



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 04:38 am GMT

PDB ID : 4COM  
Title : Crystal structure of the anaerobic ribonucleotide reductase from *Thermotoga maritima* with MES in the active site  
Authors : Aurelius, O.; Johansson, R.; Bagenholm, V.; Beck, T.; Balhuizen, A.; Lundin, D.; Sjoberg, B.M.; Mulliez, E.; Logan, D.T.  
Deposited on : 2014-01-29  
Resolution : 1.92 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

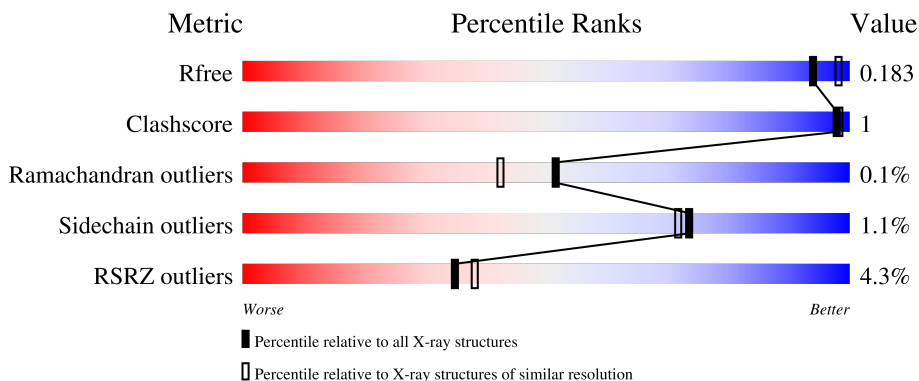
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

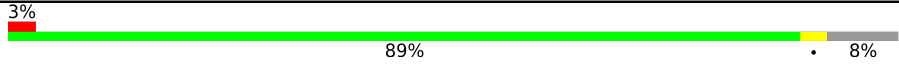
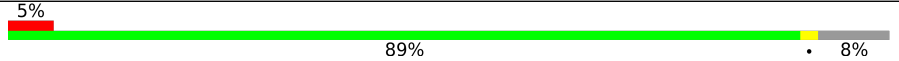
The reported resolution of this entry is 1.92 Å.

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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	651	
1	B	651	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20381 atoms, of which 9759 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.

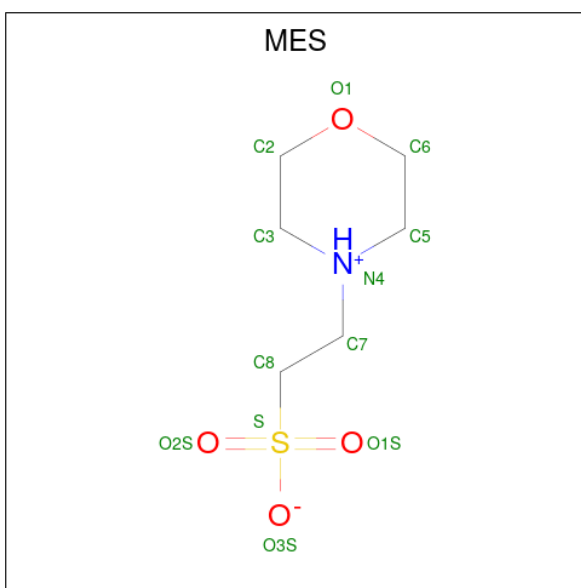
- Molecule 1 is a protein called ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	601	9771	3194	4828	813	910	26	0	7	0
1	B	596	9808	3185	4883	810	906	24	0	8	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

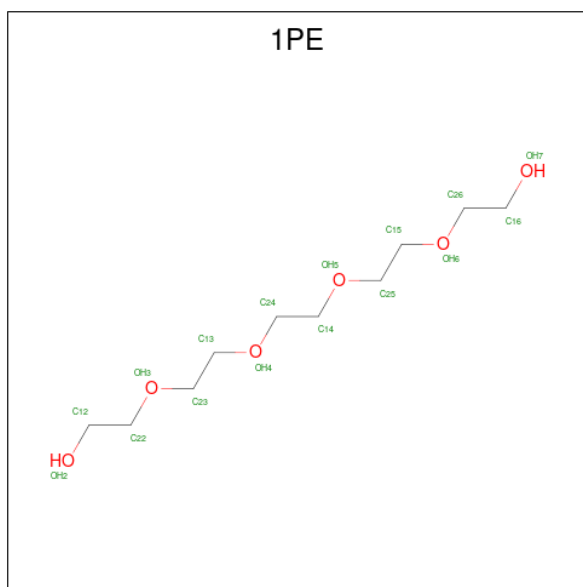
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			38	10	22	6		

