



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:38 pm BST

PDB ID : 5YFN  
Title : Human isocitrate dehydrogenase 1 bound with isocitrate  
Authors : Nordlund, P.; Chen, D.; Jansson, A.; Larsson, A.  
Deposited on : 2017-09-21  
Resolution : 2.50 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.

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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 : 1.8.5 (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

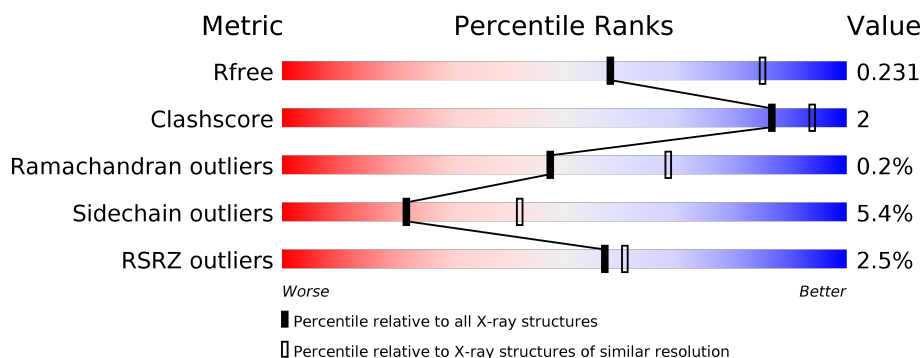
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	421	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	421	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6734 atoms, of which 10 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 [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3292	2093	555	625	19			
1	B	406	Total	C	N	O	S	0	0	0
			3197	2035	536	608	18			

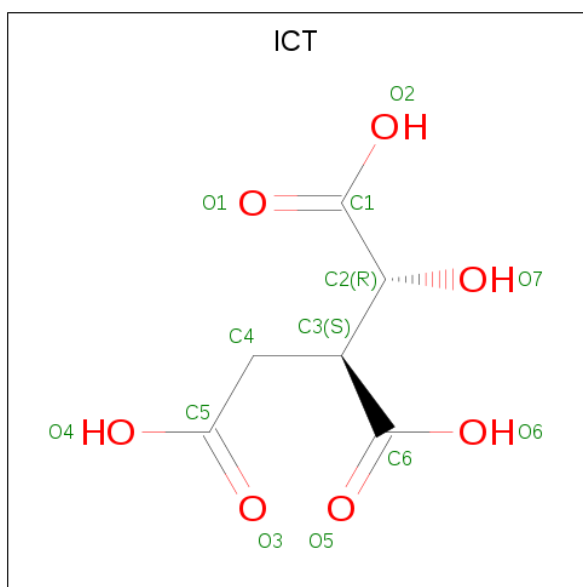
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP O75874
A	-5	LEU	-	expression tag	UNP O75874
A	-4	TYR	-	expression tag	UNP O75874
A	-3	PHE	-	expression tag	UNP O75874
A	-2	GLN	-	expression tag	UNP O75874
A	-1	SER	-	expression tag	UNP O75874
A	0	MET	-	expression tag	UNP O75874
B	-6	ASN	-	expression tag	UNP O75874
B	-5	LEU	-	expression tag	UNP O75874
B	-4	TYR	-	expression tag	UNP O75874
B	-3	PHE	-	expression tag	UNP O75874
B	-2	GLN	-	expression tag	UNP O75874
B	-1	SER	-	expression tag	UNP O75874
B	0	MET	-	expression tag	UNP O75874

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- 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	H	O	0	0
			18	6	5	7		
3	A	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

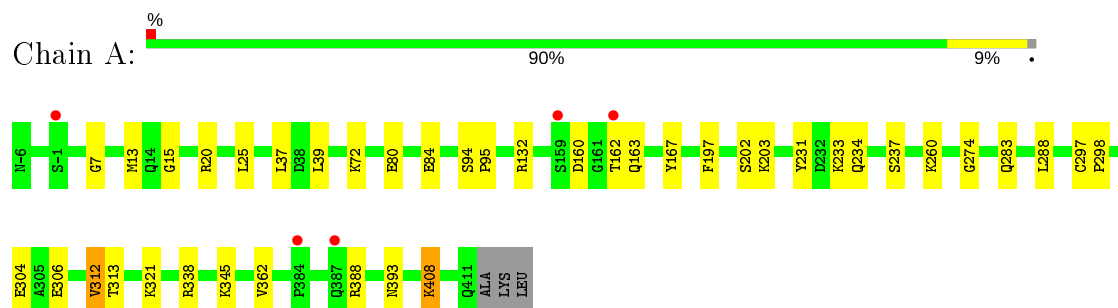
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	94	Total	O	0	0
			94	94		

