



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:27 PM UTC

PDB ID : 7CUI / pdb\_00007cui  
Title : Crystal structure of fission yeast Pot1 and Tpz1  
Authors : Sun, H.; Wu, Z.; Wu, J.; Lei, M.  
Deposited on : 2020-08-23  
Resolution : 2.60 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)

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<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)  
Xtrriage (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

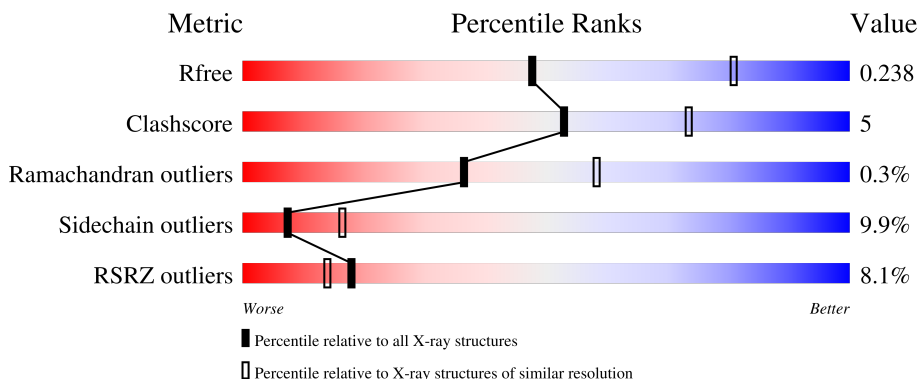
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	199	 6% 73% 11% • 13%
1	C	199	 6% 70% 14% • 13%
2	B	77	 8% 34% • 64%
2	D	77	 5% 31% 5% 64%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3397 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.

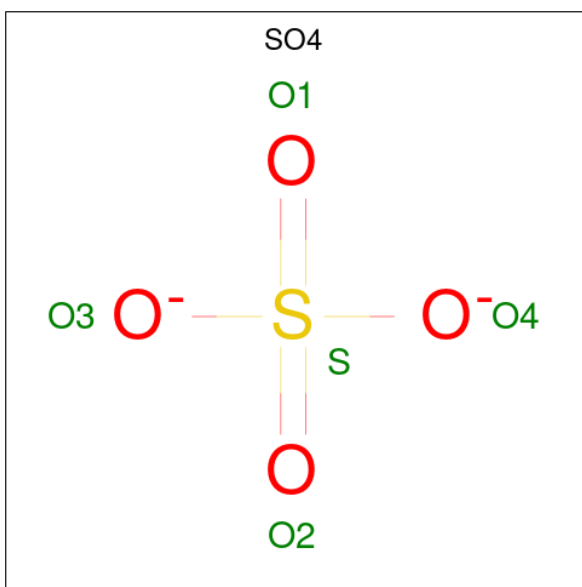
- Molecule 1 is a protein called Protection of telomeres protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	173	1410	919	239	249	1	2	0	0	0
1	C	173	1410	919	239	249	1	2	0	0	0

- Molecule 2 is a protein called Protection of telomeres protein tpz1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
2	B	28	230	148	37	43	1	1	0	0	0
2	D	28	230	148	37	43	1	1	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

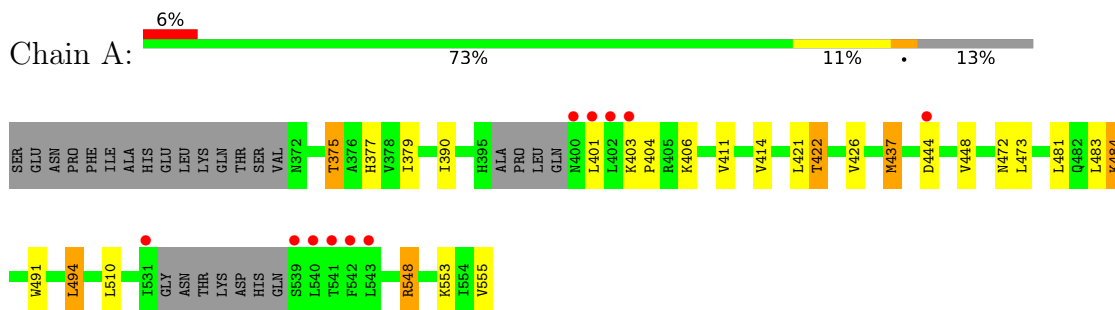
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	3	Total	O	0	0
			3	3		
4	C	54	Total	O	0	0
			54	54		
4	D	6	Total	O	0	0
			6	6		

