



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

PDB ID : 3AYG  
Title : Crystal structure of nitric oxide reductase complex with HQNO  
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Deposited on : 2011-05-06  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

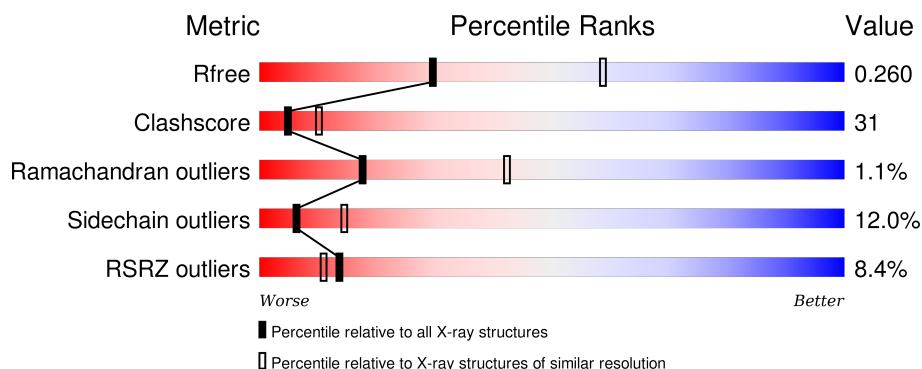
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	800	<div> <div>8%</div> <div>50%</div> <div>36%</div> <div>8%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BOG	A	805	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BOG	A	806	-	-	-	X
5	BOG	A	807	-	-	-	X
6	LOP	A	809	-	-	-	X
6	LOP	A	810	-	-	-	X
7	HQO	A	811	-	-	X	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6448 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.

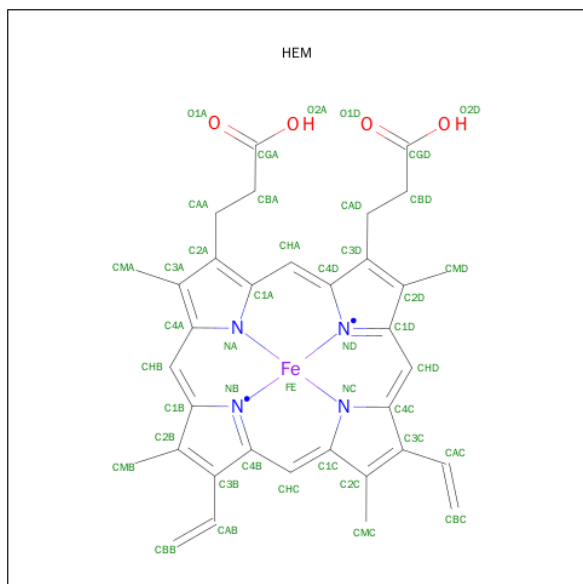
- Molecule 1 is a protein called Nitric oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	754	6078	4055	966	1034	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	793	LEU	-	EXPRESSION TAG	UNP B3Y963
A	794	GLU	-	EXPRESSION TAG	UNP B3Y963
A	795	HIS	-	EXPRESSION TAG	UNP B3Y963
A	796	HIS	-	EXPRESSION TAG	UNP B3Y963
A	797	HIS	-	EXPRESSION TAG	UNP B3Y963
A	798	HIS	-	EXPRESSION TAG	UNP B3Y963
A	799	HIS	-	EXPRESSION TAG	UNP B3Y963
A	800	HIS	-	EXPRESSION TAG	UNP B3Y963

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

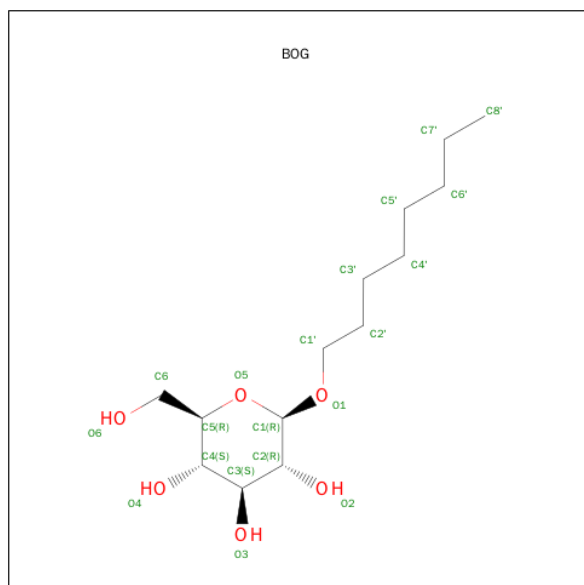
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn		
			1	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

