



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:42 pm GMT

PDB ID : 3A8R  
Title : The structure of the N-terminal regulatory domain of a plant NADPH oxidase  
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Deposited on : 2009-10-07  
Resolution : 2.40 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

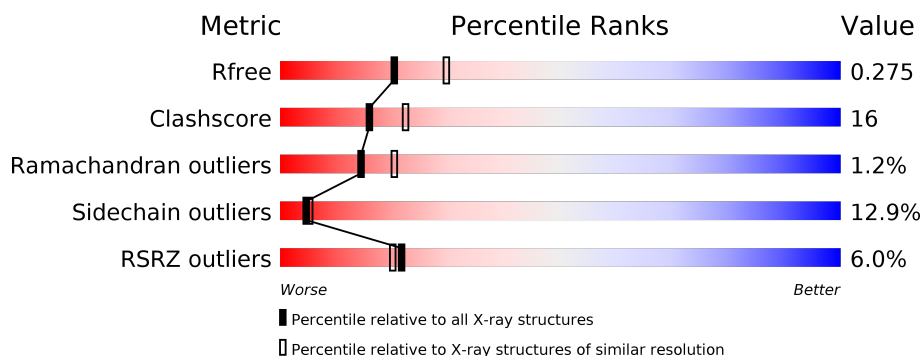
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	179	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	179	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>• • 7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2698 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1305	822	221	256	6			
1	B	167	Total	C	N	O	S	0	0	0
			1314	827	223	258	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ALA	-	EXPRESSION TAG	UNP Q5ZAJ0
A	136	MET	-	EXPRESSION TAG	UNP Q5ZAJ0
A	137	GLY	-	EXPRESSION TAG	UNP Q5ZAJ0
B	135	ALA	-	EXPRESSION TAG	UNP Q5ZAJ0
B	136	MET	-	EXPRESSION TAG	UNP Q5ZAJ0
B	137	GLY	-	EXPRESSION TAG	UNP Q5ZAJ0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

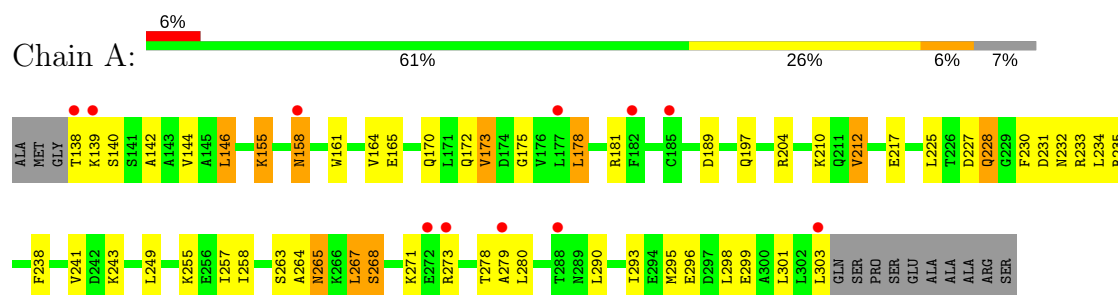
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	39	Total	O	0	0
			39	39		

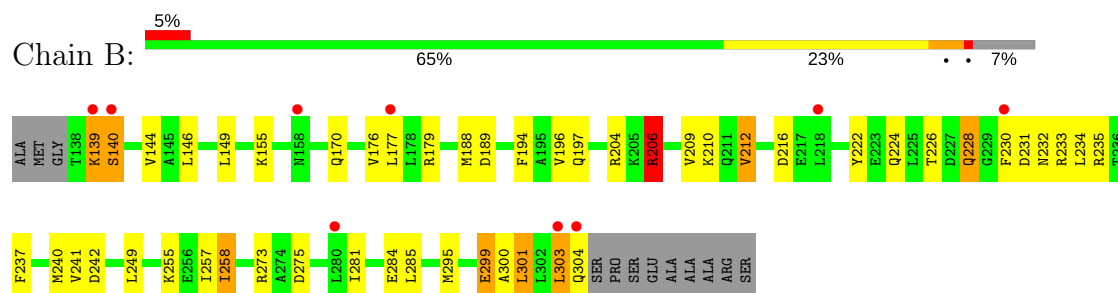
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Putative uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.42Å 72.16Å 118.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.47 – 2.40 19.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.47-2.40) 97.9 (19.47-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.10 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.6.0041	Depositor
R, $R_{free}$	0.234 , 0.266 0.238 , 0.275	Depositor DCC
$R_{free}$ test set	1047 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.75	0/1319	0.79	3/1769 (0.2%)
1	B	0.80	0/1328	0.86	4/1781 (0.2%)
All	All	0.78	0/2647	0.83	7/3550 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	273	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	206	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	204	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	181	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	204	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	216	ASP	CB-CG-OD2	5.12	122.91	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	1305	0	1314	46	0
1	B	1314	0	1322	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	38	0	0	1	0
3	B	39	0	0	1	0
All	All	2698	0	2636	82	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 16.

