



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:10 PM EDT

PDB ID : 3N60  
Title : Structure of neuronal nitric oxide synthase heme domain in complex with 6,6'-(2,2'-(5-amino-1,3-phenylene)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)  
Authors : Li, H.; Delker, S.L.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 1.98 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.

---

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

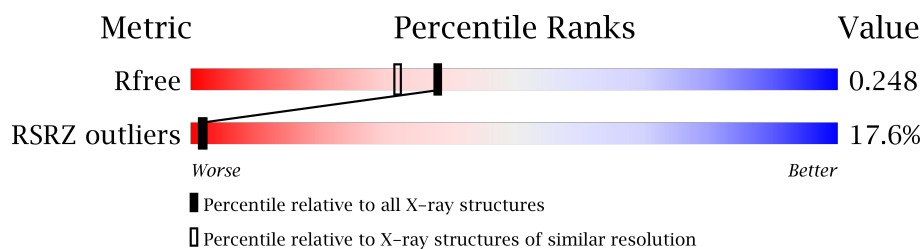
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	9293 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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
4	ACT	B	860	-	-	-	X
6	CL	B	930	-	-	-	X

## 2 Entry composition [i](#)

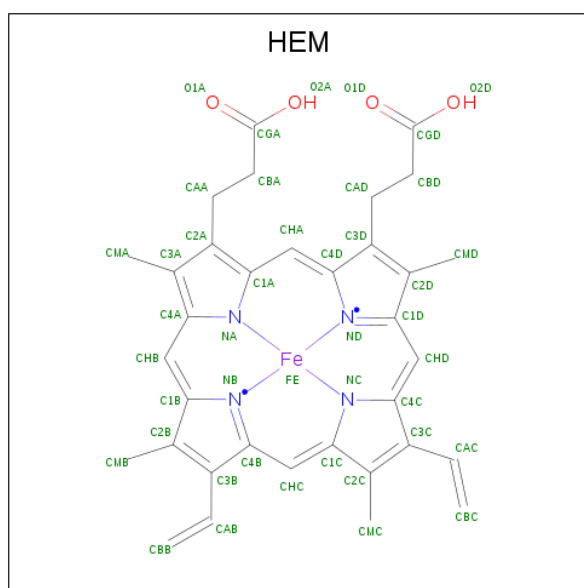
There are 7 unique types of molecules in this entry. The entry contains 7150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

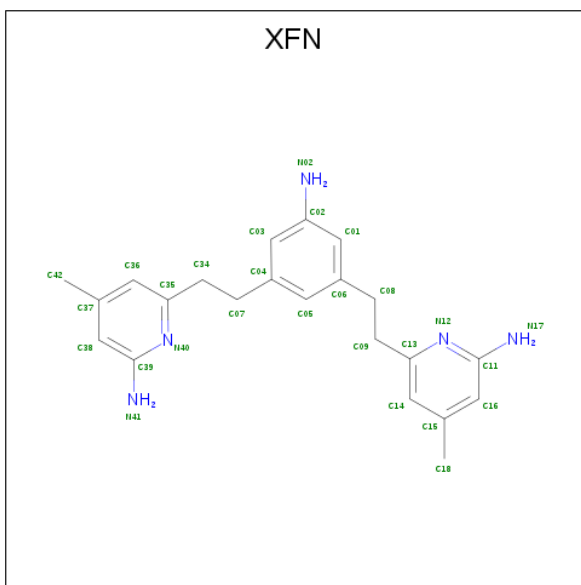
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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



