



# Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 04:22 AM EDT

PDB ID : 4ZPX  
Title : Crystal structure of Lon ATPase domain from Thermococcus onnurineus NA1  
Authors : An, Y.J.; Kim, M.I.; Na, J.H.; Cha, S.S.  
Deposited on : 2015-05-08  
Resolution : 2.03 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
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-20027457

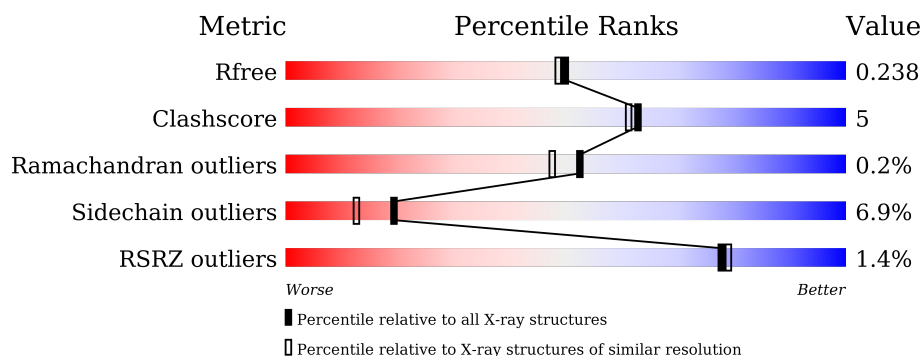
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	413	<div> <div></div> <div>64%</div> <div>14%</div> <div>•</div> <div>21%</div> </div>
1	B	413	<div> <div></div> <div>69%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>

## 2 Entry composition [i](#)

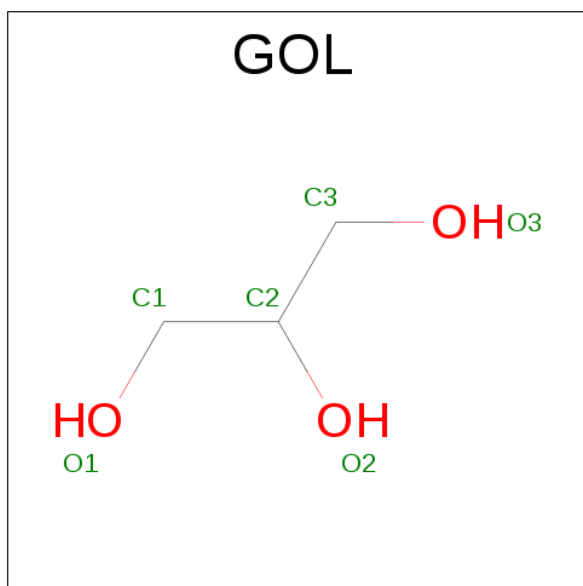
There are 3 unique types of molecules in this entry. The entry contains 5207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent protease Lon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2446	1541	441	452	12			
1	B	333	Total	C	N	O	S	0	0	0
			2512	1580	451	467	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		

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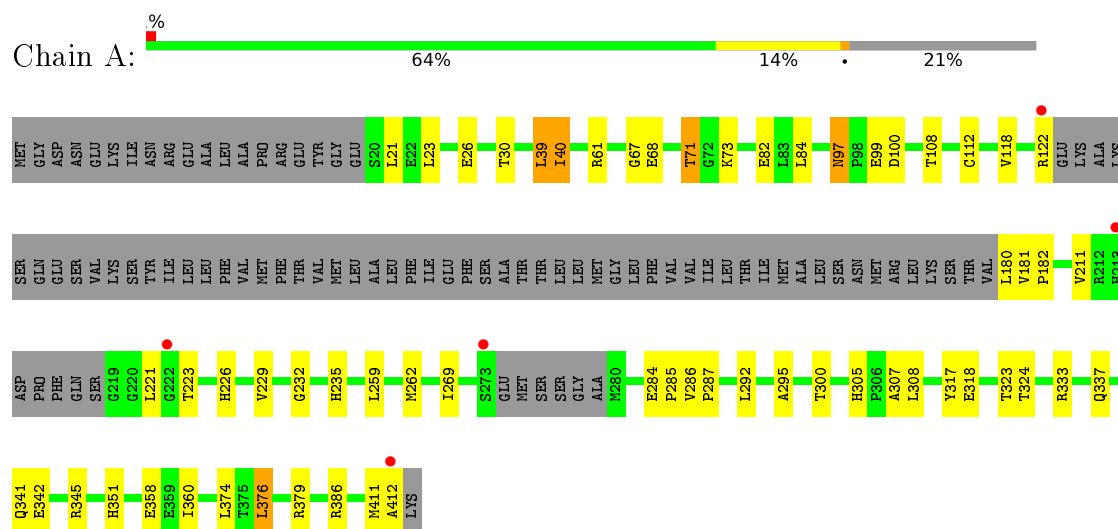
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	121	Total	O	0	0
			121	121		