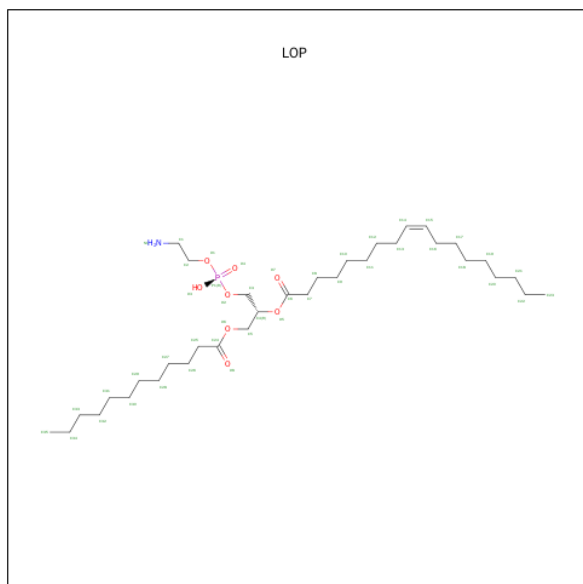
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca		
			1	1	0	0

- Molecule 5 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



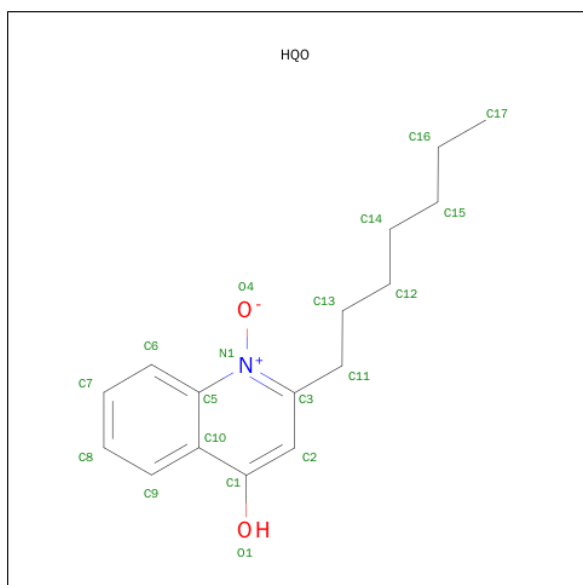
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			20	14	6	0	0
5	A	1	Total	C	O		
			20	14	6	0	0
5	A	1	Total	C	O		
			20	14	6	0	0

- Molecule 6 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 7 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total	O	0	0
			113	113		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.52Å 149.09Å 151.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.60 – 2.70 42.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.60-2.70) 99.8 (42.60-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.236 , 0.267 0.231 , 0.260	Depositor DCC
$R_{free}$ test set	1732 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 34516 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, LOP, HQO, HEM, BOG

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	0.48	0/6262	0.68	3/8517 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	435	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	220	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	602	GLY	N-CA-C	-5.10	100.34	113.10

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	6078	0	6095	387	1
2	A	86	0	60	4	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	60	0	84	3	0
6	A	90	0	134	30	0
7	A	19	0	20	9	0
8	A	113	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6448	0	6393	400	1

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 31.