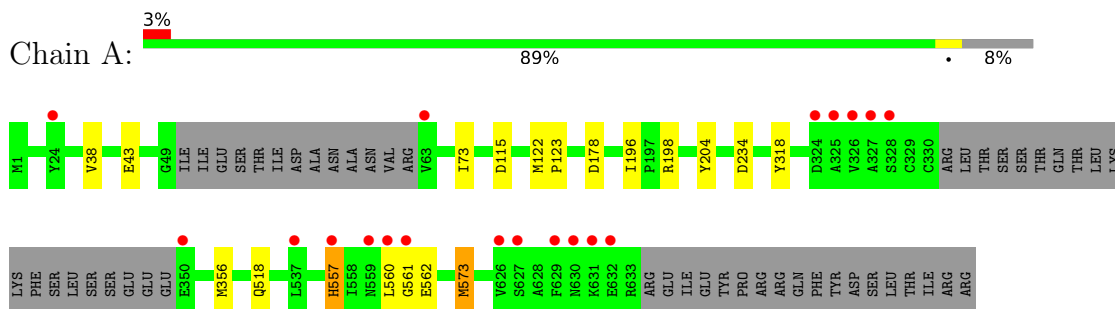
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total	O	0	0
			383	383		
5	B	329	Total	O	0	0
			329	329		

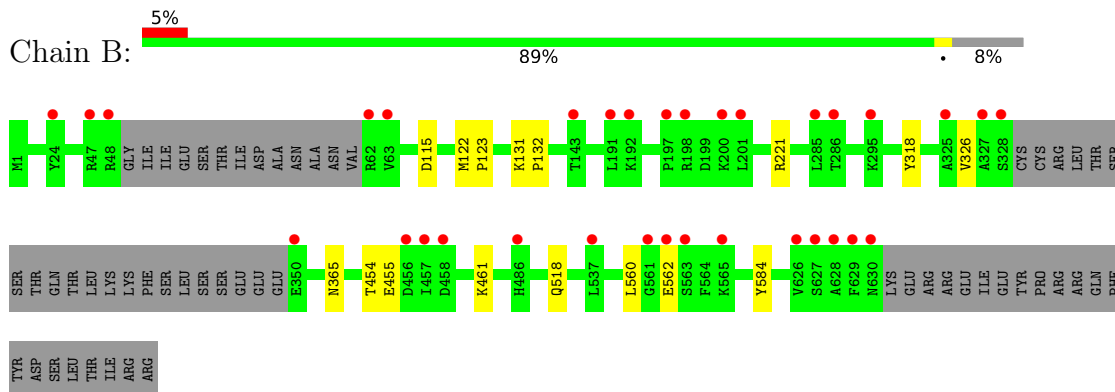
### 3 Residue-property plots [i](#)

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: ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE



- Molecule 1: ANAEROBIC RIBONUCLEOSIDE-TRIPHOSPHATE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.59Å 96.03Å 89.60Å 90.00° 112.66° 90.00°	Depositor
Resolution (Å)	29.40 – 1.92 29.40 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.40-1.92) 99.8 (29.40-1.92)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.92Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.153 , 0.182 0.155 , 0.183	Depositor DCC
$R_{free}$ test set	2410 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: MES, ZN, 1PE

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	0.92	1/5079 (0.0%)	0.72	1/6852 (0.0%)
1	B	0.93	1/5067 (0.0%)	0.72	0/6836
All	All	0.92	2/10146 (0.0%)	0.72	1/13688 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	584	TYR	CD1-CE1	6.04	1.48	1.39
1	A	43	GLU	CG-CD	5.45	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CB-CG-OD1	5.27	123.05	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	4943	4828	4878	9	0
1	B	4925	4883	4871	5	0
2	A	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	12	13	13	0	0
3	B	12	13	13	0	0
4	B	16	22	22	0	0
5	A	383	0	0	3	0
5	B	329	0	0	2	0
All	All	10622	9759	9797	14	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 1.

All (14) 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:560:LEU:HD21	1:A:573:MET:HE2	1.77	0.65
1:A:560:LEU:HD21	1:A:573:MET:CE	2.36	0.56
1:A:198[A]:ARG:NH2	5:A:2139:HOH:O	2.40	0.55
1:A:356:MET:HE3	5:A:2241:HOH:O	2.09	0.51
1:B:122:MET:HB2	1:B:123:PRO:HD2	1.94	0.49
1:A:122:MET:HB2	1:A:123:PRO:HD2	1.95	0.48
1:A:38:VAL:HG13	1:A:73:ILE:HD11	1.97	0.47
1:A:557:HIS:NE2	5:A:2355:HOH:O	2.36	0.44
1:B:454:THR:OG1	1:B:455:GLU:N	2.49	0.44
1:B:131:LYS:HB3	1:B:132:PRO:HD3	2.00	0.43
1:B:221:ARG:NH1	5:B:2126:HOH:O	2.52	0.42
1:B:326:VAL:HG12	5:B:2200:HOH:O	2.20	0.42
1:A:561:GLY:O	1:A:562:GLU:HB2	2.20	0.41
1:A:196:ILE:HD11	1:A:204:TYR:CE2	2.56	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	602/651 (92%)	592 (98%)	10 (2%)	0	100	100
1	B	598/651 (92%)	591 (99%)	6 (1%)	1 (0%)	47	38
All	All	1200/1302 (92%)	1183 (99%)	16 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	562	GLU