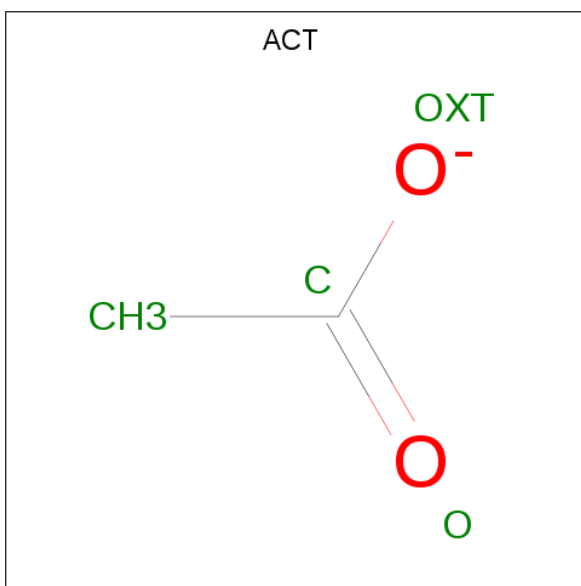
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6,6'-[(5-aminobenzene-1,3-diyl)diethane-2,1-diyl]bis(4-methylpyridin-2-amine) (three-letter code: XFN) (formula:  $C_{22}H_{27}N_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 27 22 5	0	0
3	B	1	Total C N 27 22 5	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Cl 2	0	0
6	A	2	Total 2	Cl 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total 139	O 139	0	0
7	B	198	Total 198	O 198	0	0

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

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.86Å 111.17Å 164.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.63 – 1.98 36.94 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.63-1.98) 99.8 (36.94-1.98)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.98Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.191 , 0.232 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	3282 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	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	7150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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](#)

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

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

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

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

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

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

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

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

#### 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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	13 (46%)	17,82,82	2.36	8 (47%)
3	XFN	A	800	-	29,29,29	0.99	1 (3%)	38,40,40	2.40	12 (31%)
4	ACT	A	860	-	1,3,3	1.59	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.27	11 (39%)	17,82,82	1.44	3 (17%)
3	XFN	B	800	-	29,29,29	0.92	0	38,40,40	2.11	10 (26%)
4	ACT	B	860	-	1,3,3	1.87	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	XFN	A	800	-	-	0/10/10/10	0/3/3/3
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	XFN	B	800	-	-	0/10/10/10	0/3/3/3
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-4.77	1.34	1.40
2	B	750	HEM	C3C-C2C	-4.68	1.34	1.40
2	A	750	HEM	C3B-C2B	-3.45	1.35	1.40