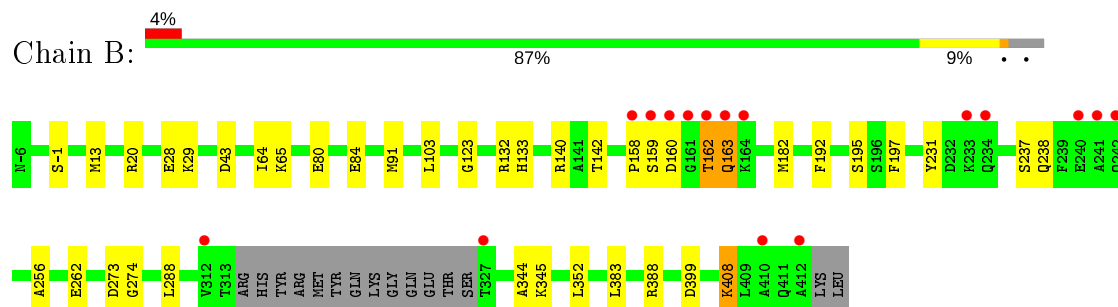
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.56Å 92.00Å 138.84Å 90.00° 109.94° 90.00°	Depositor
Resolution (Å)	41.80 – 2.50 41.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.80-2.50) 99.4 (41.80-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.173 , 0.226 0.187 , 0.231	Depositor DCC
$R_{free}$ test set	2300 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.2	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	0.95	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, 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	1.13	2/3362 (0.1%)	0.89	0/4538
1	B	1.02	0/3263	0.89	1/4404 (0.0%)
All	All	1.08	2/6625 (0.0%)	0.89	1/8942 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CD-OE1	-5.88	1.19	1.25
1	A	306	GLU	CD-OE1	-5.07	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ASP	CB-CG-OD1	7.00	124.60	118.30

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	3292	0	3225	14	0
1	B	3197	0	3149	15	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	26	10	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	111	0	0	0	0
5	B	94	0	0	1	0
All	All	6724	10	6382	27	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 2.

All (27) 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:20:ARG:NH2	1:B:43:ASP:OD1	2.21	0.74
1:B:132:ARG:HG3	1:B:274:GLY:HA3	1.71	0.71
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.84	0.60
1:B:158:PRO:HG2	1:B:162:THR:HB	1.84	0.60
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.83	0.59
1:A:132:ARG:HG3	1:A:274:GLY:HA3	1.89	0.54
1:A:297:CYS:HB3	1:A:298:PRO:HD2	1.92	0.52
1:A:160:ASP:OD1	1:A:162:THR:HG23	2.13	0.48
1:B:123:GLY:O	1:B:262:GLU:HA	2.14	0.48
1:B:13:MET:CE	1:B:64:ILE:HD11	2.44	0.47
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.49	0.47
1:B:20:ARG:HH22	1:B:43:ASP:CG	2.17	0.47
1:A:13:MET:CE	1:A:72:LYS:HB2	2.45	0.46
1:A:94:SER:HA	1:A:95:PRO:HD2	1.80	0.46
1:A:297:CYS:HB3	1:A:298:PRO:CD	2.47	0.45
1:A:283:GLN:HG2	1:B:256:ALA:O	2.16	0.45
1:B:163:GLN:N	1:B:163:GLN:OE1	2.50	0.45
1:B:344:ALA:HB2	1:B:352:LEU:HB3	1.98	0.45
1:B:133:HIS:HB2	1:B:192:PHE:CE2	2.52	0.44
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.53	0.44
1:B:408:LYS:HE2	1:B:408:LYS:HB2	1.89	0.44
1:B:29:LYS:HE2	1:B:399:ASP:OD1	2.19	0.43
1:B:182:MET:CE	5:B:610:HOH:O	2.68	0.42
1:A:13:MET:HE3	1:A:72:LYS:HB2	2.00	0.42
1:A:80:GLU:OE2	1:A:84:GLU:OE1	2.36	0.42
1:A:15:GLY:O	1:A:20:ARG:HD2	2.19	0.41
1:A:7:GLY:HA3	1:A:37:LEU:HD23	2.03	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	416/421 (99%)	398 (96%)	17 (4%)	1 (0%)	47	68
1	B	402/421 (96%)	381 (95%)	20 (5%)	1 (0%)	47	68
All	All	818/842 (97%)	779 (95%)	37 (4%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASP
1	A	312	VAL

