

All (77) 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:408:ARG:O	1:A:412:ARG:HD3	1.83	0.77
1:B:249:ARG:HG3	1:B:249:ARG:HH11	1.56	0.70
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.58	0.68
1:A:156:VAL:HG22	1:A:167:GLN:HG2	1.77	0.67
1:A:386:VAL:HA	1:A:391:HIS:CD2	2.34	0.62
1:A:379:CYS:HB3	5:A:1200:HOH:O	2.00	0.62
1:B:81:GLU:H	1:B:81:GLU:CD	2.04	0.61
1:B:386:VAL:HA	1:B:391:HIS:CD2	2.36	0.60
1:A:387:LYS:H	1:A:391:HIS:HD2	1.48	0.60
1:B:387:LYS:H	1:B:391:HIS:HD2	1.48	0.59
1:A:364:VAL:O	1:A:368:GLU:HG3	2.03	0.59
1:A:81:GLU:CD	1:A:81:GLU:H	2.06	0.57
1:A:108:VAL:HG23	1:A:135:ALA:HB2	1.85	0.57
1:A:383:LEU:HD12	1:A:384:SER:N	2.19	0.57
1:B:383:LEU:HD12	1:B:384:SER:N	2.20	0.56
1:B:108:VAL:HG23	1:B:135:ALA:HB2	1.88	0.56
1:B:314:ARG:H	1:B:314:ARG:NE	2.04	0.56
1:A:314:ARG:H	1:A:314:ARG:NE	2.05	0.55
1:A:388:LEU:HG	1:A:389:ASN:ND2	2.23	0.54
1:B:364:VAL:O	1:B:368:GLU:HG3	2.09	0.53
1:B:405:ASN:HA	1:B:408:ARG:NH1	2.25	0.52
1:B:379:CYS:HB3	5:B:1205:HOH:O	2.10	0.52
1:A:2:ASP:CG	1:A:3:GLN:H	2.11	0.52
1:A:405:ASN:HA	1:A:408:ARG:NH1	2.26	0.51
1:A:121:LEU:HD12	1:A:283:GLN:HG3	1.90	0.51
1:B:388:LEU:HG	1:B:389:ASN:ND2	2.26	0.51
1:B:405:ASN:HD22	1:B:408:ARG:HH12	1.58	0.51
1:A:409:ALA:O	1:A:413:GLN:HG3	2.11	0.50
1:A:387:LYS:H	1:A:391:HIS:CD2	2.28	0.50
1:A:405:ASN:HD22	1:A:408:ARG:HH12	1.60	0.50
1:B:249:ARG:HG3	1:B:249:ARG:NH1	2.27	0.49
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.27	0.48
1:A:277:GLN:NE2	1:A:280:ILE:HD12	2.28	0.48
1:B:398:PHE:CE2	1:B:402:ILE:HD11	2.48	0.48
1:A:25:GLN:HE21	1:A:29:GLU:CD	2.17	0.47
1:A:70:VAL:HG22	1:A:342:HIS:HD2	1.79	0.47
1:A:23:ILE:HG22	1:A:395:THR:HG21	1.95	0.47
1:A:147:VAL:HG13	1:B:157:PHE:CZ	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HE2	5:B:1139:HOH:O	2.15	0.47
1:B:387:LYS:H	1:B:391:HIS:CD2	2.29	0.47
1:A:141:LYS:HE2	5:A:1152:HOH:O	2.14	0.46
1:A:386:VAL:HA	1:A:391:HIS:HD2	1.78	0.46
1:A:225:ASP:O	1:A:229:GLU:HG3	2.15	0.46
1:A:130:THR:HG21	1:A:199:TYR:CZ	2.51	0.46
1:B:130:THR:HG21	1:B:199:TYR:CZ	2.51	0.46
1:B:25:GLN:HE21	1:B:29:GLU:CG	2.30	0.45
1:B:35:HIS:CE1	1:B:403:LYS:HE2	2.52	0.45
1:B:85:GLU:HG3	5:B:1371:HOH:O	2.15	0.45
1:A:90:LYS:O	1:A:91:LYS:HG2	2.16	0.44
1:B:386:VAL:HA	1:B:391:HIS:HD2	1.80	0.44
1:A:334:PHE:HA	1:A:337:THR:OG1	2.18	0.44
1:A:24:TRP:CD2	1:A:74:CYS:HB2	2.52	0.44
1:B:124:GLY:O	1:B:262:SER:HA	2.18	0.44
1:B:405:ASN:HD22	1:B:408:ARG:NH1	2.16	0.44
1:B:314:ARG:H	1:B:314:ARG:CD	2.30	0.43
1:B:35:HIS:HE1	1:B:403:LYS:HE2	1.83	0.43
1:B:210:SER:HA	1:B:249:ARG:O	2.18	0.43
1:A:25:GLN:HE21	1:A:29:GLU:CG	2.32	0.43
1:A:338:ARG:HA	1:A:338:ARG:HD3	1.88	0.42
1:A:80:ASP:OD1	1:A:83:ARG:HG2	2.18	0.42
1:A:25:GLN:O	1:A:29:GLU:HG3	2.19	0.42
1:B:121:LEU:HD12	1:B:283:GLN:HG3	2.00	0.42
1:B:80:ASP:OD1	1:B:83:ARG:HG2	2.20	0.42
1:A:199:TYR:OH	1:A:203:LYS:HE3	2.19	0.42
1:A:361:LYS:O	1:A:365:GLU:HG3	2.19	0.42
1:B:70:VAL:HG22	1:B:342:HIS:HD2	1.84	0.42
