



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N64  
Title : Structure of neuronal nitric oxide synthase D597N mutant 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 : 2010-05-25  
Resolution : 1.95 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

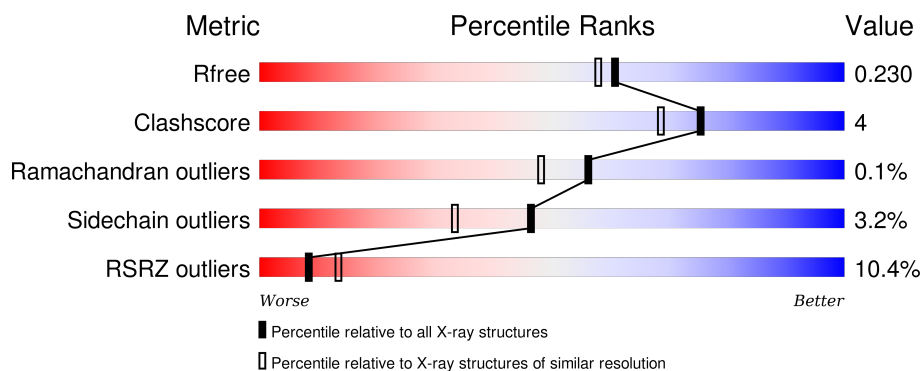
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	422	<div> <div>14%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	422	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</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
3	XFN	A	800	-	-	-	X
4	ACT	A	860	-	-	-	X
4	ACT	B	860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7189 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.

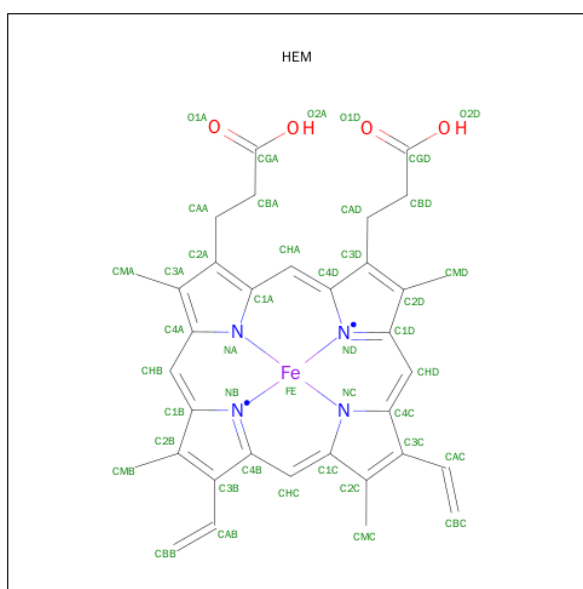
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3316	2123	567	604	22			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	575	609	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

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



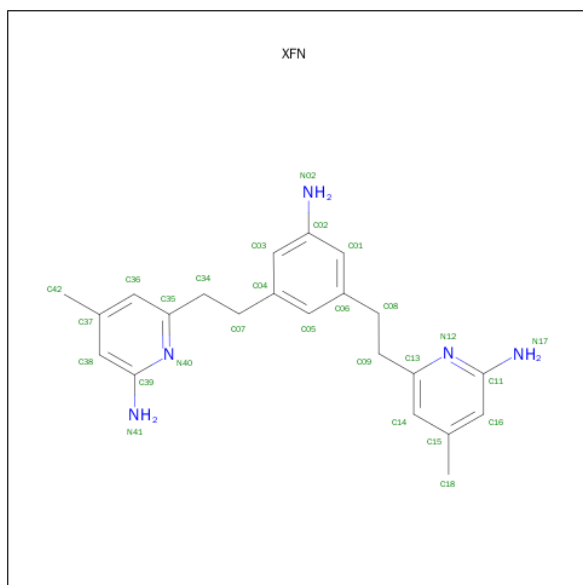
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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-METHYL PYRIDIN-2-AMINE) (three-letter code: XFN) (formula: C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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

