



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:39 PM UTC

PDB ID : 2CKO / pdb\_00002cko  
Title : Crystal structure of Human Choline Kinase alpha 2  
Authors : Malito, E.; Lavie, A.  
Deposited on : 2006-04-20  
Resolution : 2.15 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

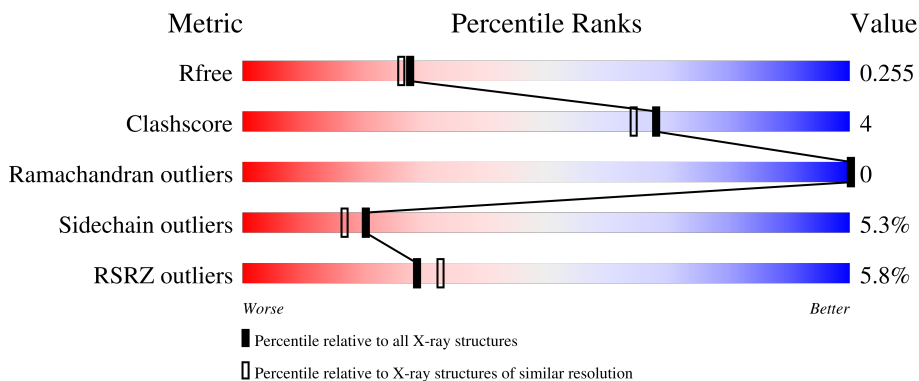
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of 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	390	 8% 79% 9% 12%
1	B	390	 2% 78% 11% 11%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6119 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.

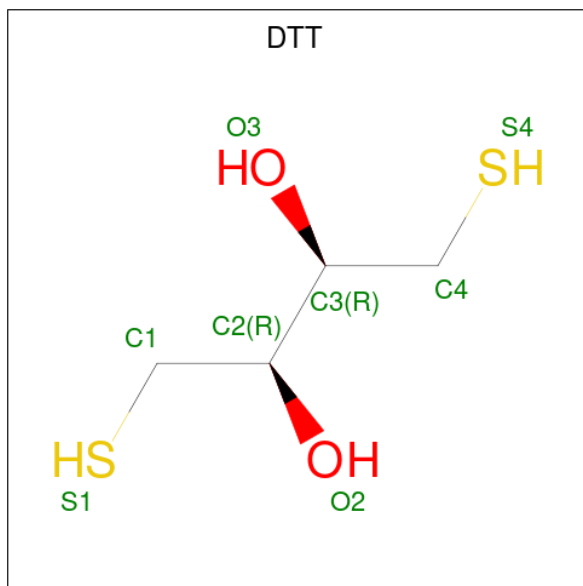
- Molecule 1 is a protein called CHOLINE KINASE ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	Total 2830	C 1836	N 476	O 502	S 16	0	0	0
1	B	346	Total 2856	C 1852	N 480	O 508	S 16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	GLY	conflict	UNP P35790
A	422	LEU	GLN	conflict	UNP P35790
B	220	SER	GLY	conflict	UNP P35790
B	422	LEU	GLN	conflict	UNP P35790

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		
2	B	1	Total	C	O	S	0	0
			8	4	2	2		

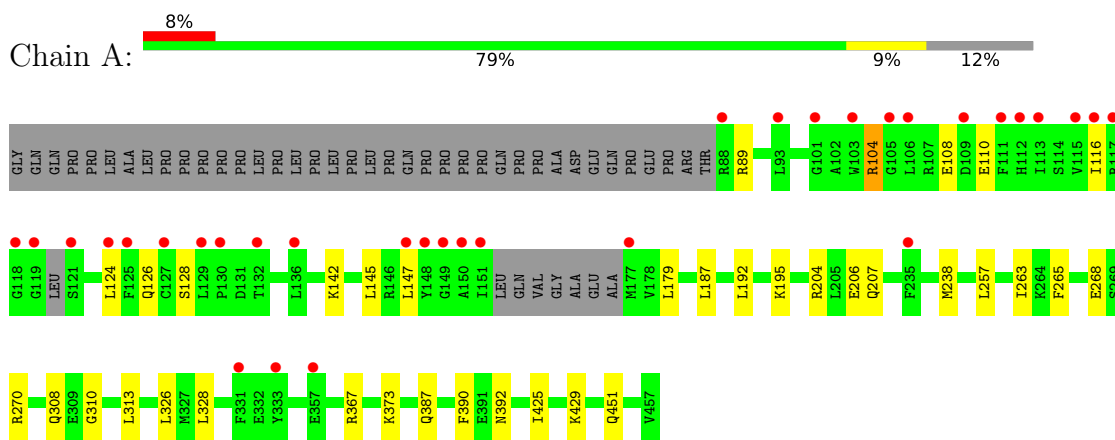
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	203	Total	O	0	0
			203	203		