1:A:327:THR:O	1:A:329:PRO:HD3	2.20	0.41
1:A:412:ARG:N	1:A:412:ARG:HD2	2.34	0.41
1:B:361:LYS:O	1:B:365:GLU:HG3	2.20	0.41
1:A:210:SER:HA	1:A:249:ARG:O	2.20	0.41
1:B:47:LEU:HB3	1:B:48:PRO:HD3	2.02	0.41
1:A:314:ARG:H	1:A:314:ARG:CD	2.34	0.41
1:A:47:LEU:HB3	1:A:48:PRO:HD3	2.02	0.41
1:B:249:ARG:NE	1:B:257:GLN:OE1	2.42	0.41
1:B:247:GLU:OE1	1:B:249:ARG:NH1	2.53	0.40
1:B:327:THR:O	1:B:329:PRO:HD3	2.20	0.40
1:A:312:VAL:HA	1:A:314:ARG:HH21	1.87	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	411/413 (100%)	390 (95%)	20 (5%)	1 (0%)	47	33
1	B	411/413 (100%)	391 (95%)	19 (5%)	1 (0%)	47	33
All	All	822/826 (100%)	781 (95%)	39 (5%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	LEU
1	B	383	LEU

### 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	354/354 (100%)	348 (98%)	6 (2%)	60	47
1	B	354/354 (100%)	346 (98%)	8 (2%)	50	34
All	All	708/708 (100%)	694 (98%)	14 (2%)	55	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	THR
1	A	111	GLU
1	A	153	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	314	ARG
1	A	329	PRO
1	B	3	GLN
1	B	20	THR
1	B	111	GLU
1	B	153	PHE
1	B	184	ASN
1	B	314	ARG
1	B	329	PRO
1	B	383	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	39	GLN
1	A	167	GLN
1	A	198	GLN
1	A	277	GLN
1	A	389	ASN
1	A	391	HIS
1	A	405	ASN
1	B	25	GLN
1	B	39	GLN
1	B	198	GLN
1	B	277	GLN
1	B	389	ASN
1	B	391	HIS
1	B	405	ASN
1	B	413	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.07	0
3	ICT	A	701	2	2,12,12	0.11	0	5,16,16	1.62	1 (20%)
3	ICT	B	702	2	2,12,12	0.34	0	5,16,16	1.63	1 (20%)
4	SO4	B	602	-	4,4,4	0.26	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ICT	B	702	2	-	0/6/16/16	-
3	ICT	A	701	2	-	0/6/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ICT	C1-C2-C3	2.62	115.19	112.25
3	B	702	ICT	C1-C2-C3	2.59	115.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	413/413 (100%)	0.16	24 (5%) 23 22	15, 26, 49, 75	0
1	B	413/413 (100%)	-0.09	6 (1%) 73 74	14, 22, 42, 65	0
All	All	826/826 (100%)	0.04	30 (3%) 42 40	14, 24, 46, 75	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	LEU	8.2
1	A	1	ALA	8.1
1	A	412	ARG	6.5
1	A	322	GLY	5.5
1	A	411	GLY	5.5
1	B	383	LEU	5.2
1	A	413	GLN	4.9
1	A	2	ASP	4.5
1	A	324	PRO	4.4
1	A	164	SER	3.8
1	B	384	SER	3.8
1	B	387	LYS	3.4
1	A	323	ARG	3.4
1	A	384	SER	3.3
1	B	390	GLU	3.1
1	A	409	ALA	3.1
1	A	408	ARG	3.0
1	A	385	ASN	3.0
1	A	390	GLU	2.9
1	A	85	GLU	2.8
1	A	321	LYS	2.7
1	A	388	LEU	2.7
1	A	389	ASN	2.7
1	B	413	GLN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	52	GLN	2.5
1	A	90	LYS	2.5
1	A	410	LEU	2.3
1	B	385	ASN	2.3
1	A	386	VAL	2.2
1	A	91	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	602	5/5	0.78	0.31	94,94,94,94	0
4	SO4	B	601	5/5	0.86	0.18	84,85,85,85	0
3	ICT	A	701	13/13	0.94	0.10	21,23,25,26	0
3	ICT	B	702	13/13	0.97	0.10	18,20,22,22	0
2	MN	A	501	1/1	1.00	0.07	21,21,21,21	0
2	MN	B	502	1/1	1.00	0.08	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.