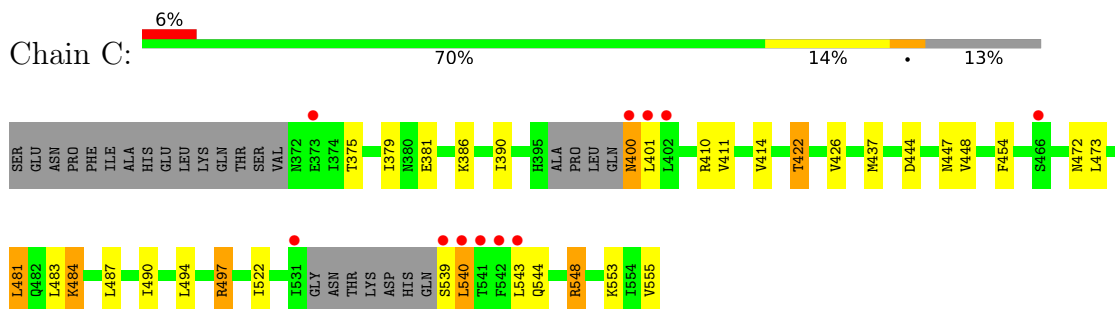
### 3 Residue-property plots [i](#)

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.

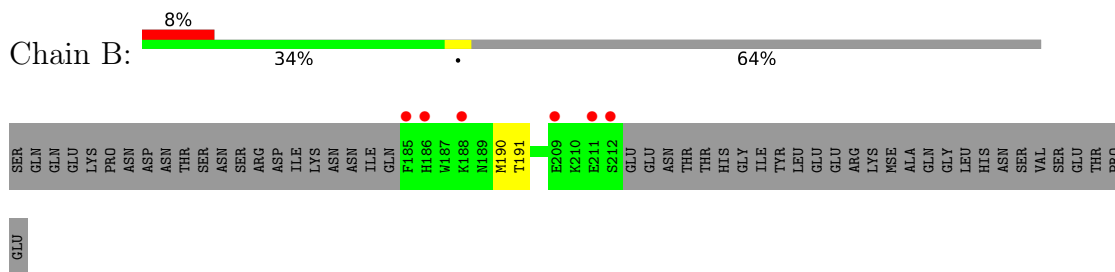
- Molecule 1: Protection of telomeres protein 1



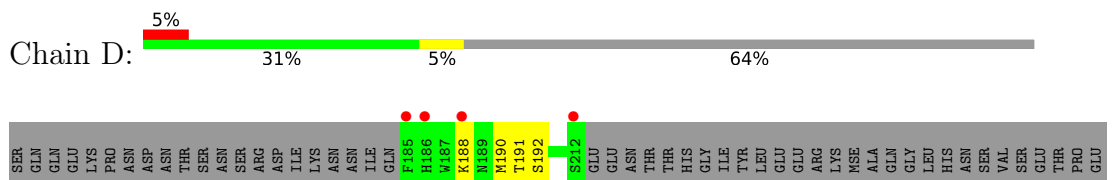
- Molecule 1: Protection of telomeres protein 1



- Molecule 2: Protection of telomeres protein tpz1



- Molecule 2: Protection of telomeres protein tpz1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.23Å 126.23Å 121.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.78 – 2.60 43.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.78-2.60) 97.9 (43.78-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.196 , 0.238 0.196 , 0.238	Depositor DCC
$R_{free}$ test set	1484 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for -h,-l,-k 0.004 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0655e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4

