



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2016 – 07:40 AM EDT

PDB ID : 4ZN0  
Title : Structure of the NADPH-dependent thioredoxin reductase from  
Methanosarcina mazei  
Authors : Buey, R.M.; de Pereda, J.M.; Balsera, M.  
Deposited on : 2015-05-04  
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)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

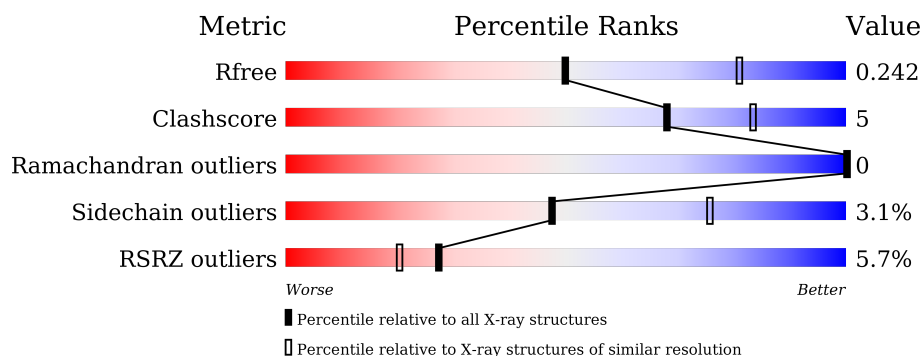
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	311	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	311	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>
1	C	311	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	311	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15485 atoms, of which 7463 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 Thioredoxin reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	H	N	O	S	0	0	0
			4137	1326	2036	360	410	5			
1	B	279	Total	C	H	N	O	S	0	0	0
			3982	1291	1950	339	397	5			
1	C	279	Total	C	H	N	O	S	0	0	0
			3804	1252	1838	332	378	4			
1	D	270	Total	C	H	N	O	S	0	0	0
			3494	1172	1639	322	357	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8PUI1
A	-1	SER	-	expression tag	UNP Q8PUI1
A	0	HIS	-	expression tag	UNP Q8PUI1
A	1	MET	-	expression tag	UNP Q8PUI1
A	2	ALA	-	expression tag	UNP Q8PUI1
A	3	SER	-	expression tag	UNP Q8PUI1
B	-2	GLY	-	expression tag	UNP Q8PUI1
B	-1	SER	-	expression tag	UNP Q8PUI1
B	0	HIS	-	expression tag	UNP Q8PUI1
B	1	MET	-	expression tag	UNP Q8PUI1
B	2	ALA	-	expression tag	UNP Q8PUI1
B	3	SER	-	expression tag	UNP Q8PUI1
C	-2	GLY	-	expression tag	UNP Q8PUI1
C	-1	SER	-	expression tag	UNP Q8PUI1
C	0	HIS	-	expression tag	UNP Q8PUI1
C	1	MET	-	expression tag	UNP Q8PUI1
C	2	ALA	-	expression tag	UNP Q8PUI1
C	3	SER	-	expression tag	UNP Q8PUI1
D	-2	GLY	-	expression tag	UNP Q8PUI1
D	-1	SER	-	expression tag	UNP Q8PUI1
D	0	HIS	-	expression tag	UNP Q8PUI1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP Q8PUI1
D	2	ALA	-	expression tag	UNP Q8PUI1
D	3	SER	-	expression tag	UNP Q8PUI1