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

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

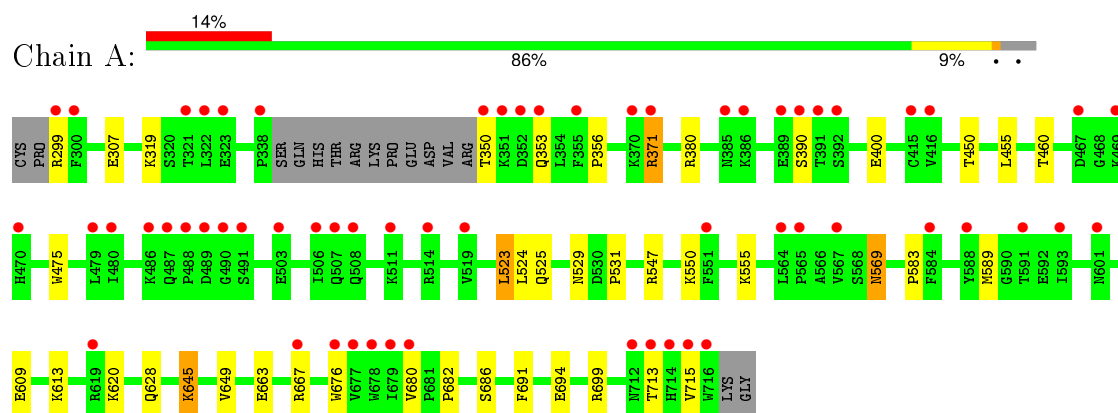
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	159	Total	O	0	0
			159	159		
7	B	214	Total	O	0	0
			214	214		

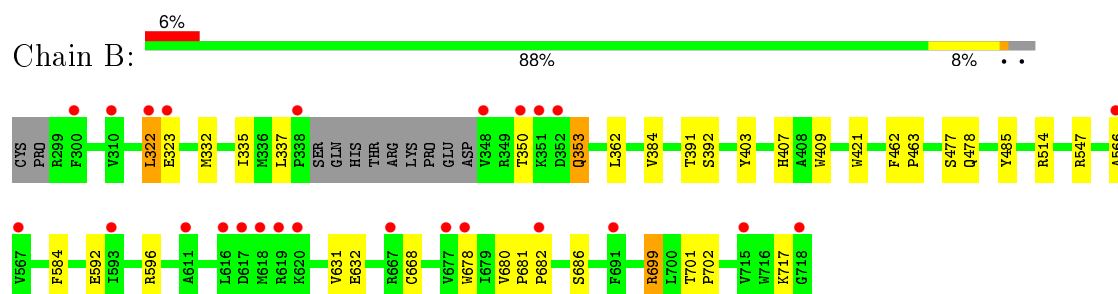
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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



#### • Molecule 1: Nitric oxide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.76Å 110.21Å 164.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.08 – 1.95 38.83 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.08-1.95) 99.7 (38.83-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.183 , 0.217 0.196 , 0.230	Depositor DCC
$R_{free}$ test set	3422 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 69402 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, HEM, ZN, CL, XFN

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	0/3412	0.63	0/4629
1	B	0.64	0/3438	0.65	0/4661
All	All	0.61	0/6850	0.64	0/9290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3316	0	3228	25	0
1	B	3345	0	3261	25	0
2	A	43	0	30	3	0
2	B	43	0	30	6	0
3	A	27	0	27	0	0
3	B	27	0	27	1	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	3	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	159	0	0	3	0
7	B	214	0	0	1	0
All	All	7189	0	6609	52	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 4.