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	0.47	0/1444	0.88	1/1962 (0.1%)
1	C	0.49	0/1444	0.90	0/1962
2	B	0.44	0/233	0.88	1/310 (0.3%)
2	D	0.44	0/233	0.94	1/310 (0.3%)
All	All	0.48	0/3354	0.90	3/4544 (0.1%)

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	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	190	MSE	CG-SE-CE	5.22	110.40	98.92
2	D	190	MSE	CG-SE-CE	5.19	110.35	98.92
1	A	437	MSE	CG-SE-CE	5.14	110.24	98.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	410	ARG	Peptide

## 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	1410	0	1435	11	0
1	C	1410	0	1435	20	0
2	B	230	0	233	0	0
2	D	230	0	233	2	0
3	A	5	0	0	0	0
3	C	5	0	0	1	0
4	A	44	0	0	4	0
4	B	3	0	0	0	0
4	C	54	0	0	6	0
4	D	6	0	0	2	0
All	All	3397	0	3336	33	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 5.

All (33) 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:C:539:SER:O	1:C:540:LEU:HG	1.56	1.04
4:A:719:HOH:O	1:C:422:THR:CG2	2.31	0.78
1:A:422:THR:CG2	4:C:721:HOH:O	2.32	0.76
1:C:379:ILE:HD12	1:C:555:VAL:HG21	1.68	0.75
4:A:719:HOH:O	1:C:422:THR:HG21	1.87	0.74
1:C:454:PHE:HZ	1:C:522:ILE:HD11	1.60	0.67
1:C:390:ILE:HD12	1:C:444:ASP:HB2	1.78	0.65
1:C:497:ARG:NH1	3:C:601:SO4:O4	2.33	0.62
1:C:540:LEU:HD22	1:C:544:GLN:HG2	1.86	0.56
1:C:400:ASN:ND2	4:C:702:HOH:O	2.39	0.55
1:A:403:LYS:HB2	1:A:404:PRO:HD2	1.90	0.54
1:A:422:THR:HG21	4:C:721:HOH:O	2.02	0.53
1:A:390:ILE:HD12	1:A:444:ASP:HB2	1.90	0.53
1:C:497:ARG:NH2	4:C:701:HOH:O	2.33	0.51
1:A:548:ARG:HD2	4:A:715:HOH:O	2.13	0.49
1:C:548:ARG:HD2	4:C:711:HOH:O	2.12	0.49
1:C:390:ILE:CD1	1:C:444:ASP:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:LYS:NZ	4:C:703:HOH:O	2.43	0.48
1:A:491:TRP:O	1:A:494:LEU:HB2	2.14	0.47
1:C:539:SER:O	1:C:540:LEU:CG	2.46	0.46
1:C:481:LEU:HD12	1:C:484:LYS:HE2	1.98	0.45
2:D:188:LYS:HG3	4:D:306:HOH:O	2.17	0.45
1:C:426:VAL:HG11	1:C:437:MSE:HE2	2.00	0.44
1:C:543:LEU:HD23	1:C:543:LEU:HA	1.88	0.42
1:C:454:PHE:CZ	1:C:522:ILE:HD11	2.46	0.42
1:C:481:LEU:HD12	1:C:481:LEU:HA	1.88	0.42
1:A:484:LYS:NZ	4:A:701:HOH:O	2.51	0.41
1:A:426:VAL:HG11	1:A:437:MSE:HE2	2.03	0.41
1:A:379:ILE:HD12	1:A:555:VAL:HG21	2.02	0.41
1:A:421:LEU:HD12	1:A:484:LYS:HG3	2.03	0.40
1:A:375:THR:HB	1:A:377:HIS:H	1.86	0.40
1:C:487:LEU:HD22	1:C:490:ILE:HD11	2.04	0.40
2:D:192:SER:HA	4:D:305:HOH:O	2.21	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	167/199 (84%)	163 (98%)	4 (2%)	0	100	100
1	C	167/199 (84%)	162 (97%)	4 (2%)	1 (1%)	21	42
2	B	26/77 (34%)	26 (100%)	0	0	100	100
2	D	26/77 (34%)	25 (96%)	1 (4%)	0	100	100
All	All	386/552 (70%)	376 (97%)	9 (2%)	1 (0%)	36	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	540	LEU