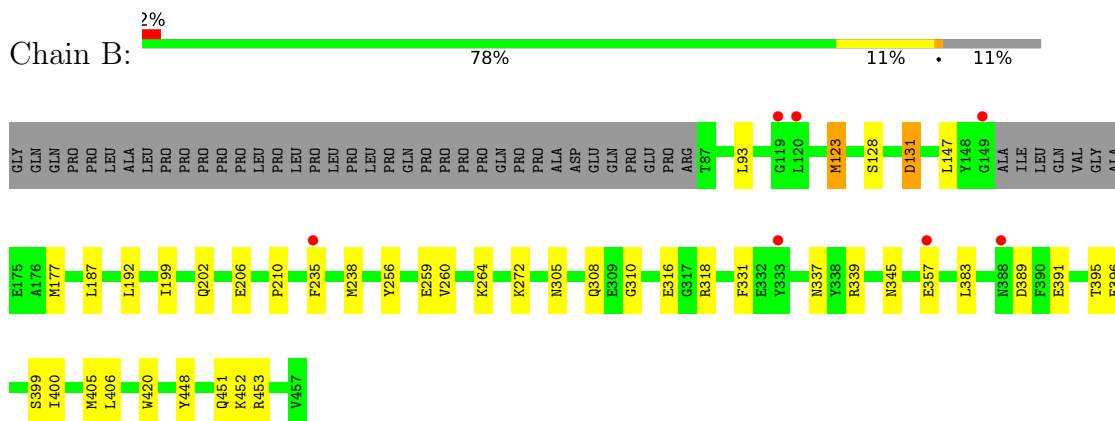
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: CHOLINE KINASE ALPHA



#### • Molecule 1: CHOLINE KINASE ALPHA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.18Å 122.82Å 132.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.15) 99.9 (30.00-2.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.256 0.199 , 0.255	Depositor DCC
$R_{free}$ test set	5080 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: DTT

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	0.78	0/2903	0.91	0/3907
1	B	0.80	0/2930	0.90	1/3945 (0.0%)
All	All	0.79	0/5833	0.91	1/7852 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	SER	N-CA-C	5.19	117.07	109.24

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	2830	0	2789	15	0
1	B	2856	0	2820	25	0
2	A	8	0	10	0	0
2	B	8	0	10	1	0
3	A	214	0	0	2	0
3	B	203	0	0	4	0
All	All	6119	0	5629	41	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 4.

All (41) 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:104:ARG:HH11	1:A:104:ARG:HG2	1.42	0.82
1:B:339:ARG:CZ	1:B:405:MET:HE2	2.11	0.80
1:B:331:PHE:HE2	3:B:2023:HOH:O	1.70	0.74
1:A:392:ASN:OD1	3:A:2183:HOH:O	2.12	0.68
1:B:305:ASN:HD21	1:B:337:ASN:HD22	1.47	0.62
1:B:331:PHE:CE2	3:B:2023:HOH:O	2.47	0.61
1:A:195:LYS:H	1:A:207:GLN:HE21	1.49	0.60
1:B:389:ASP:OD1	3:B:2169:HOH:O	2.17	0.59
1:B:308:GLN:HE21	1:B:310:GLY:H	1.50	0.57
1:B:235:PHE:HA	1:B:238:MET:HE2	1.87	0.56
1:B:305:ASN:ND2	1:B:337:ASN:HD22	2.05	0.54
1:B:383:LEU:HD21	1:B:405:MET:HE1	1.88	0.54
1:A:308:GLN:HE21	1:A:310:GLY:H	1.56	0.54
1:A:265:PHE:CD1	1:A:270:ARG:HD3	2.43	0.54
1:B:210:PRO:HB2	1:B:316:GLU:HG2	1.91	0.53
1:B:453:ARG:NH1	3:B:2200:HOH:O	2.28	0.52
1:B:383:LEU:HD21	1:B:405:MET:CE	2.39	0.51
1:A:387:GLN:NE2	3:A:2179:HOH:O	2.32	0.50
1:B:123:MET:HE3	1:B:123:MET:H	1.76	0.50
1:A:116:ILE:HD11	1:A:126:GLN:HB2	1.93	0.50
1:B:357:GLU:H	1:B:357:GLU:CD	2.19	0.50
1:B:396:GLU:O	1:B:400:ILE:HG12	2.13	0.49
1:A:126:GLN:HE21	1:A:142:LYS:NZ	2.11	0.49
1:B:131:ASP:OD1	1:B:131:ASP:N	2.44	0.48
1:A:104:ARG:HG2	1:A:104:ARG:NH1	2.18	0.48
1:A:204:ARG:HD2	1:A:206:GLU:OE1	2.14	0.48
1:A:313:LEU:O	1:A:326:LEU:HA	2.13	0.47
1:B:187:LEU:HD13	1:B:331:PHE:CD2	2.50	0.47
1:A:263:ILE:HD11	1:A:425:ILE:HG22	1.97	0.46
1:B:345:ASN:ND2	1:B:420:TRP:HE1	2.13	0.46
1:B:187:LEU:HD13	1:B:331:PHE:CE2	2.52	0.45
1:A:187:LEU:HD21	1:A:238:MET:HE1	1.97	0.45
2:B:1458:DTT:H41	2:B:1458:DTT:H12	1.57	0.44
1:B:383:LEU:CD2	1:B:405:MET:HE1	2.48	0.43
1:A:89:ARG:HG3	1:A:108:GLU:OE2	2.20	0.42
1:B:339:ARG:NH2	1:B:405:MET:HE2	2.35	0.42
1:B:123:MET:HE3	1:B:147:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:TYR:CE2	1:B:452:LYS:HD2	2.55	0.41
1:A:387:GLN:HG3	1:A:390:PHE:HB2	2.01	0.41
1:B:256:TYR:O	1:B:260:VAL:HG23	2.20	0.41
1:B:357:GLU:CD	1:B:357:GLU:N	2.79	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	338/390 (87%)	323 (96%)	15 (4%)	0	100	100
1	B	342/390 (88%)	329 (96%)	13 (4%)	0	100	100
All	All	680/780 (87%)	652 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	301/349 (86%)	286 (95%)	15 (5%)	22	18
1	B	305/349 (87%)	288 (94%)	17 (6%)	19	15
All	All	606/698 (87%)	574 (95%)	32 (5%)	20	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	110	GLU
1	A	124	LEU
1	A	128	SER
1	A	145	LEU
1	A	147	LEU
1	A	179	LEU
1	A	192	LEU
1	A	257	LEU
1	A	268	GLU
1	A	328	LEU
1	A	367	ARG
1	A	373	LYS
1	A	429	LYS
1	A	451	GLN
1	B	93	LEU
1	B	123	MET
1	B	131	ASP
1	B	177	MET
1	B	192	LEU
1	B	199	ILE
1	B	202	GLN
1	B	206	GLU
1	B	259	GLU
1	B	264	LYS
1	B	272	LYS
1	B	318	ARG
1	B	391	GLU
1	B	395	THR
1	B	399	SER
1	B	406	LEU
1	B	451	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	122	ASN
1	A	126	GLN
1	A	207	GLN
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	392	ASN
1	A	410	ASN
1	A	451	GLN
1	B	112	HIS
1	B	202	GLN
1	B	305	ASN
1	B	308	GLN
1	B	345	ASN
1	B	392	ASN
1	B	410	ASN
1	B	442	GLN
1	B	450	HIS
1	B	451	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z  > 2$
2	DTT	B	1458	-	7,7,7	0.53	0	4,8,8	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DTT	A	1458	-	7,7,7	0.59	0	4,8,8	1.96	1 (25%)

