



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:37 PM GMT

PDB ID : 4CU1  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6-[(2S)-3-amino-2-{5-[2-(6-amino-4-methylpyridin-2-yl)ethyl]pyridin-3-yl}propyl]-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-03-15  
Resolution : 1.89 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 (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

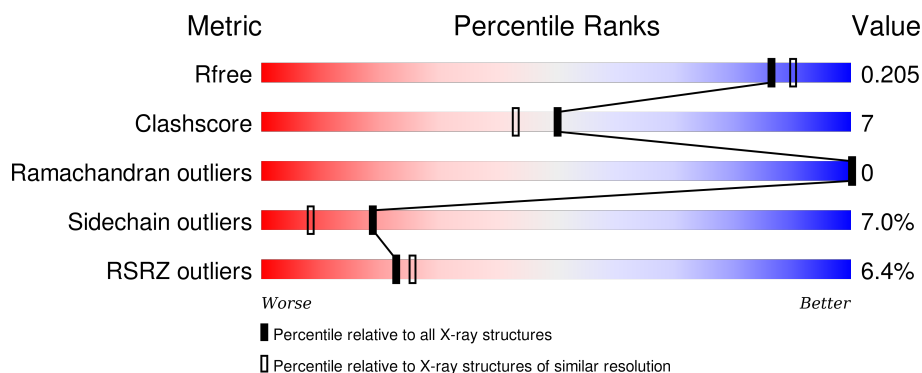
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	443	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>9%</div> </div> </div>
2	B	443	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>9%</div> </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
6	ACT	B	860	-	-	-	X
7	GOL	A	880	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6933 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 SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	VARIANT	UNP P29473

- Molecule 2 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3218	2046	568	588	16			

There is a discrepancy between the modelled and reference sequences:

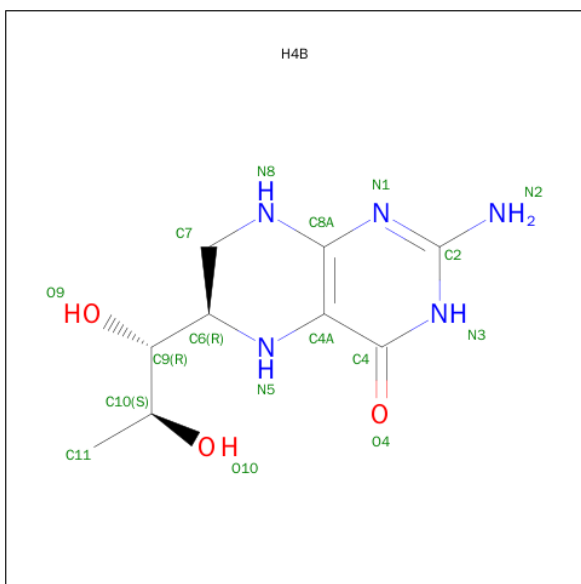
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ARG	CYS	VARIANT	UNP P29473

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



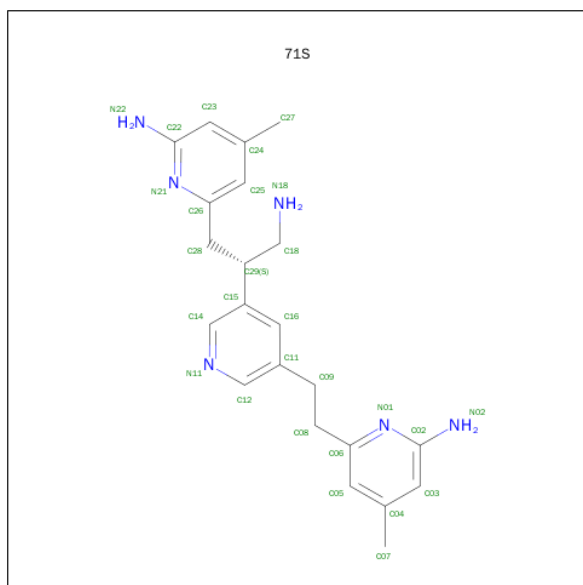
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