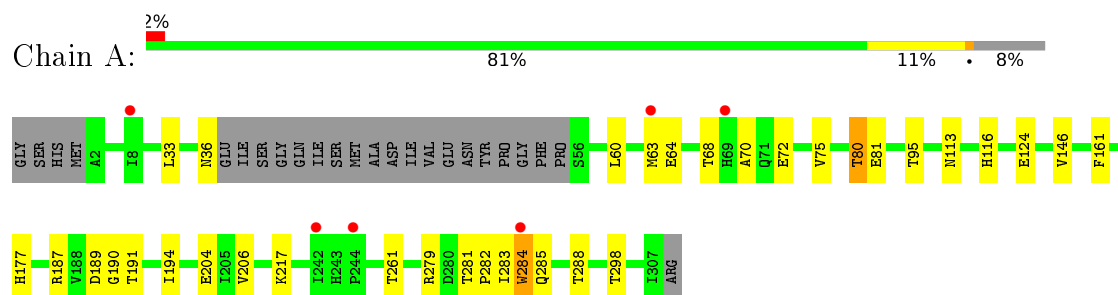
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total 22	O 22	0	0
2	B	23	Total 23	O 23	0	0
2	C	9	Total 9	O 9	0	0
2	D	14	Total 14	O 14	0	0

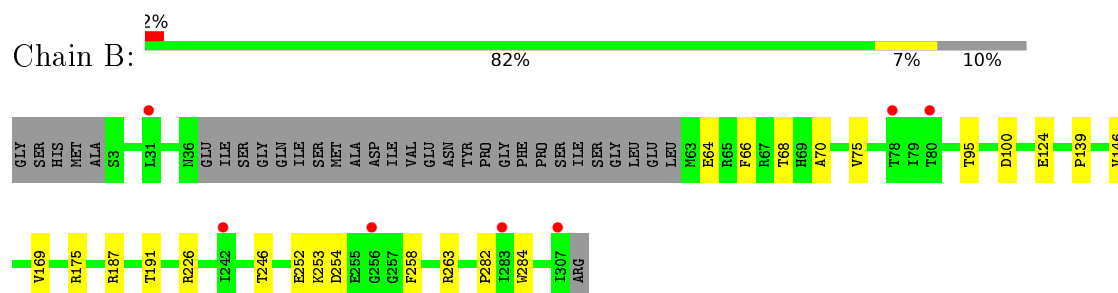
### 3 Residue-property plots [i](#)

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

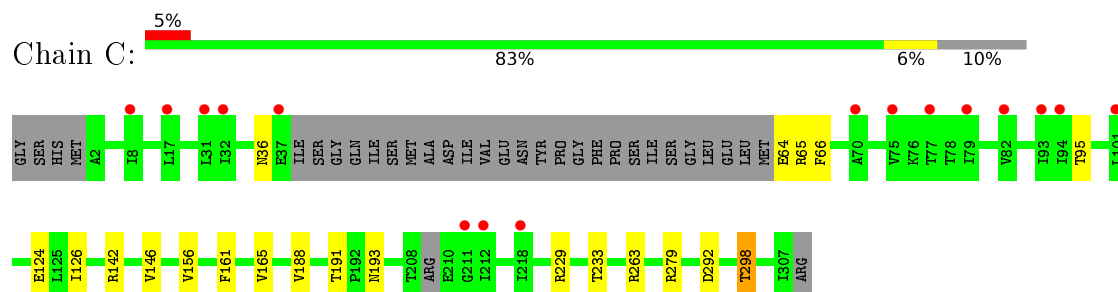
#### • Molecule 1: Thioredoxin reductase



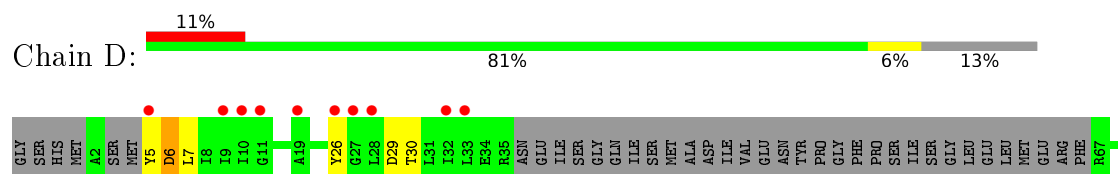
#### • Molecule 1: Thioredoxin reductase

