



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:34 PM EDT

PDB ID : 3RQL  
Title : Structure of the neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((1S,2R/1R,2S)-2-(3-Clorophenyl)cyclopropylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Delker, S.L.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 1.93 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 : **FAILED**  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

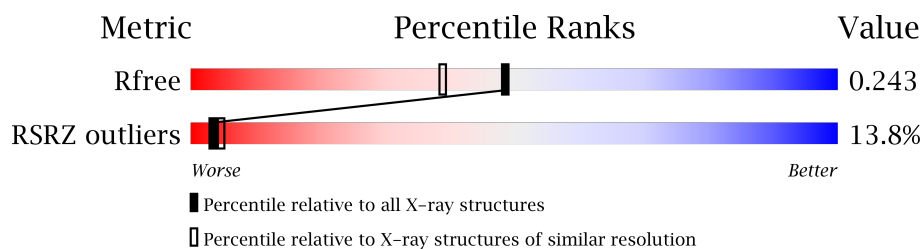
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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))
$R_{free}$	100719	3233 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
4	ACT	A	860	-	-	-	X

## 2 Entry composition [i](#)

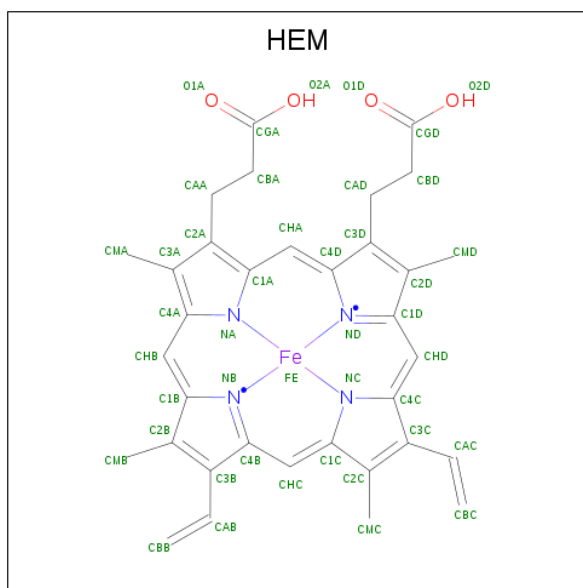
There are 7 unique types of molecules in this entry. The entry contains 7193 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, brain.

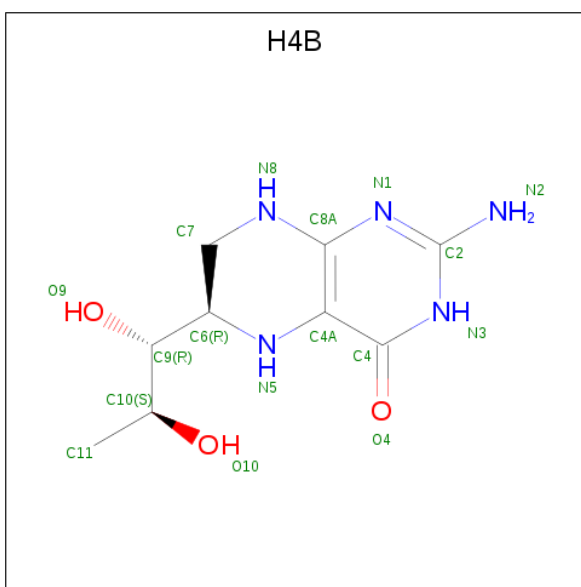
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	2	0
			3337	2136	571	608	22			
1	B	411	Total	C	N	O	S	0	4	0
			3359	2149	575	613	22			

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



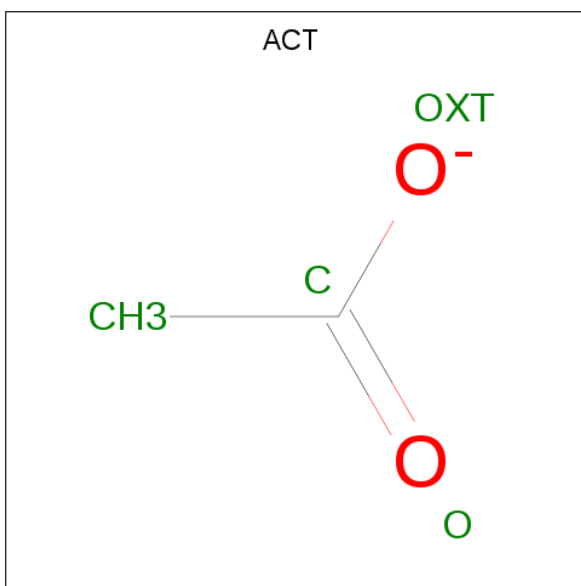
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