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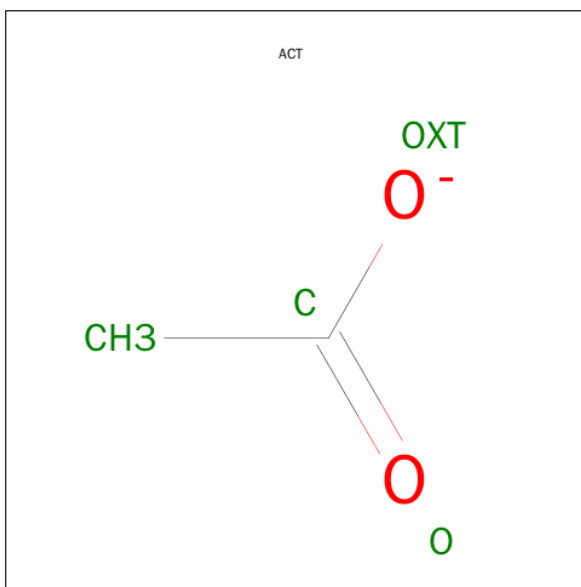
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is 6-[(2S)-3-AMINO-2-{5-[2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL]PYRIDIN-3-YL}PROPYL]-4-METHYLPYRIDIN-2-AMINE (three-letter code: 71S) (formula:  $C_{22}H_{28}N_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			28	22	6		
5	B	1	Total	C	N	0	0
			28	22	6		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Zn 1	0	0

- Molecule 9 is water.

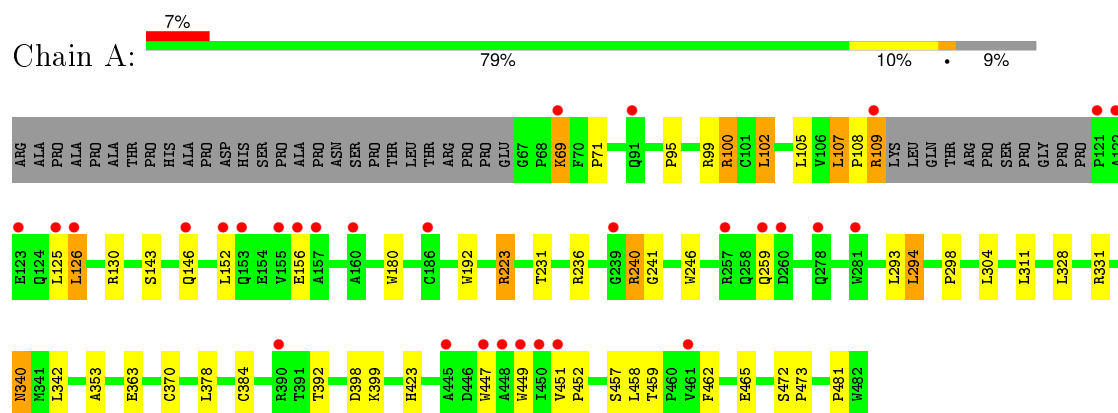
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total 170	O 170	0	0
9	B	125	Total 125	O 125	0	0



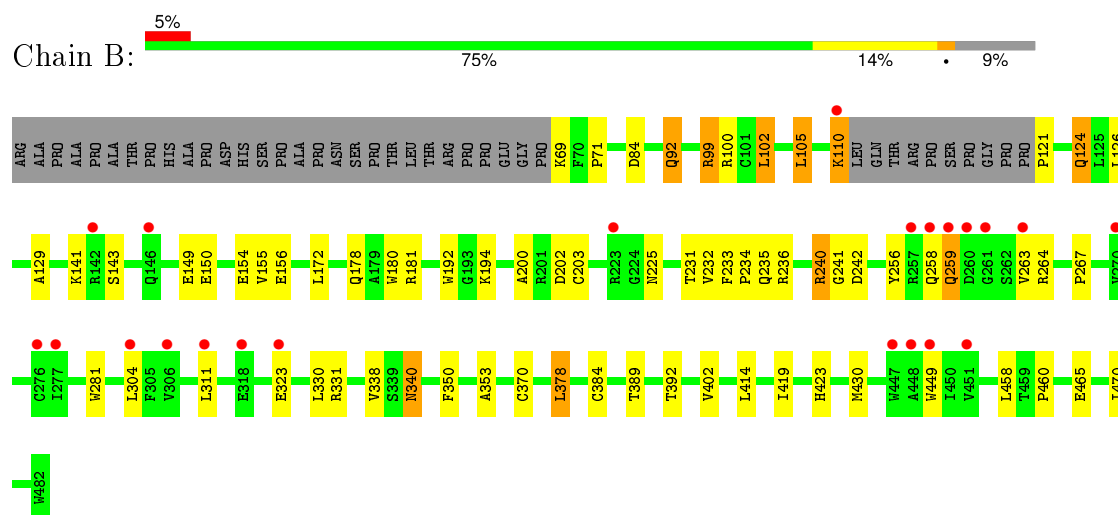
### 3 Residue-property plots

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: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