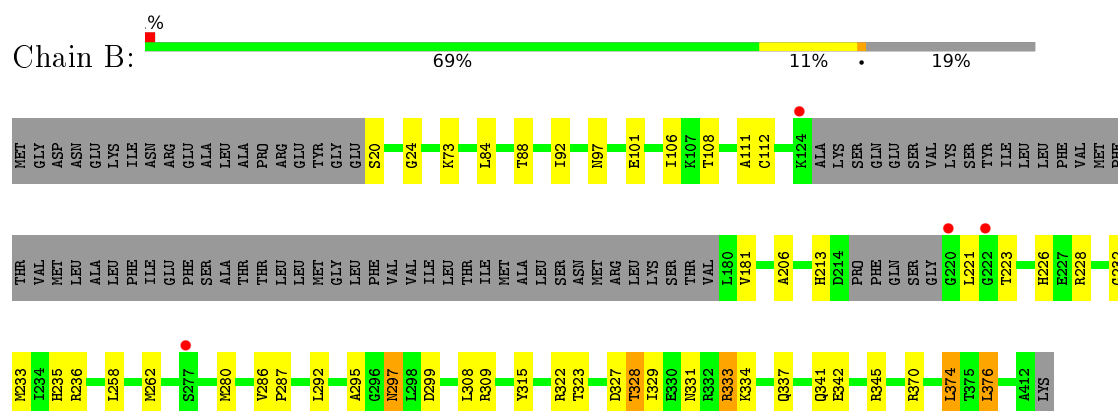
### 3 Residue-property plots [i](#)

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: ATP-dependent protease Lon



#### • Molecule 1: ATP-dependent protease Lon



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.62Å 61.60Å 76.32Å 74.61° 87.11° 83.45°	Depositor
Resolution (Å)	41.14 – 2.03 41.10 – 2.03	Depositor EDS
% Data completeness (in resolution range)	92.9 (41.14-2.03) 85.4 (41.10-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.182 , 0.239 0.189 , 0.238	Depositor DCC
$R_{free}$ test set	2130 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.4	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	0.95	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.93	1/2481 (0.0%)	0.95	1/3357 (0.0%)
1	B	0.84	0/2548	0.90	4/3445 (0.1%)
All	All	0.88	1/5029 (0.0%)	0.93	5/6802 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	TYR	CE1-CZ	-5.62	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	322	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	309	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	376	LEU	CB-CG-CD1	5.15	119.76	111.00
1	B	236	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2446	0	2458	28	0
1	B	2512	0	2527	25	0
2	A	6	0	8	0	0
3	A	122	0	0	3	0
3	B	121	0	0	2	0
All	All	5207	0	4993	53	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 (53) 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:232:GLY:H	1:A:235:HIS:HD2	1.26	0.84
1:B:232:GLY:H	1:B:235:HIS:HD2	1.25	0.81
1:B:297:ASN:C	1:B:297:ASN:HD22	1.95	0.69
1:B:342:GLU:OE2	1:B:345:ARG:NH1	2.26	0.68
1:A:232:GLY:H	1:A:235:HIS:CD2	2.11	0.65
1:B:323:THR:HG22	3:B:558:HOH:O	1.96	0.65
1:A:232:GLY:N	1:A:235:HIS:HD2	1.95	0.61
1:A:108:THR:HG21	1:A:287:PRO:HG2	1.82	0.60
1:B:106:ILE:HG13	1:B:286:VAL:HG22	1.84	0.59
1:B:333:ARG:O	1:B:333:ARG:HD3	2.03	0.58
1:A:40:ILE:HG13	3:A:692:HOH:O	2.03	0.57
1:A:379:ARG:HD3	3:A:613:HOH:O	2.04	0.57
1:A:411:MET:O	1:A:412:ALA:HB2	2.06	0.55
1:B:327:ASP:HA	1:B:374:LEU:HD22	1.88	0.55
1:A:305:HIS:HD2	1:A:307:ALA:H	1.54	0.55
1:A:342:GLU:OE2	1:A:345:ARG:NH1	2.41	0.54
1:B:331:ASN:OD1	1:B:334:LYS:HE2	2.09	0.52
1:B:337:GLN:OE1	1:B:341:GLN:NE2	2.42	0.52
1:A:337:GLN:OE1	1:A:341:GLN:NE2	2.42	0.52
1:A:118:VAL:O	1:A:122:ARG:HB2	2.11	0.51
1:A:284:GLU:HB2	1:A:285:PRO:CD	2.41	0.51
1:B:73:LYS:HD2	1:B:295:ALA:HB1	1.92	0.50
1:A:229:VAL:HG13	1:A:269:ILE:HG21	1.94	0.50
1:A:97:ASN:HB3	1:A:100:ASP:O	2.12	0.49
1:B:232:GLY:H	1:B:235:HIS:CD2	2.16	0.49
1:A:386:ARG:HD3	3:A:646:HOH:O	2.12	0.48
1:B:92:ILE:HG12	1:B:108:THR:HG22	1.96	0.48
1:A:39:LEU:HB2	1:A:82:GLU:OE2	2.14	0.47
1:B:262:MET:HE2	1:B:292:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HB2	1:A:285:PRO:HD2	1.96	0.47
1:A:68:GLU:O	1:A:71:THR:HB	2.15	0.46
1:B:232:GLY:N	1:B:235:HIS:HD2	2.05	0.45
1:B:315:TYR:CD1	1:B:315:TYR:N	2.85	0.44
1:B:299:ASP:N	3:B:506:HOH:O	2.48	0.44
1:A:181:VAL:O	1:A:226:HIS:HE1	2.01	0.44
1:A:262:MET:HE2	1:A:292:LEU:HD22	2.00	0.43
1:A:181:VAL:HG22	1:A:182:PRO:O	2.18	0.43
1:A:73:LYS:HD3	1:A:295:ALA:HB1	2.00	0.43
1:B:108:THR:HG21	1:B:287:PRO:HG2	2.00	0.43
1:B:223:THR:HB	1:B:228:ARG:HD2	1.99	0.43
1:A:235:HIS:CE1	1:A:286:VAL:HB	2.54	0.42
1:B:213:HIS:HA	1:B:228:ARG:HH21	1.84	0.42
1:A:67:GLY:O	1:A:73:LYS:HE2	2.19	0.42
1:B:297:ASN:ND2	1:B:297:ASN:C	2.66	0.42
1:B:328:THR:HG23	1:B:331:ASN:H	1.83	0.42
1:A:30:THR:OG1	1:A:351:HIS:HD2	2.02	0.42
1:B:181:VAL:O	1:B:226:HIS:HE1	2.04	0.41
1:B:111:ALA:O	1:B:112:CYS:HB2	2.19	0.41
1:B:206:ALA:O	1:B:233:MET:HG2	2.19	0.41
1:B:24:GLY:HA3	1:B:329:ILE:HG23	2.02	0.41
1:A:360:ILE:HD13	1:A:360:ILE:HA	1.93	0.41
1:A:324:THR:C	1:A:376:LEU:HD22	2.40	0.41
1:A:21:LEU:HB2	1:A:358:GLU:HG2	2.02	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	317/413 (77%)	306 (96%)	10 (3%)	1 (0%)	46 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	327/413 (79%)	319 (98%)	8 (2%)	0	100	100
All	All	644/826 (78%)	625 (97%)	18 (3%)	1 (0%)	52	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	CYS