All (52) 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:B:699:ARG:HH11	1:B:699:ARG:HG2	1.07	1.08
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.92	0.82
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.42	0.82
1:B:699:ARG:NH1	1:B:699:ARG:HG2	1.83	0.79
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.65	0.78
1:B:668:CYS:HB3	7:B:1185:HOH:O	1.89	0.70
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.74	0.70
1:A:609:GLU:HG3	7:A:1022:HOH:O	1.99	0.63
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.06	0.62
1:B:699:ARG:HH11	1:B:699:ARG:CG	1.95	0.61
2:B:750:HEM:HBA2	2:B:750:HEM:HMA1	1.85	0.59
1:A:686:SER:HB2	1:B:682:PRO:HB2	1.84	0.59
1:B:323:GLU:O	1:B:699:ARG:HD2	2.04	0.57
1:B:322:LEU:HB2	1:B:699:ARG:HD3	1.86	0.57
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.87	0.55
1:A:353:GLN:O	1:A:356:PRO:HD2	2.07	0.54
1:B:678:TRP:CZ3	3:B:800:XFN:H08	2.45	0.52
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.93	0.51
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.41	0.51
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.11	0.50
1:A:450:THR:HA	1:A:455:LEU:HD22	1.94	0.49
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.46	0.48
1:A:525:GLN:HG3	1:A:529:ASN:O	2.13	0.48
1:A:682:PRO:HB2	1:B:686:SER:HB2	1.96	0.47
2:A:750:HEM:CGA	2:A:750:HEM:HMA1	2.45	0.47
1:B:478:GLN:HA	1:B:566:ALA:O	2.15	0.47
1:B:592:GLU:HB3	1:B:596:ARG:NH2	2.29	0.47
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.46
2:A:750:HEM:HMC1	2:A:750:HEM:HBC2	1.98	0.46
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.82	0.46
1:A:307:GLU:HG2	7:A:1138:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.46
1:A:460:THR:O	1:A:583:PRO:HD2	2.15	0.46
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.52	0.44
2:B:750:HEM:CBA	2:B:750:HEM:HMA1	2.47	0.44
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.99	0.44
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.00	0.44
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.48	0.43
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.53	0.43
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.53	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:A:699:ARG:NH1	7:A:1063:HOH:O	2.51	0.43
1:B:584:PHE:CD1	2:B:750:HEM:CAC	3.02	0.43
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.42
1:A:569:ASN:H	1:A:569:ASN:HD22	1.67	0.42
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.47	0.42
1:A:663:GLU:O	1:A:667:ARG:HG2	2.21	0.41
1:B:391:THR:O	1:B:392:SER:HB2	2.20	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.95	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.21	0.41
1:B:353:GLN:HG2	1:B:353:GLN:H	1.72	0.41

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	404/422 (96%)	390 (96%)	14 (4%)	0	100	100
1	B	407/422 (96%)	398 (98%)	8 (2%)	1 (0%)	52	43
All	All	811/844 (96%)	788 (97%)	22 (3%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	LEU

### 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	364/377 (97%)	349 (96%)	15 (4%)	37	22
1	B	366/377 (97%)	358 (98%)	8 (2%)	60	51
All	All	730/754 (97%)	707 (97%)	23 (3%)	46	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	319	LYS
1	A	350	THR
1	A	371	ARG
1	A	390	SER
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	555	LYS
1	A	569	ASN
1	A	613	LYS
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	332	MET
1	B	337	LEU
1	B	350	THR
1	B	353	GLN
1	B	477	SER
1	B	547	ARG
1	B	699	ARG

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Mol	Chain	Res	Type
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	605	ASN
1	B	697	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 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	30,50,50	2.23	10 (33%)	24,82,82	2.79	12 (50%)
3	XFN	A	800	-	29,29,29	0.79	0	40,40,40	2.20	12 (30%)
4	ACT	A	860	-	1,3,3	1.48	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.08	8 (26%)	24,82,82	2.76	14 (58%)
3	XFN	B	800	-	29,29,29	0.74	0	40,40,40	1.97	13 (32%)
4	ACT	B	860	-	1,3,3	1.70	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	-	0/10/54/54	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	-	0/10/54/54	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-5.91	1.46	1.51
2	B	750	HEM	C3D-C4D	-5.89	1.44	1.51
2	A	750	HEM	C3D-C4D	-5.83	1.44	1.51
2	B	750	HEM	C3B-C4B	-5.71	1.46	1.51
2	A	750	HEM	C2C-C1C	-4.39	1.44	1.52
2	B	750	HEM	C2C-C1C	-3.70	1.45	1.52
2	A	750	HEM	C2B-C1B	-2.26	1.44	1.51
2	B	750	HEM	C2D-C1D	-2.23	1.44	1.51
2	B	750	HEM	C2B-C1B	-2.04	1.45	1.51
2	A	750	HEM	C2D-C1D	-2.03	1.45	1.51
2	B	750	HEM	C3B-CAB	2.04	1.55	1.51
2	A	750	HEM	CMA-C3A	2.34	1.56	1.51
2	A	750	HEM	CAA-C2A	2.50	1.56	1.52
2	A	750	HEM	C3B-CAB	2.52	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CMA-C3A	2.61	1.57	1.51
2	B	750	HEM	FE-NC	2.72	2.06	1.95
2	A	750	HEM	FE-NB	2.79	2.12	1.97
2	A	750	HEM	FE-NC	2.85	2.07	1.95