### 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	534/577 (92%)	528 (99%)	6 (1%)	73	72
1	B	533/577 (92%)	527 (99%)	6 (1%)	73	72
All	All	1067/1154 (92%)	1055 (99%)	12 (1%)	73	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASP
1	A	234	ASP
1	A	318	TYR
1	A	518	GLN
1	A	557	HIS
1	A	573	MET
1	B	115	ASP
1	B	318	TYR
1	B	365	ASN
1	B	461	LYS
1	B	518	GLN
1	B	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	557	HIS

### 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 monosaccharides in this entry.

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

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	MES	B	1631	-	12,12,12	1.67	2 (16%)	14,16,16	1.54	3 (21%)
3	MES	A	1634	-	12,12,12	1.60	1 (8%)	14,16,16	1.48	2 (14%)
4	1PE	B	1632	-	15,15,15	0.71	0	14,14,14	0.70	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	MES	B	1631	-	-	3/6/14/14	0/1/1/1
3	MES	A	1634	-	-	0/6/14/14	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	B	1632	-	-	5/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1634	MES	C8-S	-5.18	1.70	1.77
3	B	1631	MES	C8-S	-5.11	1.70	1.77
3	B	1631	MES	O2S-S	2.10	1.51	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1634	MES	O3S-S-C8	3.62	111.62	105.77
3	B	1631	MES	O3S-S-C8	3.28	111.07	105.77
3	B	1631	MES	C5-N4-C3	2.90	115.36	108.83
3	A	1634	MES	C5-N4-C3	2.67	114.83	108.83
3	B	1631	MES	O2S-S-C8	2.24	109.61	106.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1632	1PE	OH5-C14-C24-OH4
4	B	1632	1PE	OH6-C15-C25-OH5
3	B	1631	MES	C7-C8-S-O3S
4	B	1632	1PE	C15-C25-OH5-C14
3	B	1631	MES	C7-C8-S-O1S
4	B	1632	1PE	OH2-C12-C22-OH3
3	B	1631	MES	C8-C7-N4-C5
4	B	1632	1PE	OH4-C13-C23-OH3

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

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	601/651 (92%)	-0.11	19 (3%) 47 50	16, 29, 56, 99	0
1	B	596/651 (91%)	-0.01	33 (5%) 25 28	16, 30, 62, 115	0
All	All	1197/1302 (91%)	-0.06	52 (4%) 35 38	16, 30, 61, 115	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	ILE	8.7
1	B	629	PHE	5.9
1	B	63	VAL	5.3
1	A	560	LEU	5.2
1	B	563	SER	4.7
1	A	63	VAL	4.6
1	A	324	ASP	4.3
1	A	350	GLU	3.9
1	B	628	ALA	3.8
1	A	328	SER	3.8
1	B	458	ASP	3.7
1	B	565	LYS	3.6
1	B	328	SER	3.6
1	B	191	LEU	3.6
1	B	561	GLY	3.6
1	B	537	LEU	3.4
1	B	562	GLU	3.3
1	B	456	ASP	3.3
1	B	630	ASN	3.2
1	A	561	GLY	3.1
1	B	325	ALA	3.1
1	A	537	LEU	3.1
1	B	350	GLU	3.0
1	B	627	SER	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	486	HIS	2.8
1	B	197	PRO	2.8
1	A	632	GLU	2.8
1	B	198	ARG	2.8
1	A	24	TYR	2.8
1	B	192	LYS	2.7
1	B	200[A]	LYS	2.6
1	B	62	ARG	2.6
1	A	626	VAL	2.6
1	A	631	LYS	2.5
1	A	559	ASN	2.5
1	B	327	ALA	2.4
1	B	295	LYS	2.4
1	B	626	VAL	2.4
1	B	201	LEU	2.4
1	B	143	THR	2.4
1	B	48	ARG	2.3
1	B	24	TYR	2.3
1	A	627	SER	2.3
1	A	629	PHE	2.2
1	B	47	ARG	2.2
1	A	325	ALA	2.2
1	A	326	VAL	2.1
1	A	557	HIS	2.1
1	A	327	ALA	2.1
1	B	285	LEU	2.1
1	A	630	ASN	2.0
1	B	286	THR	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 monosaccharides 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	1PE	B	1632	16/16	0.77	0.18	49,61,71,73	3
3	MES	B	1631	12/12	0.95	0.10	28,35,41,42	21
2	ZN	A	700	1/1	0.97	0.05	28,28,28,28	1
3	MES	A	1634	12/12	0.97	0.09	23,30,36,37	22
2	ZN	B	652	1/1	0.98	0.04	27,27,27,27	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.