### 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	160/181 (88%)	144 (90%)	16 (10%)	7 16
1	C	160/181 (88%)	141 (88%)	19 (12%)	5 10
2	B	27/71 (38%)	26 (96%)	1 (4%)	30 57
2	D	27/71 (38%)	26 (96%)	1 (4%)	30 57
All	All	374/504 (74%)	337 (90%)	37 (10%)	7 16

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

Mol	Chain	Res	Type
1	A	375	THR
1	A	401	LEU
1	A	406	LYS
1	A	411	VAL
1	A	414	VAL
1	A	422	THR
1	A	448	VAL
1	A	472	ASN
1	A	473	LEU
1	A	481	LEU
1	A	483	LEU
1	A	484	LYS
1	A	494	LEU
1	A	510	LEU
1	A	548	ARG
1	A	553	LYS
2	B	191	THR
1	C	375	THR
1	C	381	GLU
1	C	386	LYS
1	C	400	ASN

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Mol	Chain	Res	Type
1	C	401	LEU
1	C	411	VAL
1	C	414	VAL
1	C	422	THR
1	C	447	ASN
1	C	448	VAL
1	C	472	ASN
1	C	473	LEU
1	C	481	LEU
1	C	483	LEU
1	C	484	LYS
1	C	494	LEU
1	C	497	ARG
1	C	548	ARG
1	C	553	LYS
2	D	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	469	GLN
1	A	472	ASN
1	A	499	GLN
1	C	372	ASN
1	C	380	ASN
1	C	423	GLN
1	C	469	GLN
1	C	482	GLN
1	C	499	GLN
2	D	189	ASN

### 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	$\# Z  > 2$
3	SO4	A	601	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	C	601	-	4,4,4	0.38	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	SO4	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	171/199 (85%)	-0.11	11 (6%) 25 20	20, 38, 86, 111	0
1	C	171/199 (85%)	0.02	11 (6%) 25 20	21, 40, 84, 101	0
2	B	27/77 (35%)	1.17	6 (22%) 2 2	39, 64, 128, 135	0
2	D	27/77 (35%)	0.96	4 (14%) 5 4	41, 63, 112, 129	0
All	All	396/552 (71%)	0.11	32 (8%) 18 14	20, 44, 92, 135	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	185	PHE	7.5
2	B	185	PHE	6.5
1	A	541	THR	5.5
1	C	540	LEU	5.5
2	B	186	HIS	4.9
2	D	212	SER	4.9
2	D	186	HIS	4.8
1	A	540	LEU	4.7
1	A	401	LEU	4.0
1	C	539	SER	3.9
2	B	211	GLU	3.8
2	B	212	SER	3.8
1	C	402	LEU	3.6
1	A	539	SER	3.6
1	C	543	LEU	3.6
2	B	188	LYS	3.3
1	A	400	ASN	3.3
1	A	543	LEU	3.3
1	C	466	SER	3.2
1	A	402	LEU	3.2
1	C	401	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	373	GLU	2.5
1	A	531	ILE	2.5
1	C	542	PHE	2.3
2	D	188	LYS	2.3
1	A	542	PHE	2.2
1	A	444	ASP	2.2
1	C	400	ASN	2.1
2	B	209	GLU	2.1
1	C	531	ILE	2.1
1	A	403	LYS	2.1
1	C	541	THR	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 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(Å <sup>2</sup> )	Q<0.9
3	SO4	A	601	5/5	0.96	0.10	62,66,68,71	5
3	SO4	C	601	5/5	0.98	0.07	49,52,53,54	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.