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CAA-C2A-C1A	-6.11	120.38	127.01
2	A	750	HEM	CAA-C2A-C1A	-4.52	122.10	127.01
3	A	800	XFN	C36-C35-N40	-3.73	118.75	122.96
2	A	750	HEM	C3C-CAC-CBC	-3.50	119.08	124.46
2	B	750	HEM	CMA-C3A-C4A	-3.47	122.63	128.36
2	A	750	HEM	CBD-CAD-C3D	-3.34	103.82	113.55
3	A	800	XFN	C14-C13-N12	-3.31	119.23	122.96
2	A	750	HEM	CMA-C3A-C4A	-2.90	123.57	128.36
3	A	800	XFN	C37-C36-C35	-2.82	118.51	120.28
3	B	800	XFN	C15-C14-C13	-2.80	118.53	120.28
3	A	800	XFN	C08-C06-C01	-2.75	115.95	120.56
2	B	750	HEM	C3C-CAC-CBC	-2.68	120.34	124.46
3	B	800	XFN	C36-C35-N40	-2.62	120.00	122.96
2	B	750	HEM	CBD-CAD-C3D	-2.61	105.96	113.55
3	B	800	XFN	C37-C36-C35	-2.55	118.68	120.28
3	B	800	XFN	C14-C13-N12	-2.52	120.12	122.96
3	B	800	XFN	C02-C01-C06	-2.38	118.94	120.84
3	B	800	XFN	C07-C04-C03	-2.37	116.59	120.56
2	B	750	HEM	C3B-C4B-NB	-2.02	107.76	111.63
3	A	800	XFN	C16-C15-C14	2.01	120.64	118.08
3	B	800	XFN	N41-C39-N40	2.19	120.49	116.50
3	B	800	XFN	C08-C09-C13	2.23	116.82	112.53
3	A	800	XFN	C38-C37-C36	2.35	121.08	118.08
2	B	750	HEM	C3B-C4B-CHC	2.36	126.49	123.16
3	B	800	XFN	N17-C11-N12	2.37	120.83	116.50
3	A	800	XFN	N17-C11-N12	2.38	120.85	116.50
2	A	750	HEM	CMD-C2D-C3D	2.42	125.06	114.35
2	B	750	HEM	CMA-C3A-C2A	2.49	130.44	125.24
2	B	750	HEM	CMD-C2D-C3D	2.52	125.49	114.35
3	B	800	XFN	C07-C04-C05	2.55	124.83	120.56
2	B	750	HEM	C2D-C3D-C4D	2.70	106.08	101.50
2	B	750	HEM	C2C-C1C-CHC	2.80	127.94	123.68
3	A	800	XFN	C08-C06-C05	2.88	125.39	120.56
3	A	800	XFN	C34-C35-C36	3.03	125.39	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C2D-C3D-C4D	3.11	106.77	101.50
2	A	750	HEM	C3B-C4B-CHC	3.18	127.64	123.16
2	A	750	HEM	CBA-CAA-C2A	3.55	118.89	112.53
3	B	800	XFN	C34-C35-N40	3.85	121.38	115.69
2	A	750	HEM	CAD-C3D-C4D	3.92	126.28	112.47
2	B	750	HEM	CAD-C3D-C2D	4.13	125.08	113.22
2	B	750	HEM	CMC-C2C-C3C	4.25	127.14	116.53
3	A	800	XFN	C09-C13-N12	4.32	122.08	115.69
2	B	750	HEM	CMB-C2B-C3B	4.34	127.37	116.53
2	A	750	HEM	CMB-C2B-C3B	4.43	127.59	116.53
2	B	750	HEM	CAD-C3D-C4D	4.63	128.80	112.47
2	A	750	HEM	CAD-C3D-C2D	4.77	126.94	113.22
3	A	800	XFN	C11-N12-C13	4.81	121.65	118.23
3	B	800	XFN	C39-N40-C35	4.92	121.73	118.23
3	B	800	XFN	C11-N12-C13	5.27	121.97	118.23
2	A	750	HEM	CMC-C2C-C3C	5.44	130.11	116.53
3	A	800	XFN	C39-N40-C35	7.47	123.54	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	3	0
2	B	750	HEM	6	0
3	B	800	XFN	1	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 ⓘ