All (82) 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:267:LEU:HD11	1:A:271:LYS:NZ	1.88	0.88
1:A:228:GLN:HE21	1:A:233:ARG:HD3	1.51	0.76
1:B:284:GLU:HG2	1:B:285:LEU:HD12	1.68	0.75
1:B:228:GLN:HE21	1:B:228:GLN:HA	1.51	0.74
1:B:303:LEU:HD12	1:B:303:LEU:O	1.88	0.74
1:A:197:GLN:HE21	1:A:243:LYS:NZ	1.86	0.73
1:B:140:SER:O	1:B:144:VAL:HG23	1.90	0.71
1:A:234:LEU:HG	1:B:295:MET:HE1	1.73	0.69
1:A:267:LEU:HD11	1:A:271:LYS:HZ1	1.56	0.68
1:A:267:LEU:HD11	1:A:271:LYS:HZ2	1.59	0.68
1:A:172:GLN:NE2	1:A:175:GLY:H	1.92	0.68
1:A:172:GLN:HE21	1:A:175:GLY:H	1.42	0.67
1:A:255:LYS:NZ	1:B:275:ASP:OD1	2.27	0.66
1:A:142:ALA:HB2	1:B:301:LEU:HD22	1.76	0.66
1:A:158:ASN:O	1:A:158:ASN:ND2	2.25	0.64
1:A:241:VAL:HG22	1:A:257:ILE:HG12	1.79	0.63
1:B:285:LEU:HD11	1:B:301:LEU:HG	1.80	0.63
1:B:188:MET:CE	1:B:194:PHE:HE2	2.11	0.63
1:B:179:ARG:CZ	1:B:196:VAL:HG13	2.29	0.63
1:B:257:ILE:HD12	1:B:258:ILE:N	2.13	0.63
1:A:228:GLN:NE2	1:A:233:ARG:HD3	2.14	0.61
1:A:197:GLN:HE21	1:A:243:LYS:HZ2	1.47	0.61
1:B:235:ARG:HD3	3:B:49:HOH:O	1.99	0.61
1:B:206:ARG:HH22	1:B:224:GLN:NE2	1.99	0.60
1:B:242:ASP:HB2	1:B:249:LEU:HD21	1.82	0.60
1:B:139:LYS:HG3	1:B:140:SER:N	2.17	0.58
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.16	0.58
1:B:188:MET:CE	1:B:194:PHE:CE2	2.87	0.58
1:B:179:ARG:NH2	1:B:196:VAL:CG1	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:HE21	1:B:233:ARG:HD3	1.69	0.58
1:B:179:ARG:CZ	1:B:196:VAL:CG1	2.83	0.56
1:B:231:ASP:O	1:B:235:ARG:HG3	2.05	0.56
1:A:140:SER:O	1:A:144:VAL:HG23	2.06	0.56
1:A:295:MET:HE1	1:B:235:ARG:HA	1.88	0.56
1:A:267:LEU:HG	1:A:268:SER:N	2.21	0.55
1:A:138:THR:O	1:A:142:ALA:N	2.27	0.55
1:B:300:ALA:HA	1:B:304:GLN:OE1	2.07	0.54
1:B:197:GLN:HG2	1:B:240:MET:SD	2.48	0.54
1:A:257:ILE:HG23	3:A:15:HOH:O	2.08	0.53
1:B:237:PHE:O	1:B:241:VAL:HG23	2.08	0.53
1:A:161:TRP:CE3	1:A:164:VAL:CG2	2.92	0.53
1:A:257:ILE:HD12	1:A:258:ILE:N	2.24	0.52
1:A:265:ASN:OD1	1:A:265:ASN:N	2.42	0.52
1:B:176:VAL:HG13	1:B:212:VAL:HG22	1.92	0.52
1:B:144:VAL:CG1	1:B:258:ILE:HD13	2.41	0.50
1:A:197:GLN:NE2	1:A:243:LYS:NZ	2.59	0.50
1:A:267:LEU:CD1	1:A:271:LYS:NZ	2.68	0.49
1:A:296:GLU:HA	1:A:299:GLU:HB2	1.94	0.49
1:A:228:GLN:O	1:A:233:ARG:NH1	2.46	0.49
1:B:222:TYR:CZ	1:B:226:THR:HG21	2.48	0.49
1:B:232:ASN:HA	1:B:235:ARG:NH1	2.28	0.49
1:A:278:THR:C	1:A:280:LEU:H	2.17	0.49
1:B:242:ASP:HB2	1:B:249:LEU:CD2	2.43	0.48
1:A:241:VAL:CG2	1:A:257:ILE:HG12	2.41	0.48
1:B:300:ALA:O	1:B:304:GLN:OE1	2.30	0.48
1:B:301:LEU:O	1:B:301:LEU:HD22	2.13	0.48
1:A:197:GLN:HE21	1:A:243:LYS:HZ1	1.63	0.46
1:A:230:PHE:O	1:A:231:ASP:C	2.54	0.46
1:A:146:LEU:HD22	1:A:146:LEU:O	2.17	0.45
1:B:176:VAL:CG1	1:B:212:VAL:HG22	2.47	0.45
1:A:172:GLN:NE2	1:A:173:VAL:CA	2.80	0.45
1:A:293:ILE:HG21	1:A:293:ILE:HD13	1.74	0.44
1:B:230:PHE:CE2	1:B:234:LEU:HD12	2.53	0.44
1:A:172:GLN:NE2	1:A:173:VAL:HA	2.34	0.43
1:A:238:PHE:CZ	1:A:249:LEU:HD13	2.54	0.43
1:A:298:LEU:HB3	1:B:234:LEU:HD21	1.99	0.43
1:B:299:GLU:O	1:B:300:ALA:C	2.57	0.43
1:A:234:LEU:HG	1:B:295:MET:CE	2.45	0.43
1:B:295:MET:HA	1:B:295:MET:HE3	2.01	0.43
1:A:155:LYS:HD2	1:A:155:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ALA:HB2	1:B:301:LEU:CD2	2.46	0.42
1:A:263:SER:O	1:A:264:ALA:C	2.58	0.42
1:B:144:VAL:CG1	1:B:258:ILE:CD1	2.98	0.42
1:B:257:ILE:C	1:B:257:ILE:HD12	2.40	0.42
1:A:178:LEU:HD12	1:A:212:VAL:HG23	2.02	0.42
1:B:228:GLN:NE2	1:B:233:ARG:HD3	2.33	0.41
1:A:280:LEU:O	1:A:280:LEU:HD13	2.20	0.41
1:A:227:ASP:HB3	1:A:232:ASN:ND2	2.35	0.41
1:A:172:GLN:HE21	1:A:173:VAL:C	2.25	0.41
1:A:295:MET:CE	1:B:235:ARG:HA	2.50	0.41
1:B:284:GLU:HG2	1:B:285:LEU:CD1	2.43	0.40
1:A:210:LYS:NZ	1:A:217:GLU:OE2	2.52	0.40