#### • Molecule 2: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.34Å 105.17Å 155.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.04 – 1.89 47.88 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.04-1.89) 98.6 (47.88-1.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.170 , 0.205 0.170 , 0.205	Depositor DCC
$R_{free}$ test set	3704 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 74408 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: GOL, ZN, H4B, CAS, 71S, ACT, HEM

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	0.59	0/3303	0.74	1/4497 (0.0%)
2	B	0.56	0/3307	0.72	0/4502
All	All	0.57	0/6610	0.73	1/8999 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	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 [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	3223	0	3127	46	0
2	B	3218	0	3131	41	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
4	A	17	0	15	2	0
4	B	17	0	15	1	0
5	A	28	0	28	8	0
5	B	28	0	28	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	A	6	0	8	1	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
9	A	170	0	0	2	0
9	B	125	0	0	2	0
All	All	6933	0	6426	92	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 7.

All (92) 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:223:ARG:HH11	1:A:223:ARG:HG3	1.24	1.01
3:A:500:HEM:O1D	5:A:800:71S:H282	1.72	0.90
1:A:384:CAS:AS	1:A:384:CAS:SG	2.93	0.87
2:B:384:CYS:SG	9:B:2096:HOH:O	2.39	0.79
1:A:109:ARG:HH11	1:A:109:ARG:HA	1.47	0.79
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.68	0.76
1:A:384:CAS:CE2	1:A:384:CAS:SG	2.78	0.72
3:B:500:HEM:O1D	5:B:800:71S:H282	1.92	0.69
2:B:236:ARG:CD	2:B:242:ASP:OD1	2.40	0.69
2:B:178:GLN:HE22	2:B:181:ARG:HH11	1.42	0.67
2:B:236:ARG:HD2	2:B:242:ASP:OD1	1.94	0.66
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.05	0.65
1:A:109:ARG:NH1	1:A:109:ARG:HA	2.12	0.64
2:B:92:GLN:HG3	2:B:470:ILE:HG21	1.78	0.64
1:A:223:ARG:NH1	1:A:223:ARG:HG3	2.03	0.63
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.79	0.62
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.29	0.62
3:A:500:HEM:HBB2	3:A:500:HEM:HHC	1.82	0.62
2:B:449:TRP:CH2	5:B:800:71S:H182	2.35	0.61
1:A:107:LEU:HD21	5:A:800:71S:H273	1.83	0.60
1:A:105:LEU:HD22	2:B:465:GLU:HB3	1.83	0.59
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.83	0.59
3:B:500:HEM:HBB2	3:B:500:HEM:HHC	1.85	0.57
1:A:449:TRP:CH2	5:A:800:71S:H182	2.40	0.56
2:B:150:GLU:O	2:B:154:GLU:HG3	2.04	0.56
1:A:126:LEU:O	1:A:130:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TRP:HA	4:A:600:H4B:N1	2.21	0.56
2:B:281:TRP:HB2	2:B:304:LEU:HD21	1.88	0.55
2:B:236:ARG:HD3	2:B:242:ASP:OD1	2.06	0.55
2:B:178:GLN:HE22	2:B:181:ARG:NH1	2.04	0.55
2:B:378:LEU:HB2	9:B:2094:HOH:O	2.06	0.54
2:B:338:VAL:CG2	5:B:800:71S:H092	2.39	0.53
2:B:240:ARG:HD2	2:B:241:GLY:O	2.09	0.53
2:B:121:PRO:HG2	2:B:124:GLN:HB2	1.92	0.52
2:B:129:ALA:HB1	2:B:155:VAL:HG11	1.92	0.52
2:B:92:GLN:HG3	2:B:470:ILE:CG2	2.39	0.52