### 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	251/348 (72%)	231 (92%)	20 (8%)	15	9
1	B	259/348 (74%)	244 (94%)	15 (6%)	25	18
All	All	510/696 (73%)	475 (93%)	35 (7%)	19	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	GLU
1	A	39	LEU
1	A	40	ILE
1	A	71	THR
1	A	84	LEU
1	A	97	ASN
1	A	99	GLU
1	A	180	LEU
1	A	211	VAL
1	A	221	LEU
1	A	223	THR
1	A	259	LEU
1	A	300	THR
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	318	GLU
1	A	323	THR
1	A	333	ARG
1	A	374	LEU
1	A	376	LEU
1	B	20	SER
1	B	84	LEU
1	B	88	THR
1	B	97	ASN
1	B	101	GLU
1	B	221	LEU
1	B	258	LEU
1	B	280	MET
1	B	297	ASN
1	B	308	LEU
1	B	328	THR
1	B	333	ARG
1	B	370	ARG
1	B	374	LEU
1	B	376	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	59	GLN
1	A	97	ASN
1	A	226	HIS
1	A	235	HIS
1	A	263	GLN
1	A	297	ASN
1	A	305	HIS
1	A	337	GLN
1	A	341	GLN
1	A	351	HIS
1	A	365	GLN
1	B	59	GLN
1	B	97	ASN
1	B	226	HIS
1	B	235	HIS
1	B	256	GLN
1	B	263	GLN

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Mol	Chain	Res	Type
1	B	297	ASN
1	B	305	HIS
1	B	337	GLN
1	B	341	GLN
1	B	351	HIS
1	B	373	HIS

### 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 ⓘ

1 ligand is 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	GOL	A	501	-	5,5,5	0.30	0	5,5,5	0.72	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
2	GOL	A	501	-	-	0/4/4/4	0/0/0/0

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.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	325/413 (78%)	-0.27	5 (1%) 76 77	15, 29, 59, 93	0
1	B	333/413 (80%)	-0.32	4 (1%) 81 82	17, 33, 63, 82	0
All	All	658/826 (79%)	-0.30	9 (1%) 78 79	15, 31, 61, 93	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	SER	6.0
1	A	222	GLY	3.7
1	B	222	GLY	3.2
1	A	412	ALA	2.5
1	A	213	HIS	2.4
1	A	122	ARG	2.4
1	B	220	GLY	2.2
1	B	277	SER	2.1
1	B	124	LYS	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 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	501	6/6	0.90	0.11	1.16	32,44,50,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.