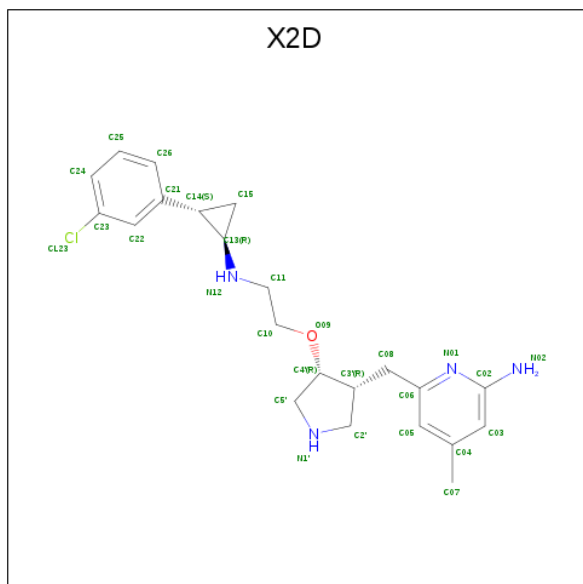
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[(1R,2S)-2-(3-chlorophenyl)cyclopropyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: X2D) (formula:  $C_{22}H_{29}ClN_4O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
5	B	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	131	Total	O	0	0
			131	131		
7	B	181	Total	O	0	0
			181	181		

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.70Å 110.78Å 163.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.93 37.80 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.64-1.93) 99.1 (37.80-1.93)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.235 0.204 , 0.243	Depositor DCC
$R_{free}$ test set	3533 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	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	0.96	EDS
Total number of atoms	7193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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.

## 4 Model quality [i](#)

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

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is 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	750	1	28,50,50	2.19	8 (28%)	17,82,82	2.06	6 (35%)
3	H4B	A	760	-	14,18,18	0.63	0	12,26,26	2.29	5 (41%)
5	X2D	A	800	-	26,31,31	1.07	2 (7%)	30,43,43	2.22	9 (30%)
4	ACT	A	860	-	1,3,3	1.39	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.16	10 (35%)	17,82,82	2.43	7 (41%)
3	H4B	B	760	-	14,18,18	0.91	0	12,26,26	2.54	3 (25%)
5	X2D	B	800	-	26,31,31	0.89	2 (7%)	30,43,43	1.94	6 (20%)
4	ACT	B	860	-	1,3,3	1.94	0	0,3,3	0.00	-