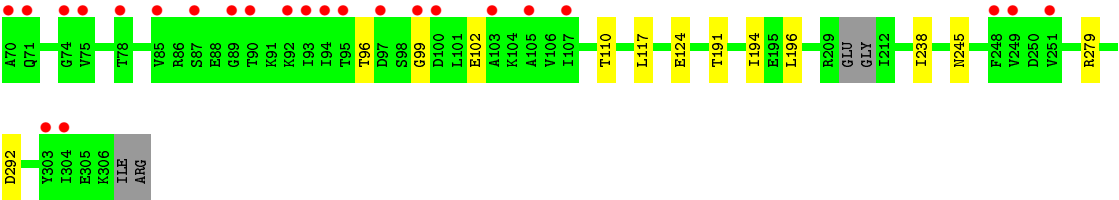


#### • Molecule 1: Thioredoxin reductase



#### • Molecule 1: Thioredoxin reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.14Å 182.50Å 152.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.89 – 2.60 46.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.89-2.60) 100.0 (46.89-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.217 , 0.241 0.222 , 0.242	Depositor DCC
$R_{free}$ test set	2410 reflections (4.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

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	0.24	0/2132	0.45	0/2899
1	B	0.23	0/2063	0.43	0/2813
1	C	0.24	0/1996	0.43	0/2728
1	D	0.24	0/1882	0.46	0/2564
All	All	0.24	0/8073	0.45	0/11004