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	164/179 (92%)	155 (94%)	7 (4%)	2 (1%)	14	20
1	B	165/179 (92%)	157 (95%)	6 (4%)	2 (1%)	14	20
All	All	329/358 (92%)	312 (95%)	13 (4%)	4 (1%)	14	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	B	303	LEU
1	A	279	ALA
1	B	299	GLU

### 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	139/147 (95%)	120 (86%)	19 (14%)	4	4
1	B	140/147 (95%)	123 (88%)	17 (12%)	5	7
All	All	279/294 (95%)	243 (87%)	36 (13%)	5	5

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	155	LYS
1	A	158	ASN
1	A	165	GLU
1	A	170	GLN
1	A	173	VAL
1	A	178	LEU
1	A	189	ASP
1	A	212	VAL
1	A	225	LEU
1	A	228	GLN
1	A	235	ARG
1	A	265	ASN
1	A	267	LEU
1	A	268	SER
1	A	273	ARG
1	A	290	LEU
1	A	301	LEU
1	A	303	LEU
1	B	139	LYS
1	B	140	SER
1	B	146	LEU
1	B	149	LEU
1	B	155	LYS
1	B	170	GLN
1	B	177	LEU
1	B	189	ASP

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Mol	Chain	Res	Type
1	B	206	ARG
1	B	209	VAL
1	B	210	LYS
1	B	212	VAL
1	B	228	GLN
1	B	255	LYS
1	B	258	ILE
1	B	281	ILE
1	B	301	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	170	GLN
1	A	172	GLN
1	A	197	GLN
1	A	211	GLN
1	A	228	GLN
1	A	289	ASN
1	B	170	GLN
1	B	197	GLN
1	B	211	GLN
1	B	224	GLN
1	B	228	GLN
1	B	289	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	166/179 (92%)	0.26	11 (6%) 18 16	42, 54, 76, 86	0
1	B	167/179 (93%)	0.16	9 (5%) 26 24	37, 51, 68, 82	0
All	All	333/358 (93%)	0.21	20 (6%) 22 20	37, 53, 75, 86	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	GLN	4.5
1	A	139	LYS	4.4
1	A	138	THR	4.0
1	B	303	LEU	3.8
1	B	139	LYS	3.2
1	A	288	THR	2.8
1	A	185	CYS	2.8
1	A	177	LEU	2.8
1	A	182	PHE	2.7
1	B	280	LEU	2.6
1	B	140	SER	2.6
1	A	273	ARG	2.6
1	B	218	LEU	2.4
1	A	279	ALA	2.4
1	A	272	GLU	2.3
1	A	158	ASN	2.3
1	B	230	PHE	2.2
1	B	177	LEU	2.1
1	B	158	ASN	2.1
1	A	303	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](#)

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	CA	B	402	1/1	0.95	0.11	53,53,53,53	0
2	CA	A	401	1/1	0.98	0.02	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.