### 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	407/422 (96%)	0.76	60 (14%) 3 5	22, 39, 66, 85	0
1	B	411/422 (97%)	0.38	25 (6%) 25 34	21, 32, 55, 73	0
All	All	818/844 (96%)	0.57	85 (10%) 8 13	21, 36, 61, 85	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	8.4
1	A	716	TRP	7.4
1	B	718	GLY	7.1
1	A	300	PHE	6.9
1	B	300	PHE	6.6
1	A	488	PRO	5.8
1	A	299	ARG	5.5
1	A	352	ASP	5.3
1	B	348	VAL	5.3
1	B	350	THR	5.2
1	B	619	ARG	5.2
1	A	713	THR	5.0
1	B	338	PRO	4.4
1	A	355	PHE	4.2
1	A	350	THR	4.2
1	B	351	LYS	4.1
1	B	322	LEU	4.1
1	A	322	LEU	4.1
1	B	616	LEU	3.9
1	A	351	LYS	3.8
1	B	620	LYS	3.6
1	A	619	ARG	3.6
1	A	677	VAL	3.6
1	A	593	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	390	SER	3.3
1	A	507	GLN	3.3
1	B	611	ALA	3.2
1	A	321	THR	3.2
1	A	338	PRO	3.1
1	A	678	TRP	3.1
1	A	712	ASN	3.1
1	A	714	HIS	3.0
1	A	389	GLU	3.0
1	B	352	ASP	2.9
1	B	677	VAL	2.9
1	A	385	ASN	2.8
1	A	490	GLY	2.8
1	A	588	TYR	2.7
1	A	415	CYS	2.7
1	A	676	TRP	2.7
1	A	667	ARG	2.7
1	A	679	ILE	2.6
1	A	680	VAL	2.6
1	A	514	ARG	2.6
1	A	491	SER	2.6
1	A	479	LEU	2.5
1	A	470	HIS	2.5
1	A	386	LYS	2.5
1	B	667	ARG	2.5
1	A	567	VAL	2.5
1	A	503	GLU	2.5
1	A	551	PHE	2.4
1	B	678	TRP	2.4
1	B	691	PHE	2.4
1	B	323	GLU	2.4
1	A	489	ASP	2.4
1	A	323	GLU	2.4
1	A	467	ASP	2.4
1	A	591	THR	2.4
1	A	370	LYS	2.4
1	A	486	LYS	2.4
1	B	617	ASP	2.4
1	A	519	VAL	2.4
1	A	480	ILE	2.3
1	A	469	LYS	2.3
1	B	715	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	511	LYS	2.3
1	A	584	PHE	2.2
1	A	371	ARG	2.2
1	A	487	GLN	2.2
1	B	566	ALA	2.2
1	A	506	ILE	2.2
1	A	508	GLN	2.2
1	A	391	THR	2.1
1	A	601	ASN	2.1
1	B	593	ILE	2.1
1	A	565	PRO	2.1
1	B	310	VAL	2.1
1	A	392	SER	2.1
1	A	416	VAL	2.1
1	B	682	PRO	2.1
1	A	564	LEU	2.0
1	B	567	VAL	2.0
1	A	353	GLN	2.0
1	B	618	MET	2.0

## 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
4	ACT	A	860	4/4	0.86	0.29	7.53	55,56,56,57	0
4	ACT	B	860	4/4	0.90	0.16	5.32	39,40,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	XFN	A	800	27/27	0.91	0.27	2.26	25,30,35,36	0
3	XFN	B	800	27/27	0.94	0.18	0.67	24,29,32,34	0
2	HEM	A	750	43/43	0.98	0.19	0.61	19,24,34,35	0
2	HEM	B	750	43/43	0.98	0.15	0.42	21,24,35,38	0
6	CL	A	930	1/1	0.98	0.15	-0.84	32,32,32,32	0
6	CL	B	930	1/1	0.99	0.14	-1.46	29,29,29,29	0
5	ZN	A	900	1/1	0.99	0.07	-2.22	30,30,30,30	0
5	ZN	A	719	1/1	0.99	0.13	-	24,24,24,24	1
5	ZN	A	901	1/1	1.00	0.13	-	23,23,23,23	1
6	CL	B	910	1/1	0.99	0.14	-	33,33,33,33	0
6	CL	A	910	1/1	0.99	0.13	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.