2	A	750	HEM	C3C-C2C	-3.30	1.36	1.40
2	B	750	HEM	CMB-C2B	2.04	1.55	1.51
2	A	750	HEM	CMB-C2B	2.04	1.55	1.51
2	A	750	HEM	CMD-C2D	2.11	1.55	1.51
2	B	750	HEM	CAA-C2A	2.22	1.55	1.52
2	B	750	HEM	CMD-C2D	2.25	1.56	1.51
2	A	750	HEM	CMC-C2C	2.32	1.56	1.51
2	A	750	HEM	CMA-C3A	2.33	1.56	1.51
2	B	750	HEM	CAD-C3D	2.36	1.56	1.52
2	A	750	HEM	C1C-NC	2.42	1.39	1.36
2	A	750	HEM	CAA-C2A	2.54	1.56	1.52
3	A	800	XFN	C05-C04	2.71	1.44	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C1B-NB	2.75	1.40	1.36
2	B	750	HEM	CMA-C3A	2.82	1.57	1.51
2	A	750	HEM	C3C-CAC	3.23	1.54	1.47
2	B	750	HEM	C3B-CAB	3.34	1.54	1.47
2	B	750	HEM	C3C-CAC	3.49	1.54	1.47
2	B	750	HEM	C4D-ND	3.61	1.41	1.36
2	A	750	HEM	C4D-ND	3.63	1.41	1.36
2	A	750	HEM	C3B-CAB	3.90	1.55	1.47
2	A	750	HEM	C3D-C2D	4.47	1.50	1.37
2	B	750	HEM	C3D-C2D	4.60	1.51	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	XFN	C15-C14-C13	-4.68	117.32	120.26
2	A	750	HEM	CBD-CAD-C3D	-3.83	105.15	112.47
3	A	800	XFN	C36-C35-N40	-3.79	118.80	122.91
2	A	750	HEM	CMA-C3A-C4A	-3.79	122.64	128.46
3	B	800	XFN	C36-C35-N40	-3.36	119.27	122.91
3	A	800	XFN	C14-C13-N12	-3.28	119.35	122.91
3	A	800	XFN	C07-C04-C03	-3.25	115.23	120.56
2	A	750	HEM	C1D-C2D-C3D	-3.11	104.83	107.00
2	B	750	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
3	B	800	XFN	C15-C14-C13	-2.91	118.44	120.26
3	B	800	XFN	C14-C13-N12	-2.85	119.82	122.91
3	A	800	XFN	C18-C15-C16	-2.65	117.04	120.94
2	B	750	HEM	CBD-CAD-C3D	-2.43	107.83	112.47
2	A	750	HEM	C4A-C3A-C2A	2.04	108.41	107.00
2	A	750	HEM	CMA-C3A-C2A	2.12	128.95	124.94
3	B	800	XFN	N41-C39-N40	2.16	120.28	116.64
3	B	800	XFN	C07-C04-C05	2.20	124.17	120.56
3	B	800	XFN	C08-C09-C13	2.22	117.34	112.71
3	A	800	XFN	N41-C39-N40	2.43	120.73	116.64
3	B	800	XFN	C09-C13-C14	2.45	124.49	121.19
3	A	800	XFN	C16-C15-C14	2.67	121.39	118.09
2	B	750	HEM	CMA-C3A-C2A	2.77	130.17	124.94
2	A	750	HEM	CBA-CAA-C2A	3.13	118.47	112.48
3	A	800	XFN	C07-C04-C05	3.14	125.71	120.56
3	B	800	XFN	C34-C35-N40	3.17	120.37	115.78
2	A	750	HEM	C4C-C3C-C2C	3.19	109.12	106.90
2	A	750	HEM	CMC-C2C-C3C	3.60	131.56	124.89
3	A	800	XFN	C34-C35-N40	3.67	121.09	115.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	XFN	C09-C13-C14	3.69	126.16	121.19
3	B	800	XFN	C39-N40-C35	5.08	121.76	118.17
3	A	800	XFN	C39-N40-C35	5.11	121.78	118.17
3	B	800	XFN	C11-N12-C13	7.57	123.52	118.17
3	A	800	XFN	C11-N12-C13	8.04	123.85	118.17