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	2101	2036	2030	31	0
1	B	2032	1950	1947	18	0
1	C	1966	1838	1836	11	0
1	D	1855	1639	1635	24	0
2	A	22	0	0	0	0
2	B	23	0	0	2	0
2	C	9	0	0	0	0
2	D	14	0	0	2	0
All	All	8022	7463	7448	73	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 (73) 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:D:96:THR:HG22	1:D:99:GLY:O	1.35	1.22
1:D:96:THR:HG23	1:D:99:GLY:H	1.27	0.99
1:C:279:ARG:NH1	1:C:292:ASP:OD2	1.96	0.98
1:A:282:PRO:HG3	1:B:252:GLU:OE1	1.66	0.94
1:D:6:ASP:HB2	1:D:29:ASP:O	1.75	0.85
1:D:96:THR:CG2	1:D:99:GLY:O	2.21	0.85
1:D:5:TYR:HB2	1:D:102:GLU:O	1.78	0.83
1:A:206:VAL:CG1	1:A:217:LYS:HB2	2.09	0.83
1:A:191:THR:HG21	1:A:194:ILE:HD12	1.61	0.81
1:D:6:ASP:CB	1:D:29:ASP:O	2.29	0.80
1:B:95:THR:HG22	1:B:100:ASP:OD1	1.84	0.78
1:A:68:THR:O	1:A:72:GLU:HG3	1.84	0.77
1:A:282:PRO:O	1:A:284:TRP:CZ3	2.39	0.76
1:A:282:PRO:CG	1:B:252:GLU:OE1	2.36	0.74
1:A:281:THR:O	1:A:284:TRP:HZ3	1.71	0.72
1:B:146:VAL:CG1	1:B:169:VAL:HG22	2.23	0.68
1:A:204:GLU:OE1	1:B:226:ARG:NH1	2.28	0.67
1:A:283:ILE:HG22	1:A:285:GLN:H	1.61	0.66
1:A:298:THR:HG21	1:C:161:PHE:CE1	2.31	0.65
1:A:64:GLU:O	1:A:68:THR:HG23	1.95	0.65
1:D:96:THR:CG2	1:D:99:GLY:H	2.06	0.63
1:B:175:ARG:NH1	2:B:401:HOH:O	2.33	0.61
1:A:187:ARG:NH1	1:C:263:ARG:HE	1.98	0.60
1:D:6:ASP:HB2	1:D:29:ASP:CA	2.32	0.60
1:D:6:ASP:HB2	1:D:29:ASP:N	2.16	0.60
1:A:191:THR:HG21	1:A:194:ILE:CD1	2.31	0.59
1:A:187:ARG:HH12	1:C:263:ARG:HE	1.51	0.58
1:A:281:THR:O	1:A:284:TRP:CZ3	2.56	0.57
1:A:284:TRP:N	1:A:284:TRP:CE3	2.73	0.56
1:A:206:VAL:HG12	1:A:217:LYS:HB2	1.86	0.56
1:A:282:PRO:C	1:A:284:TRP:CZ3	2.79	0.56
1:B:139:PRO:HA	1:D:26:TYR:HE1	1.71	0.55
1:D:279:ARG:NH1	1:D:292:ASP:OD2	2.39	0.55
1:D:124:GLU:N	1:D:124:GLU:OE1	2.40	0.54
1:B:263:ARG:NH2	2:B:403:HOH:O	2.41	0.54
1:C:124:GLU:N	1:C:124:GLU:OE1	2.39	0.54
1:D:124:GLU:OE2	2:D:401:HOH:O	2.18	0.53
1:A:283:ILE:C	1:A:284:TRP:CE3	2.82	0.53
1:A:124:GLU:N	1:A:124:GLU:OE1	2.41	0.53
1:D:6:ASP:HB2	1:D:29:ASP:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:OE1	1:B:124:GLU:N	2.42	0.52
1:D:6:ASP:HB2	1:D:29:ASP:CB	2.40	0.51
1:D:110:THR:HB	1:D:245:ASN:HB2	1.92	0.51
1:A:284:TRP:N	1:A:284:TRP:CD2	2.79	0.51
1:C:64:GLU:HG2	1:C:65:ARG:H	1.76	0.51
1:B:282:PRO:O	1:B:284:TRP:N	2.43	0.51
1:A:282:PRO:O	1:A:284:TRP:CH2	2.64	0.50
1:B:187:ARG:O	1:B:191:THR:OG1	2.29	0.50
1:A:261:THR:OG1	1:A:279:ARG:HD2	2.13	0.49
1:D:6:ASP:CB	1:D:29:ASP:N	2.76	0.49
1:B:64:GLU:O	1:B:68:THR:HG23	2.13	0.49
1:D:124:GLU:CD	2:D:401:HOH:O	2.51	0.49
1:B:70:ALA:HB1	1:B:75:VAL:HG21	1.94	0.48
1:C:156:VAL:HG13	1:C:188:VAL:HG21	1.95	0.48
1:A:190:GLY:HA2	1:A:191:THR:C	2.34	0.48
1:B:139:PRO:HA	1:D:26:TYR:CE1	2.49	0.47
1:D:6:ASP:CB	1:D:29:ASP:H	2.28	0.47
1:A:80:THR:OG1	1:A:81:GLU:N	2.48	0.47
1:D:117:LEU:HD11	1:D:238:ILE:HG12	1.96	0.46
1:C:191:THR:HG22	1:C:193:ASN:OD1	2.15	0.45
1:B:254:ASP:OD1	1:B:258:PHE:N	2.46	0.45
1:C:142:ARG:HA	1:C:165:VAL:HG22	1.99	0.45
1:D:6:ASP:HB2	1:D:29:ASP:H	1.83	0.44
1:A:70:ALA:HB1	1:A:75:VAL:CG2	2.48	0.43
1:B:246:THR:O	1:B:253:LYS:NZ	2.47	0.43
1:D:7:LEU:O	1:D:30:THR:HA	2.19	0.43
1:D:191:THR:OG1	1:D:194:ILE:HD12	2.18	0.43
1:A:70:ALA:HB1	1:A:75:VAL:HG21	2.01	0.42
1:A:161:PHE:CE1	1:C:298:THR:HG21	2.54	0.42
1:A:282:PRO:HB3	1:B:252:GLU:HG3	2.02	0.41
1:A:285:GLN:O	1:A:288:THR:OG1	2.36	0.41
1:B:75:VAL:HG23	1:B:75:VAL:O	2.20	0.41
1:A:161:PHE:CZ	1:C:298:THR:HG21	2.55	0.41