The worst 5 of 400 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:168:ARG:NE	1:A:208:GLN:HE21	1.33	1.27
1:A:164:LEU:O	1:A:168:ARG:HG3	1.41	1.16
1:A:110:MET:CE	1:A:138:VAL:HG23	1.74	1.14
1:A:168:ARG:HE	1:A:208:GLN:NE2	1.48	1.12
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.06	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:NH2	1:A:334:ASP:OD1[8_455]	2.03	0.17

## 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	750/800 (94%)	690 (92%)	52 (7%)	8 (1%)	17 42

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASP
1	A	199	ALA

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Mol	Chain	Res	Type
1	A	204	SER
1	A	157	THR
1	A	194	PRO

### 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	631/675 (94%)	555 (88%)	76 (12%)	6	14

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	LEU
1	A	462	ARG
1	A	739	LEU
1	A	400	LEU
1	A	440	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	471	HIS
1	A	622	ASN
1	A	357	GLN
1	A	595	GLN

### 5.3.3 RNA [i](#)

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 ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
2	HEM	A	801	1,4	30,50,50	2.70	10 (33%)	24,82,82	2.51	9 (37%)
2	HEM	A	802	1,8,4	30,50,50	2.52	11 (36%)	24,82,82	2.16	8 (33%)
5	BOG	A	805	-	20,20,20	1.29	3 (15%)	25,25,25	0.73	0
5	BOG	A	806	-	20,20,20	1.42	3 (15%)	25,25,25	0.78	0
5	BOG	A	807	-	20,20,20	1.23	3 (15%)	25,25,25	0.83	0
6	LOP	A	809	-	43,44,44	0.78	2 (4%)	44,49,49	1.21	4 (9%)
6	LOP	A	810	-	43,44,44	0.78	2 (4%)	44,49,49	1.19	3 (6%)
7	HQO	A	811	-	20,20,20	1.37	2 (10%)	21,26,26	0.98	1 (4%)

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	HEM	A	801	1,4	-	0/10/54/54	0/0/8/8
2	HEM	A	802	1,8,4	-	0/10/54/54	0/0/8/8
5	BOG	A	805	-	-	0/11/31/31	0/1/1/1
5	BOG	A	806	-	-	0/11/31/31	0/1/1/1
5	BOG	A	807	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LOP	A	809	-	-	0/48/48/48	0/0/0/0
6	LOP	A	810	-	-	0/48/48/48	0/0/0/0
7	HQO	A	811	-	-	0/7/7/7	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C4B	-7.08	1.45	1.51
2	A	802	HEM	C3C-CAC	-5.72	1.40	1.51
2	A	801	HEM	C2D-C3D	-5.52	1.38	1.54
2	A	802	HEM	C2D-C3D	-5.45	1.38	1.54
2	A	802	HEM	C3B-C4B	-5.40	1.47	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	809	LOP	C4-O5-C6	-3.93	108.45	117.89
6	A	810	LOP	C4-O5-C6	-3.85	108.64	117.89
6	A	809	LOP	C5-O6-C24	-2.17	110.78	116.85
2	A	802	HEM	C2D-C3D-C4D	2.18	105.20	101.50
7	A	811	HQO	O1-C1-C10	2.31	119.55	116.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	3	0
2	A	802	HEM	1	0
5	A	806	BOG	1	0
5	A	807	BOG	2	0
6	A	809	LOP	12	0
6	A	810	LOP	18	0
7	A	811	HQO	9	0

## 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 [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	754/800 (94%)	0.30	63 (8%) 14 11	39, 67, 96, 108	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	6.3
1	A	113	TYR	4.9
1	A	125	ASP	4.8
1	A	458	ARG	4.8
1	A	79	TYR	4.2

### 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
5	BOG	A	807	20/20	0.82	0.49	7.29	95,107,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	LOP	A	809	45/45	0.66	0.68	6.54	94,104,125,126	0
5	BOG	A	806	20/20	0.78	0.45	4.78	94,106,109,110	0
7	HQO	A	811	19/19	0.91	0.42	3.35	67,71,85,86	0
5	BOG	A	805	20/20	0.75	0.34	2.58	94,107,112,113	0
6	LOP	A	810	45/45	0.74	0.33	2.16	64,80,113,114	0
4	CA	A	804	1/1	0.97	0.24	0.51	49,49,49,49	0
2	HEM	A	801	43/43	0.97	0.21	0.39	45,52,58,60	0
2	HEM	A	802	43/43	0.97	0.20	-0.42	33,41,54,59	0
3	ZN	A	803	1/1	0.99	0.15	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.