



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:29 AM GMT

PDB ID : 3A8R  
Title : The structure of the N-terminal regulatory domain of a plant NADPH oxidase  
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Wong, H.L.; Kawasaki, T.; Shimamoto, K.; Sato, M.; Shimizu, T.  
Deposited on : 2009-10-07  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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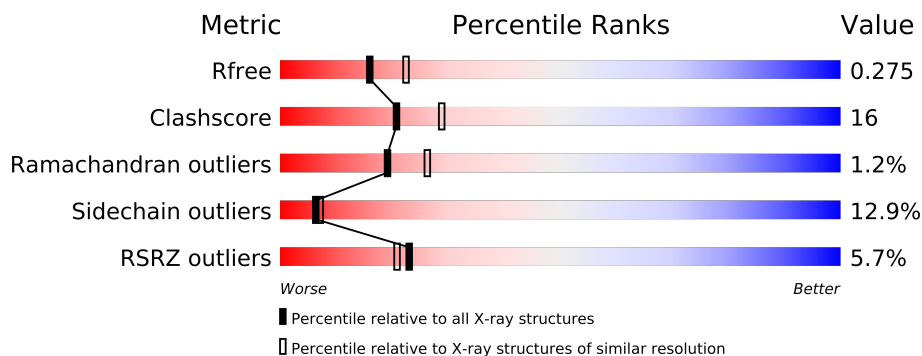
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	179	
1	B	179	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2698 atoms, of which 0 are hydrogen and 0 are deuterium.

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		

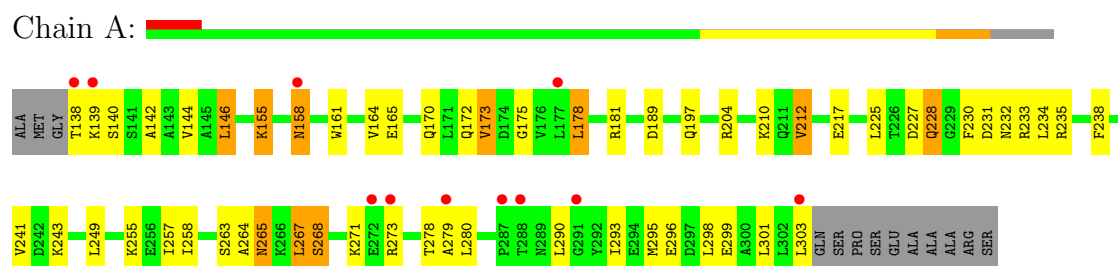
- Molecule 3 is water.

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

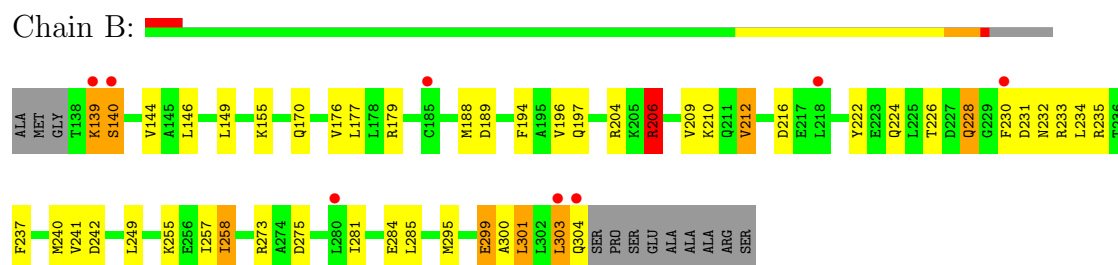
### 3 Residue-property plots

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: 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 0.241 , 0.275	Depositor DCC
$R_{free}$ test set	1047 reflections (5.39%)	DCC
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> )	0.35 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 20484 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	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.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HA	1:B:228:GLN:NE2	2.16	0.58
1:B:188:MET:CE	1:B:194:PHE:CE2	2.87	0.58
1:B:228:GLN:HE21	1:B:233:ARG:HD3	1.69	0.58
1:B:179:ARG:NH2	1:B:196:VAL:CG1	2.67	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:295:MET:HE1	1:B:235:ARG:HA	1.88	0.56
1:A:140:SER:O	1:A:144:VAL:HG23	2.06	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:232:ASN:HA	1:B:235:ARG:NH1	2.28	0.49
1:B:222:TYR:CZ	1:B:226:THR:HG21	2.48	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:B:301:LEU:O	1:B:301:LEU:HD22	2.13	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: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:B:176:VAL:CG1	1:B:212:VAL:HG22	2.47	0.45
1:A:146:LEU:HD22	1:A:146:LEU:O	2.17	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:227:ASP:HB3	1:A:232:ASN:ND2	2.35	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%)	19	26
1	B	165/179 (92%)	157 (95%)	6 (4%)	2 (1%)	19	26
All	All	329/358 (92%)	312 (95%)	13 (4%)	4 (1%)	19	26

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%)	5	6
1	B	140/147 (95%)	123 (88%)	17 (12%)	7	9
All	All	279/294 (95%)	243 (87%)	36 (13%)	6	7

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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

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.

## 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%)	0.35	11 (6%) 18 16	42, 54, 76, 86	0
1	B	167/179 (93%)	0.26	8 (4%) 29 27	37, 51, 68, 82	0
All	All	333/358 (93%)	0.31	19 (5%) 23 21	37, 53, 75, 86	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	5.2
1	B	304	GLN	4.7
1	B	303	LEU	4.0
1	A	138	THR	4.0
1	B	139	LYS	3.7
1	A	279	ALA	3.6
1	B	280	LEU	3.3
1	A	303	LEU	3.1
1	A	288	THR	3.0
1	A	273	ARG	3.0
1	B	140	SER	2.7
1	A	158	ASN	2.6
1	A	272	GLU	2.5
1	A	291	GLY	2.4
1	A	177	LEU	2.4
1	B	185	CYS	2.3
1	B	230	PHE	2.3
1	A	287	PRO	2.2
1	B	218	LEU	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	401	1/1	0.12	-0.76	42,42,42,42	0
2	CA	B	402	1/1	0.04	-3.48	53,53,53,53	0

### 6.5 Other polymers

There are no such residues in this entry.