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	283/311 (91%)	267 (94%)	16 (6%)	0	100	100
1	B	275/311 (88%)	264 (96%)	11 (4%)	0	100	100
1	C	273/311 (88%)	258 (94%)	15 (6%)	0	100	100
1	D	263/311 (85%)	253 (96%)	10 (4%)	0	100	100
All	All	1094/1244 (88%)	1042 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	209/255 (82%)	197 (94%)	12 (6%)	25	49
1	B	200/255 (78%)	199 (100%)	1 (0%)	92	98
1	C	182/255 (71%)	174 (96%)	8 (4%)	35	63
1	D	152/255 (60%)	150 (99%)	2 (1%)	76	91
All	All	743/1020 (73%)	720 (97%)	23 (3%)	47	76

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	63	MET
1	A	80	THR
1	A	95	THR
1	A	113	ASN
1	A	116	HIS
1	A	146	VAL
1	A	177	HIS
1	A	189	ASP
1	A	284	TRP
1	B	66	PHE
1	C	36	ASN
1	C	66	PHE
1	C	95	THR
1	C	126	ILE
1	C	146	VAL
1	C	229	ARG
1	C	233	THR
1	C	298	THR
1	D	6	ASP
1	D	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	113	ASN
1	D	245	ASN

### 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 [i](#)

There are no ligands in this entry.

## 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	287/311 (92%)	0.57	6 (2%) 67 61	41, 59, 106, 132	0
1	B	279/311 (89%)	0.43	7 (2%) 61 54	45, 63, 96, 122	0
1	C	279/311 (89%)	0.49	16 (5%) 27 20	54, 72, 105, 127	0
1	D	270/311 (86%)	0.77	34 (12%) 5 3	44, 76, 111, 136	0
All	All	1115/1244 (89%)	0.56	63 (5%) 27 20	41, 66, 106, 136	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	TYR	4.8
1	D	103	ALA	4.5
1	D	10	ILE	4.4
1	C	37	GLU	4.4
1	D	32	ILE	4.4
1	C	77	THR	4.3
1	D	78	THR	4.2
1	D	33	LEU	4.1
1	D	100	ASP	4.0
1	D	9	ILE	4.0
1	D	248	PHE	3.5
1	C	70	ALA	3.5
1	C	211	GLY	3.4
1	C	94	ILE	3.4
1	D	99	GLY	3.4
1	D	105	ALA	3.3
1	D	93	ILE	3.3
1	D	90	THR	3.2
1	C	31	LEU	3.1
1	D	19	ALA	3.0
1	D	70	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	249	VAL	2.9
1	C	212	ILE	2.9
1	C	32	ILE	2.9
1	D	107	ILE	2.9
1	A	284	TRP	2.9
1	C	101	LEU	2.9
1	D	85	VAL	2.9
1	D	304	ILE	2.9
1	D	75	VAL	2.8
1	D	87	SER	2.7
1	D	94	ILE	2.6
1	D	28	LEU	2.6
1	D	74	GLY	2.6
1	A	63	MET	2.5
1	C	82	VAL	2.5
1	B	283	ILE	2.4
1	B	307	ILE	2.4
1	D	92	LYS	2.4
1	C	75	VAL	2.4
1	A	8	ILE	2.3
1	A	69	HIS	2.3
1	D	303	TYR	2.3
1	B	256	GLY	2.2
1	C	8	ILE	2.2
1	C	79	ILE	2.2
1	B	242	ILE	2.2
1	A	242	ILE	2.2
1	C	17	LEU	2.1
1	D	11	GLY	2.1
1	D	89	GLY	2.1
1	C	218	ILE	2.1
1	D	251	VAL	2.1
1	B	78	THR	2.1
1	D	97	ASP	2.1
1	C	93	ILE	2.1
1	D	71	GLN	2.1
1	D	27	GLY	2.1
1	A	244	PRO	2.0
1	D	26	TYR	2.0
1	D	95	THR	2.0
1	B	80	THR	2.0
1	B	31	LEU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.