2:B:340:ASN:OD1	5:B:800:71S:N22	2.43	0.52
2:B:236:ARG:HD3	2:B:242:ASP:CG	2.30	0.51
1:A:236:ARG:NH1	1:A:236:ARG:HB2	2.26	0.51
3:A:500:HEM:CBB	3:A:500:HEM:HHC	2.41	0.50
2:B:99:ARG:HB2	2:B:99:ARG:HH11	1.76	0.50
1:A:392:THR:HB	2:B:423:HIS:HB2	1.93	0.50
2:B:126:LEU:HD11	2:B:156:GLU:HA	1.94	0.49
2:B:231:THR:O	2:B:353:ALA:HA	2.11	0.49
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.51	0.49
2:B:338:VAL:HG23	5:B:800:71S:H05	1.94	0.49
2:B:110:LYS:O	2:B:110:LYS:HE2	2.12	0.49
2:B:370:CYS:SG	2:B:378:LEU:HD13	2.53	0.48
2:B:449:TRP:HA	4:B:600:H4B:N1	2.28	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.47
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.96	0.47
1:A:423:HIS:HB2	2:B:392:THR:HB	1.98	0.46
1:A:340:ASN:HD22	1:A:340:ASN:H	1.63	0.46
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.30	0.46
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.28	0.46
2:B:256:TYR:O	2:B:258:GLN:NE2	2.49	0.45
1:A:236:ARG:HB2	1:A:236:ARG:HH11	1.81	0.45
1:A:363:GLU:OE1	5:A:800:71S:N01	2.49	0.45
1:A:378:LEU:HB2	9:A:2125:HOH:O	2.16	0.44
1:A:294:LEU:HD13	1:A:304:LEU:HD12	1.99	0.44
2:B:235:GLN:HB3	2:B:350:PHE:CE1	2.53	0.44
2:B:200:ALA:O	2:B:203:CYS:HB2	2.17	0.44
3:A:500:HEM:HBB2	3:A:500:HEM:CHC	2.47	0.44
1:A:152:LEU:O	1:A:156:GLU:HG3	2.17	0.44
2:B:259:GLN:HG3	2:B:259:GLN:H	1.64	0.44
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.53	0.43
1:A:457:SER:HA	1:A:462:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:HEM:C1C	5:A:800:71S:H073	2.53	0.43
1:A:240:ARG:HD3	1:A:298:PRO:CG	2.47	0.43
3:B:500:HEM:O2A	5:B:800:71S:C16	2.65	0.43
1:A:447:TRP:CE2	1:A:451:VAL:HG21	2.53	0.43
1:A:95:PRO:HB3	1:A:108:PRO:CB	2.48	0.43
1:A:340:ASN:HD21	5:A:800:71S:H222	1.66	0.43
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.74	0.43
2:B:233:PHE:HB3	2:B:234:PRO:CD	2.48	0.43
1:A:240:ARG:HD2	1:A:241:GLY:O	2.18	0.42
2:B:430:MET:HG3	2:B:460:PRO:HB2	2.01	0.42
5:A:800:71S:H181	7:A:880:GOL:H32	2.00	0.42
1:A:452:PRO:HG2	1:A:459:THR:HG21	2.01	0.42
2:B:180:TRP:CE3	2:B:192:TRP:HA	2.54	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.42
2:B:263:VAL:HG11	2:B:267:PRO:HA	2.01	0.42
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.81	0.42
1:A:465:GLU:HB3	2:B:105:LEU:HD22	2.01	0.41
2:B:71:PRO:HG2	2:B:84:ASP:HB3	2.02	0.41
3:B:500:HEM:CBB	3:B:500:HEM:HHC	2.49	0.41
1:A:143:SER:HB3	9:A:2031:HOH:O	2.20	0.41
1:A:71:PRO:HB3	2:B:102:LEU:HD11	2.02	0.41
2:B:172:LEU:HD11	2:B:232:VAL:HG11	2.02	0.41
3:A:500:HEM:O1A	4:A:600:H4B:N3	2.45	0.41
1:A:449:TRP:HH2	5:A:800:71S:H281	1.86	0.41
1:A:399:LYS:HG2	2:B:402:VAL:HG11	2.02	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	400/443 (90%)	389 (97%)	11 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	400/443 (90%)	390 (98%)	10 (2%)	0	100	100
All	All	800/886 (90%)	779 (97%)	21 (3%)	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	343/375 (92%)	322 (94%)	21 (6%)	23	11
2	B	344/376 (92%)	317 (92%)	27 (8%)	16	6
All	All	687/751 (92%)	639 (93%)	48 (7%)	19	8