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	750	1	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	X2D	A	800	-	-	0/13/30/30	0/3/4/4
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	X2D	B	800	-	-	0/13/30/30	0/3/4/4
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C2B	-5.37	1.33	1.40
2	B	750	HEM	C3B-C2B	-4.12	1.34	1.40
2	B	750	HEM	C3C-C2C	-3.88	1.35	1.40
2	A	750	HEM	C3C-C2C	-3.19	1.36	1.40
5	B	800	X2D	C23-CL23	2.00	1.78	1.74
2	A	750	HEM	CMA-C3A	2.11	1.55	1.51
2	B	750	HEM	CMB-C2B	2.20	1.56	1.51
5	A	800	X2D	C15-C14	2.30	1.54	1.50
2	B	750	HEM	C3B-CAB	2.39	1.52	1.47
5	B	800	X2D	C15-C14	2.40	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CMA-C3A	2.42	1.56	1.51
5	A	800	X2D	C23-CL23	2.54	1.80	1.74
2	A	750	HEM	C1B-NB	2.59	1.39	1.36
2	B	750	HEM	C4A-NA	2.92	1.42	1.36
2	B	750	HEM	C3C-CAC	2.94	1.53	1.47
2	A	750	HEM	C1C-NC	2.95	1.40	1.36
2	B	750	HEM	C4D-ND	3.06	1.40	1.36
2	A	750	HEM	C3C-CAC	3.14	1.54	1.47
2	A	750	HEM	C3B-CAB	3.30	1.54	1.47
2	B	750	HEM	C1C-NC	3.46	1.40	1.36
2	B	750	HEM	C3D-C2D	4.06	1.49	1.37
2	A	750	HEM	C3D-C2D	5.14	1.52	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	X2D	C15-C14-C21	-7.40	108.73	122.31
5	B	800	X2D	C15-C14-C21	-6.75	109.94	122.31
2	B	750	HEM	CBD-CAD-C3D	-5.65	101.70	112.47
2	B	750	HEM	CBA-CAA-C2A	-4.94	103.05	112.48
2	A	750	HEM	CBA-CAA-C2A	-4.31	104.25	112.48
2	A	750	HEM	CBD-CAD-C3D	-3.70	105.42	112.47
2	B	750	HEM	C3B-C4B-NB	-3.25	105.01	109.21
3	A	760	H4B	N3-C2-N1	-2.58	121.26	125.45
5	A	800	X2D	C05-C06-N01	-2.58	120.11	122.91
5	A	800	X2D	C22-C23-CL23	-2.57	115.93	119.14
2	A	750	HEM	CAA-CBA-CGA	-2.55	108.30	112.66
2	A	750	HEM	C3C-C4C-NC	-2.38	106.45	110.94
5	B	800	X2D	C05-C06-N01	-2.36	120.35	122.91
5	A	800	X2D	O09-C4'-C5'	-2.34	105.19	111.42
3	B	760	H4B	C4A-N5-C6	-2.11	115.42	121.16
2	B	750	HEM	CAA-CBA-CGA	-2.07	109.12	112.66
2	B	750	HEM	CAD-C3D-C2D	-2.00	123.28	129.00
5	A	800	X2D	C26-C25-C24	-2.00	117.42	120.24
2	A	750	HEM	CMC-C2C-C3C	2.01	128.62	124.89
5	B	800	X2D	C22-C21-C14	2.05	123.85	120.10
5	A	800	X2D	C2'-N1'-C5'	2.07	110.21	105.40
5	B	800	X2D	C10-C11-N12	2.14	116.97	111.55
2	B	750	HEM	CMB-C2B-C3B	2.36	129.28	124.89
3	A	760	H4B	N2-C2-N1	2.42	121.11	117.24
5	B	800	X2D	C2'-N1'-C5'	2.60	111.46	105.40
3	A	760	H4B	C4-N3-C2	2.70	119.95	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C2-N1-C8A	2.74	120.68	114.51
5	A	800	X2D	C08-C06-N01	2.82	121.57	117.12
5	A	800	X2D	N02-C02-N01	2.82	121.39	116.64
2	B	750	HEM	C4C-C3C-C2C	2.84	108.88	106.90
2	A	750	HEM	C4C-C3C-C2C	3.22	109.15	106.90
3	B	760	H4B	C4-N3-C2	3.29	120.80	116.06
5	B	800	X2D	C02-N01-C06	4.30	121.21	118.17
3	A	760	H4B	C4-C4A-C8A	5.30	119.36	114.56
5	A	800	X2D	C02-N01-C06	5.45	122.03	118.17
3	B	760	H4B	C4-C4A-C8A	6.96	120.87	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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	409/422 (96%)	1.01	77 (18%) 1 1	27, 52, 90, 117	0