### 5.3.2 Protein sidechains [i](#)

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	348/357 (98%)	330 (95%)	18 (5%)	23	44
1	B	340/357 (95%)	321 (94%)	19 (6%)	21	40
All	All	688/714 (96%)	651 (95%)	37 (5%)	22	42

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	163	GLN
1	A	202	SER
1	A	203	LYS
1	A	233	LYS
1	A	234	GLN
1	A	237	SER
1	A	260	LYS
1	A	288	LEU
1	A	312	VAL
1	A	313	THR
1	A	321	LYS
1	A	338	ARG
1	A	345	LYS
1	A	388	ARG
1	A	393	ASN
1	A	408	LYS
1	B	-1	SER
1	B	28	GLU
1	B	65	LYS
1	B	80	GLU
1	B	84	GLU
1	B	91	MET
1	B	103	LEU
1	B	140	ARG
1	B	159	SER
1	B	162	THR
1	B	163	GLN
1	B	195	SER
1	B	237	SER
1	B	238	GLN
1	B	288	LEU
1	B	345	LYS
1	B	383	LEU
1	B	388	ARG
1	B	408	LYS

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
3	ICT	A	505	2	2,12,12	2.94	1 (50%)	5,16,16	2.47	4 (80%)
3	ICT	A	502	2	2,12,12	1.75	1 (50%)	5,16,16	4.72	4 (80%)

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	A	505	2	-	2/6/16/16	-
3	ICT	A	502	2	-	4/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	ICT	O7-C2	-4.00	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ICT	O7-C2	-2.28	1.38	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ICT	C1-C2-C3	-6.63	104.78	112.25
3	A	502	ICT	O7-C2-C3	5.76	124.69	108.56
3	A	502	ICT	C4-C3-C6	4.77	119.16	112.70
3	A	505	ICT	C4-C3-C6	3.52	117.48	112.70
3	A	502	ICT	C4-C3-C2	3.39	119.81	110.29
3	A	505	ICT	O7-C2-C3	2.72	116.16	108.56
3	A	505	ICT	C4-C3-C2	2.21	116.50	110.29
3	A	505	ICT	C1-C2-C3	-2.07	109.92	112.25

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	ICT	C1-C2-C3-C4
3	A	502	ICT	C1-C2-C3-C4
3	A	502	ICT	O7-C2-C3-C4
3	A	502	ICT	C1-C2-C3-C6
3	A	502	ICT	C6-C3-C4-C5
3	A	505	ICT	O7-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 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	418/421 (99%)	-0.23	5 (1%) 79 80	19, 35, 62, 119	0
1	B	406/421 (96%)	-0.09	16 (3%) 39 42	19, 37, 70, 104	0
All	All	824/842 (97%)	-0.16	21 (2%) 57 61	19, 36, 66, 119	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ALA	3.9
1	B	159	SER	3.7
1	B	161	GLY	3.6
1	A	162	THR	3.5
1	B	163	GLN	2.6
1	B	162	THR	2.5
1	B	327	THR	2.5
1	B	242	GLN	2.4
1	B	241	ALA	2.4
1	B	233	LYS	2.4
1	B	312	VAL	2.3
1	B	164	LYS	2.2
1	B	158	PRO	2.2
1	A	159	SER	2.2
1	B	160	ASP	2.2
1	B	412	ALA	2.1
1	A	387	GLN	2.1
1	B	240	GLU	2.1
1	A	-1	SER	2.1
1	B	234	GLN	2.0
1	A	384	PRO	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](#)

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
2	MG	A	503	1/1	0.77	0.37	36,36,36,36	0
2	MG	A	501	1/1	0.88	0.37	34,34,34,34	0
3	ICT	A	505	13/13	0.96	0.11	20,20,20,20	0
3	ICT	A	502	13/13	0.96	0.12	20,20,20,20	0
4	K	A	504	1/1	0.98	0.29	30,30,30,30	0
4	K	B	501	1/1	0.99	0.34	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.