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	107	LEU
1	A	109	ARG
1	A	125	LEU
1	A	126	LEU
1	A	146	GLN
1	A	223	ARG
1	A	259	GLN
1	A	293	LEU
1	A	294	LEU
1	A	311	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	398	ASP
1	A	458	LEU
1	A	481	PRO
2	B	69	LYS
2	B	92	GLN
2	B	99	ARG
2	B	100	ARG
2	B	102	LEU
2	B	105	LEU
2	B	110	LYS
2	B	124	GLN
2	B	141	LYS
2	B	143	SER
2	B	149	GLU
2	B	194	LYS
2	B	202	ASP
2	B	225	ASN
2	B	240	ARG
2	B	259	GLN
2	B	264	ARG
2	B	311	LEU
2	B	323	GLU
2	B	330	LEU
2	B	331	ARG
2	B	340	ASN
2	B	378	LEU
2	B	389	THR
2	B	414	LEU
2	B	419	ILE
2	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	249	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
2	B	178	GLN

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Mol	Chain	Res	Type
2	B	191	GLN
2	B	207	GLN
2	B	222	ASN
2	B	225	ASN
2	B	258	GLN
2	B	376	ASN
2	B	405	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	CAS	A	384	1	5,8,9	1.14	0	2,9,11	1.40	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
1	CAS	A	384	1	-	0/0/7/9	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z  > 2$
3	HEM	A	500	1	30,50,50	2.11	7 (23%)	24,82,82	2.75	12 (50%)
4	H4B	A	600	-	13,18,18	0.68	0	11,26,26	2.73	5 (45%)
5	71S	A	800	-	30,30,30	0.97	2 (6%)	37,41,41	2.30	16 (43%)
6	ACT	A	860	-	1,3,3	1.18	0	0,3,3	0.00	-
7	GOL	A	880	-	5,5,5	0.19	0	5,5,5	0.70	0
3	HEM	B	500	2	30,50,50	2.00	7 (23%)	24,82,82	2.72	12 (50%)
4	H4B	B	600	-	13,18,18	0.72	0	11,26,26	2.13	5 (45%)
5	71S	B	800	-	30,30,30	0.91	2 (6%)	37,41,41	2.44	14 (37%)
6	ACT	B	860	-	1,3,3	1.42	0	0,3,3	0.00	-
7	GOL	B	880	-	5,5,5	0.29	0	5,5,5	0.83	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
3	HEM	A	500	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
5	71S	A	800	-	-	0/15/15/15	0/3/3/3
6	ACT	A	860	-	-	0/0/0/0	0/0/0/0
7	GOL	A	880	-	-	0/4/4/4	0/0/0/0
3	HEM	B	500	2	-	0/10/54/54	0/0/8/8
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	71S	B	800	-	-	0/15/15/15	0/3/3/3
6	ACT	B	860	-	-	0/0/0/0	0/0/0/0
7	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C2D-C3D	-6.55	1.34	1.54
3	B	500	HEM	C2D-C3D	-6.37	1.35	1.54
3	A	500	HEM	C2C-C1C	-5.73	1.41	1.52
3	B	500	HEM	C2C-C1C	-5.34	1.42	1.52
3	B	500	HEM	C3D-C4D	-3.28	1.47	1.51
3	A	500	HEM	C3B-C4B	-3.24	1.49	1.51
3	A	500	HEM	C3D-C4D	-3.00	1.47	1.51
3	B	500	HEM	C3B-C4B	-2.84	1.49	1.51
5	B	800	71S	C08-C09	-2.78	1.34	1.53
5	A	800	71S	C08-C09	-2.68	1.35	1.53
3	A	500	HEM	C2B-C1B	-2.31	1.44	1.51
3	B	500	HEM	C2B-C1B	-2.16	1.44	1.51
3	A	500	HEM	C3B-CAB	-2.06	1.47	1.51
3	B	500	HEM	FE-NB	2.12	2.08	1.97
5	A	800	71S	C16-C15	2.14	1.42	1.39
5	B	800	71S	C16-C15	2.26	1.42	1.39
3	A	500	HEM	FE-NC	2.48	2.05	1.95
3	B	500	HEM	FE-NC	2.69	2.06	1.95