1	B	411/422 (97%)	0.47	36 (8%) 11 16	27, 42, 66, 83	0
All	All	820/844 (97%)	0.74	113 (13%) 3 5	27, 47, 83, 117	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	10.0
1	A	488	PRO	7.5
1	A	716	TRP	6.3
1	A	300	PHE	6.3
1	A	348	VAL	6.0
1	A	713	THR	5.9
1	A	355	PHE	5.7
1	A	486	LYS	5.6
1	A	715	VAL	5.6
1	B	348	VAL	5.0
1	A	352	ASP	5.0
1	B	619	ARG	4.6
1	A	712	ASN	4.4
1	A	299	ARG	4.2
1	A	552	ASP	4.2
1	A	321	THR	4.1
1	A	506	ILE	4.0
1	A	619	ARG	4.0
1	A	351	LYS	4.0
1	A	322	LEU	3.8
1	A	388	ILE	3.8
1	A	386	LYS	3.8
1	A	503	GLU	3.7
1	B	310	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	350	THR	3.6
1	A	678	TRP	3.6
1	A	551	PHE	3.6
1	A	487	GLN	3.6
1	B	715	VAL	3.5
1	A	349	ARG	3.5
1	A	593	ILE	3.5
1	B	301	LEU	3.5
1	A	507	GLN	3.4
1	A	415	CYS	3.4
1	A	491	SER	3.3
1	A	390	SER	3.3
1	A	679	ILE	3.3
1	A	682	PRO	3.3
1	A	567	VAL	3.2
1	A	492	THR	3.2
1	A	514	ARG	3.1
1	A	490	GLY	3.1
1	B	667	ARG	3.1
1	A	714	HIS	3.0
1	B	680	VAL	3.0
1	A	385	ASN	3.0
1	A	392	SER	3.0
1	B	299	ARG	3.0
1	B	616	LEU	3.0
1	B	351	LYS	3.0
1	A	416	VAL	3.0
1	A	511	LYS	2.9
1	A	479	LEU	2.9
1	A	591	THR	2.9
1	B	561	TRP	2.9
1	A	489	ASP	2.9
1	A	389	GLU	2.8
1	A	677	VAL	2.8
1	A	480	ILE	2.8
1	A	588	TYR	2.8
1	A	469	LYS	2.8
1	B	691	PHE	2.8
1	A	330	ILE	2.7
1	A	391	THR	2.7
1	A	504	ILE	2.7
1	A	311	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	595	VAL	2.7
1	A	615	ASP	2.6
1	A	508	GLN	2.6
1	A	550	LYS	2.6
1	A	350	THR	2.6
1	A	676	TRP	2.6
1	A	681	PRO	2.6
1	A	680	VAL	2.6
1	A	584	PHE	2.5
1	B	620	LYS	2.5
1	B	611	ALA	2.5
1	B	677	VAL	2.5
1	A	667	ARG	2.5
1	A	617	ASP	2.4
1	A	565	PRO	2.4
1	A	509	GLY	2.4
1	A	302	LYS	2.4
1	B	375	LYS	2.4
1	B	682	PRO	2.4
1	A	412	ALA	2.4
1	B	352	ASP	2.4
1	A	505	CYS	2.3
1	B	567	VAL	2.3
1	B	322	LEU	2.3
1	B	584	PHE	2.3
1	A	612	LYS	2.3
1	B	591	THR	2.3
1	A	318	LEU	2.3
1	A	645	LYS	2.3
1	B	593	ILE	2.2
1	B	713	THR	2.2
1	B	718	GLY	2.2
1	B	389	GLU	2.2
1	A	370	LYS	2.2
1	B	321	THR	2.1
1	A	601	ASN	2.1
1	A	686	SER	2.1
1	B	590	GLY	2.1
1	B	617	ASP	2.1
1	B	681	PRO	2.1
1	B	676	TRP	2.1
1	B	479	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	467	ASP	2.0
1	A	519	VAL	2.0
1	A	409	TRP	2.0
1	B	615	ASP	2.0
1	B	684	SER	2.0

## 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.4 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
4	ACT	A	860	4/4	0.92	0.33	9.85	59,60,62,64	0
4	ACT	B	860	4/4	0.94	0.13	1.43	48,50,51,52	0
2	HEM	A	750	43/43	0.97	0.23	1.16	29,34,38,39	0
2	HEM	B	750	43/43	0.98	0.18	0.90	25,32,39,44	0
5	X2D	B	800	28/28	0.93	0.20	0.87	35,41,45,52	0
3	H4B	B	760	17/17	0.97	0.18	0.83	28,33,38,40	0
3	H4B	A	760	17/17	0.94	0.19	0.57	30,33,40,40	0
5	X2D	A	800	28/28	0.90	0.16	-0.44	27,33,36,46	0
6	ZN	A	900	1/1	1.00	0.06	-1.71	38,38,38,38	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.