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
2	DTT	B	1458	-	-	6/8/8/8	-
2	DTT	A	1458	-	-	4/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1458	DTT	C3-C4-S4	-3.52	104.59	114.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1458	DTT	C1-C2-C3-O3
2	A	1458	DTT	C1-C2-C3-C4
2	A	1458	DTT	O2-C2-C3-O3
2	A	1458	DTT	O2-C2-C3-C4
2	B	1458	DTT	S1-C1-C2-O2
2	B	1458	DTT	S1-C1-C2-C3
2	B	1458	DTT	C1-C2-C3-O3
2	B	1458	DTT	C1-C2-C3-C4
2	B	1458	DTT	O2-C2-C3-O3
2	B	1458	DTT	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1458	DTT	1	0

## 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	344/390 (88%)	0.27	33 (9%) 13 15	17, 31, 68, 75	0
1	B	346/390 (88%)	0.08	7 (2%) 65 69	19, 33, 56, 65	0
All	All	690/780 (88%)	0.17	40 (5%) 29 32	17, 32, 63, 75	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	PHE	3.8
1	A	88	ARG	3.8
1	A	113	ILE	3.7
1	A	116	ILE	3.4
1	A	115	VAL	3.3
1	A	136	LEU	3.3
1	B	235	PHE	3.1
1	A	331	PHE	3.1
1	A	148	TYR	3.1
1	A	129	LEU	3.1
1	A	111	PHE	3.0
1	A	112	HIS	2.9
1	A	124	LEU	2.8
1	A	119	GLY	2.8
1	A	333	TYR	2.8
1	B	333	TYR	2.8
1	A	147	LEU	2.7
1	A	151	ILE	2.7
1	B	120	LEU	2.6
1	B	388	ASN	2.6
1	A	109	ASP	2.5
1	A	150	ALA	2.5
1	A	177	MET	2.5
1	A	125	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	93	LEU	2.3
1	A	118	GLY	2.3
1	A	357	GLU	2.3
1	B	149	GLY	2.3
1	A	130	PRO	2.2
1	A	149	GLY	2.2
1	A	132	THR	2.2
1	A	101	GLY	2.2
1	B	357	GLU	2.2
1	A	121	SER	2.1
1	A	117	ARG	2.1
1	A	127	CYS	2.1
1	A	106	LEU	2.0
1	A	103	TRP	2.0
1	A	105	GLY	2.0
1	B	119	GLY	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 oligosaccharides 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	DTT	A	1458	8/8	0.87	0.17	68,69,70,73	0
2	DTT	B	1458	8/8	0.87	0.15	66,66,67,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.