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	CBA-CAA-C2A	-5.94	101.89	112.53
3	A	500	HEM	C1D-CHD-C4C	-5.37	116.84	125.82
5	B	800	71S	C05-C06-N01	-4.64	117.73	122.96
4	A	600	H4B	N3-C2-N1	-3.83	119.26	125.53
3	A	500	HEM	CBA-CAA-C2A	-3.81	105.70	112.53
5	A	800	71S	C09-C11-C12	-3.78	115.42	121.85
3	B	500	HEM	C1D-CHD-C4C	-3.69	119.65	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	71S	C05-C06-N01	-3.63	118.87	122.96
5	B	800	71S	C09-C11-C12	-3.62	115.69	121.85
3	A	500	HEM	C3B-C4B-NB	-2.86	106.15	111.63
5	B	800	71S	C24-C25-C26	-2.85	118.50	120.28
4	B	600	H4B	N3-C2-N1	-2.76	121.00	125.53
5	A	800	71S	C14-C15-C29	-2.76	114.96	121.36
5	A	800	71S	C15-C16-C11	-2.61	116.92	120.96
3	B	500	HEM	CBD-CAD-C3D	-2.49	106.31	113.55
5	A	800	71S	C18-C29-C28	-2.45	105.03	110.11
3	B	500	HEM	C3C-CAC-CBC	-2.32	120.89	124.46
5	A	800	71S	C24-C25-C26	-2.32	118.83	120.28
5	B	800	71S	C14-C15-C29	-2.25	116.14	121.36
3	B	500	HEM	C3B-C4B-NB	-2.19	107.43	111.63
5	A	800	71S	C15-C14-N11	-2.17	120.77	124.27
3	B	500	HEM	CMA-C3A-C4A	-2.07	124.93	128.36
3	A	500	HEM	C4B-CHC-C1C	-2.03	122.42	125.82
5	B	800	71S	C16-C15-C14	2.01	118.99	116.78
5	B	800	71S	C16-C11-C12	2.05	118.81	116.57
5	B	800	71S	C08-C09-C11	2.08	120.11	113.27
5	B	800	71S	C05-C04-C03	2.10	120.77	118.08
4	B	600	H4B	C4A-C8A-N8	2.14	120.95	118.43
5	A	800	71S	C12-N11-C14	2.19	120.80	117.50
3	A	500	HEM	C2D-C3D-C4D	2.23	105.28	101.50
3	A	500	HEM	CAA-CBA-CGA	2.29	116.94	112.75
5	A	800	71S	C08-C06-N01	2.31	119.10	115.69
4	B	600	H4B	C2-N1-C8A	2.32	119.75	114.54
3	A	500	HEM	CHC-C4B-NB	2.40	130.31	124.52
3	A	500	HEM	CMD-C2D-C3D	2.46	125.25	114.35
4	A	600	H4B	C2-N1-C8A	2.50	120.16	114.54
4	A	600	H4B	N2-C2-N3	2.54	121.40	117.20
5	A	800	71S	C16-C15-C29	2.56	124.65	120.89
5	A	800	71S	C16-C11-C12	2.60	119.41	116.57
5	B	800	71S	C16-C15-C29	2.71	124.87	120.89
5	A	800	71S	C09-C11-C16	2.75	125.17	120.56
5	B	800	71S	C09-C11-C16	2.93	125.47	120.56
5	A	800	71S	C22-N21-C26	3.16	120.47	118.23
4	B	600	H4B	C4-N3-C2	3.23	120.42	115.94
3	B	500	HEM	C2D-C3D-C4D	3.23	106.97	101.50
5	A	800	71S	C16-C15-C14	3.29	120.39	116.78
3	B	500	HEM	CMD-C2D-C3D	3.30	128.94	114.35
3	B	500	HEM	CAD-C3D-C4D	3.70	125.51	112.47
4	B	600	H4B	C4-C4A-C8A	3.82	118.02	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	800	71S	C22-N21-C26	3.89	120.99	118.23
5	B	800	71S	C08-C06-N01	3.96	121.54	115.69
3	B	500	HEM	CMB-C2B-C3B	4.09	126.75	116.53
3	B	500	HEM	CMC-C2C-C3C	4.18	126.97	116.53
3	A	500	HEM	CAD-C3D-C2D	4.40	125.86	113.22
3	A	500	HEM	CMC-C2C-C3C	4.40	127.52	116.53
4	A	600	H4B	C4-C4A-C8A	4.46	118.60	114.56
3	A	500	HEM	CMB-C2B-C3B	4.63	128.09	116.53
3	A	500	HEM	CAD-C3D-C4D	4.65	128.86	112.47
3	B	500	HEM	CAD-C3D-C2D	4.97	127.52	113.22
4	A	600	H4B	C4-N3-C2	5.42	123.47	115.94
5	A	800	71S	C02-N01-C06	5.89	122.42	118.23
5	B	800	71S	C09-C08-C06	6.09	124.25	112.53
5	A	800	71S	C09-C08-C06	6.45	124.94	112.53
5	B	800	71S	C02-N01-C06	6.82	123.08	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	6	0
4	A	600	H4B	2	0
5	A	800	71S	8	0
7	A	880	GOL	1	0
3	B	500	HEM	4	0
4	B	600	H4B	1	0
5	B	800	71S	6	0