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	407/422 (96%)	1.17	96 (23%)  	31, 56, 96, 124	0
1	B	411/422 (97%)	0.68	48 (11%)  	31, 45, 71, 87	0
All	All	818/844 (96%)	0.92	144 (17%)  	31, 50, 89, 124	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.3
1	A	716	TRP	8.5
1	B	348	VAL	6.4
1	A	300	PHE	6.2
1	B	718	GLY	5.9
1	A	715	VAL	5.8
1	A	355	PHE	5.8
1	A	488	PRO	5.8
1	A	322	LEU	5.0
1	B	619	ARG	4.8
1	A	567	VAL	4.6
1	A	479	LEU	4.5
1	A	338	PRO	4.5
1	A	352	ASP	4.5
1	A	489	ASP	4.3
1	A	351	LYS	4.2
1	A	486	LYS	4.2
1	A	593	ILE	4.2
1	A	491	SER	4.1
1	A	485	TYR	4.0
1	A	678	TRP	4.0
1	A	490	GLY	3.9
1	A	591	THR	3.9
1	B	616	LEU	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	554	PHE	3.8
1	A	713	THR	3.7
1	A	712	ASN	3.7
1	A	584	PHE	3.7
1	A	311	VAL	3.7
1	A	619	ARG	3.7
1	B	338	PRO	3.6
1	A	415	CYS	3.6
1	A	667	ARG	3.6
1	B	567	VAL	3.6
1	A	507	GLN	3.6
1	A	679	ILE	3.5
1	A	390	SER	3.5
1	A	514	ARG	3.5
1	B	620	LYS	3.5
1	A	677	VAL	3.4
1	A	487	GLN	3.3
1	B	310	VAL	3.3
1	A	680	VAL	3.3
1	A	389	GLU	3.2
1	B	350	THR	3.2
1	A	566	ALA	3.2
1	A	676	TRP	3.2
1	A	508	GLN	3.2
1	A	388	ILE	3.2
1	A	511	LYS	3.2
1	A	714	HIS	3.2
1	A	681	PRO	3.1
1	A	299	ARG	3.1
1	A	685	GLY	3.1
1	B	351	LYS	3.1
1	A	321	THR	3.1
1	B	299	ARG	3.1
1	B	667	ARG	3.0
1	A	492	THR	3.0
1	A	354	LEU	3.0
1	A	704	PHE	3.0
1	A	350	THR	3.0
1	A	682	PRO	3.0
1	B	680	VAL	3.0
1	A	503	GLU	2.9
1	A	565	PRO	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	2.9
1	A	392	SER	2.9
1	B	591	THR	2.9
1	B	311	VAL	2.9
1	B	677	VAL	2.8
1	B	715	VAL	2.8
1	A	594	GLY	2.8
1	A	393	THR	2.8
1	A	588	TYR	2.8
1	B	566	ALA	2.7
1	A	385	ASN	2.7
1	A	506	ILE	2.7
1	A	416	VAL	2.7
1	B	322	LEU	2.7
1	A	509	GLY	2.6
1	A	595	VAL	2.6
1	B	691	PHE	2.6
1	B	309	ASP	2.6
1	B	561	TRP	2.6
1	A	596	ARG	2.6
1	A	686	SER	2.6
1	A	391	THR	2.6
1	B	679	ILE	2.5
1	B	352	ASP	2.5
1	B	678	TRP	2.5
1	B	301	LEU	2.5
1	B	617	ASP	2.5
1	B	565	PRO	2.5
1	B	409	TRP	2.5
1	A	480	ILE	2.4
1	B	584	PHE	2.4
1	A	668	CYS	2.4
1	A	467	ASP	2.4
1	A	706	TYR	2.4
1	B	704	PHE	2.4
1	A	568	SER	2.4
1	A	323	GLU	2.4
1	B	593	ILE	2.4
1	A	366	TYR	2.4
1	B	582	CYS	2.4
1	B	630	LEU	2.3
1	B	713	THR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	590	GLY	2.3
1	A	550	LYS	2.3
1	A	442	ILE	2.3
1	B	615	ASP	2.3
1	B	588	TYR	2.3
1	A	561	TRP	2.2
1	A	630	LEU	2.2
1	A	589	MET	2.2
1	B	572	LEU	2.2
1	B	323	GLU	2.2
1	B	618	MET	2.2
1	A	581	ALA	2.2
1	A	564	LEU	2.1
1	A	582	CYS	2.1
1	A	386	LYS	2.1
1	A	482	TYR	2.1
1	A	412	ALA	2.1
1	A	371	ARG	2.1
1	B	329	HIS	2.1
1	B	389	GLU	2.1
1	A	315	THR	2.1
1	B	415	CYS	2.1
1	A	469	LYS	2.1
1	A	512	ALA	2.1
1	A	504	ILE	2.1
1	B	480	ILE	2.1
1	A	620	LYS	2.1
1	A	470	HIS	2.0
1	A	552	ASP	2.0
1	A	617	ASP	2.0
1	A	570	MET	2.0
1	A	618	MET	2.0
1	B	353	GLN	2.0
1	B	302	LYS	2.0
1	A	394	TYR	2.0
1	B	683	MET	2.0

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

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	0.86	0.40	12.76	75,77,77,77	0
4	ACT	B	860	4/4	0.87	0.27	9.55	64,67,67,67	0
6	CL	B	930	1/1	0.97	0.28	4.90	50,50,50,50	0
3	XFN	A	800	27/27	0.90	0.28	1.22	36,42,47,47	0
3	XFN	B	800	27/27	0.92	0.23	0.92	35,41,44,45	0
6	CL	A	930	1/1	0.98	0.24	0.49	49,49,49,49	0
2	HEM	B	750	43/43	0.98	0.18	0.47	28,35,47,51	0
2	HEM	A	750	43/43	0.97	0.21	0.18	29,33,47,54	0
5	ZN	A	900	1/1	0.99	0.07	-1.49	40,40,40,40	0
6	CL	A	910	1/1	0.99	0.12	-	45,45,45,45	0
6	CL	B	910	1/1	0.98	0.12	-	45,45,45,45	0
5	ZN	A	901	1/1	0.99	0.12	-	35,35,35,35	1
5	ZN	A	719	1/1	0.99	0.13	-	35,35,35,35	1

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

There are no such residues in this entry.