## 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	404/443 (91%)	0.58	30 (7%) 17 19	27, 40, 69, 91	0
2	B	404/443 (91%)	0.43	22 (5%) 29 33	27, 45, 74, 110	0
All	All	808/886 (91%)	0.50	52 (6%) 23 25	27, 43, 72, 110	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	259	GLN	7.8
1	A	123	GLU	5.1
1	A	122	ALA	4.9
1	A	160	ALA	4.4
2	B	260	ASP	4.4
2	B	110	LYS	4.2
1	A	121	PRO	4.1
1	A	259	GLN	4.1
1	A	153	GLN	3.7
1	A	450	ILE	3.7
1	A	126	LEU	3.6
2	B	257	ARG	3.5
2	B	263	VAL	3.4
1	A	448	ALA	3.2
2	B	261	GLY	3.2
2	B	146	GLN	3.2
2	B	447	TRP	3.0
1	A	69	LYS	3.0
1	A	109	ARG	2.9
1	A	449	TRP	2.9
1	A	155	VAL	2.8
2	B	449	TRP	2.8
1	A	257	ARG	2.7
2	B	448	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	447	TRP	2.7
2	B	223	ARG	2.7
2	B	270	VAL	2.6
2	B	306	VAL	2.6
1	A	461	VAL	2.6
2	B	258	GLN	2.6
2	B	276	CYS	2.5
1	A	125	LEU	2.5
1	A	451	VAL	2.5
1	A	91	GLN	2.5
2	B	323	GLU	2.5
1	A	239	GLY	2.4
2	B	311	LEU	2.4
1	A	157	ALA	2.4
1	A	281	TRP	2.4
1	A	445	ALA	2.4
2	B	277	ILE	2.3
1	A	186	CYS	2.3
2	B	318	GLU	2.3
1	A	278	GLN	2.3
1	A	390	ARG	2.2
2	B	304	LEU	2.2
2	B	451	VAL	2.2
1	A	146	GLN	2.1
1	A	260	ASP	2.1
2	B	142	ARG	2.0
1	A	156	GLU	2.0
1	A	152	LEU	2.0

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

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
1	CAS	A	384	9/10	0.93	0.12	-	40,42,82,108	0

### 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( $\text{\AA}^2$ )	Q<0.9
6	ACT	B	860	4/4	0.95	0.33	21.38	53,59,60,62	0
7	GOL	A	880	6/6	0.90	0.21	2.06	50,56,59,69	0
7	GOL	B	880	6/6	0.84	0.19	1.74	51,54,57,58	0
5	71S	A	800	28/28	0.92	0.19	1.60	31,56,106,112	0
5	71S	B	800	28/28	0.93	0.16	1.58	35,58,94,98	0
3	HEM	B	500	43/43	0.98	0.13	0.65	29,33,40,43	0
3	HEM	A	500	43/43	0.98	0.17	0.56	25,28,39,43	0
4	H4B	B	600	17/17	0.98	0.17	0.21	25,29,32,34	0
4	H4B	A	600	17/17	0.98	0.17	0.04	28,31,35,35	0
6	ACT	A	860	4/4	0.95	0.12	-1.72	48,53,54,57	0
8	ZN	B	900	1/1	0.99	0.09	-2.10	37,37,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.