



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

PDB ID : 3JX1  
Title : Structure of rat neuronal nitric oxide synthase D597N mutant heme domain  
in complex with N1-{(3'R,4'R)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]  
pyrrolidin-3'-yl}-N2-(3'-fluorophenethyl)ethane-1,2-diamine  
Authors : Delker, S.L.; Li, H.; Poulos, T.L.  
Deposited on : 2009-09-18  
Resolution : 2.00 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

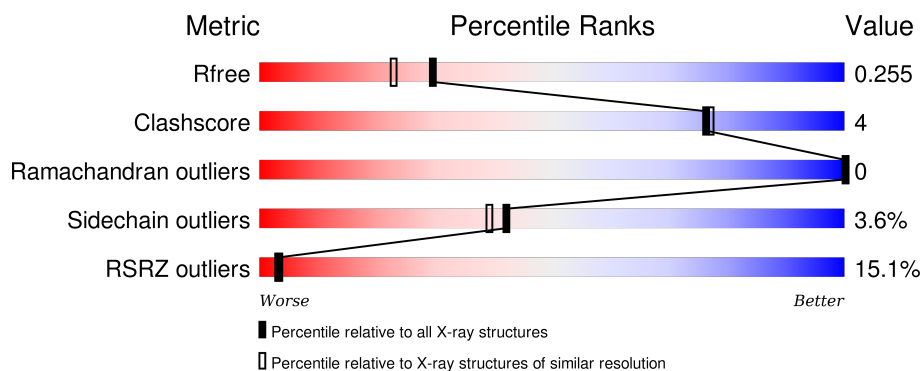
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>19%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	422	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>9%</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
5	ACT	A	860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7215 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	407	Total	C	N	O	S	0	0	0
			3313	2121	567	604	21			
1	B	410	Total	C	N	O	S	0	0	0
			3340	2138	574	607	21			

There are 2 discrepancies between the modelled and reference sequences:

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

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



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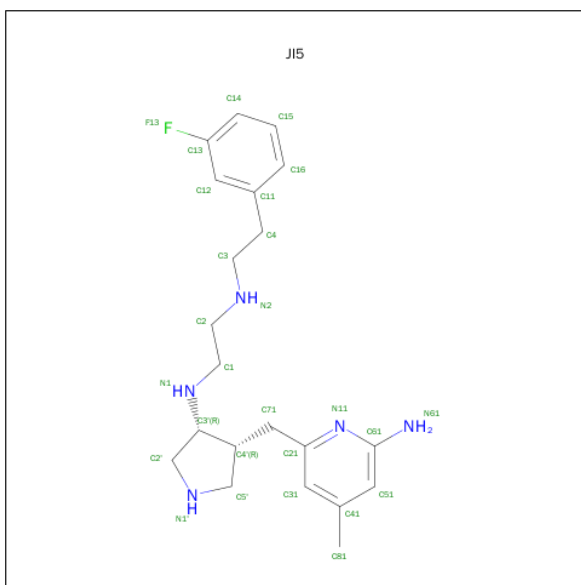
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 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 N-{(3R,4R)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-[2-(3-FLUOROPHENYL)ETHYL]ETHANE-1,2-DIAMINE (three-letter code: JI5) (formula:  $C_{21}H_{30}FN_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	21	1	5		
4	B	1	Total	C	F	N	0	0
			27	21	1	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

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

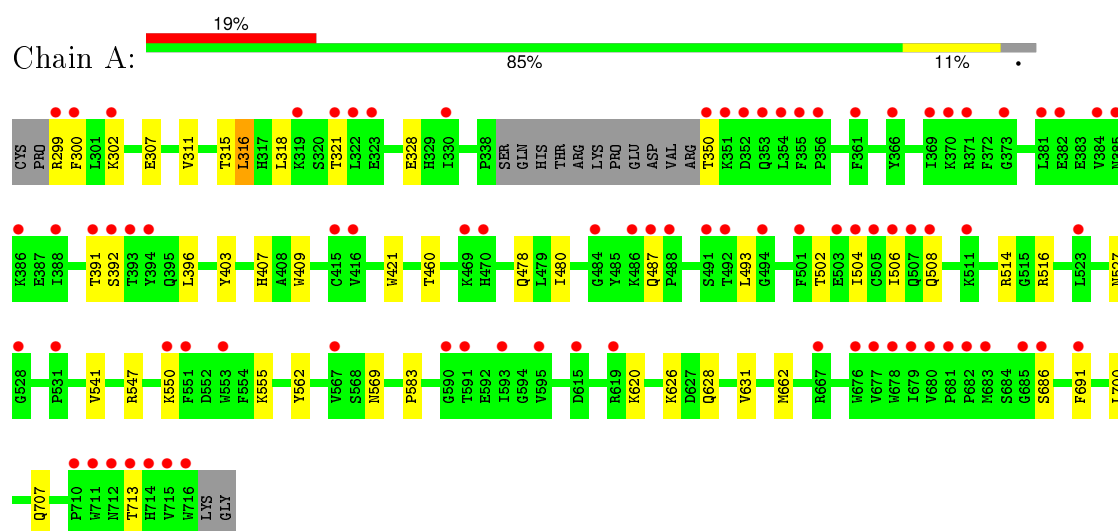
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total 165	O 165	0	0
7	B	214	Total 214	O 214	0	0

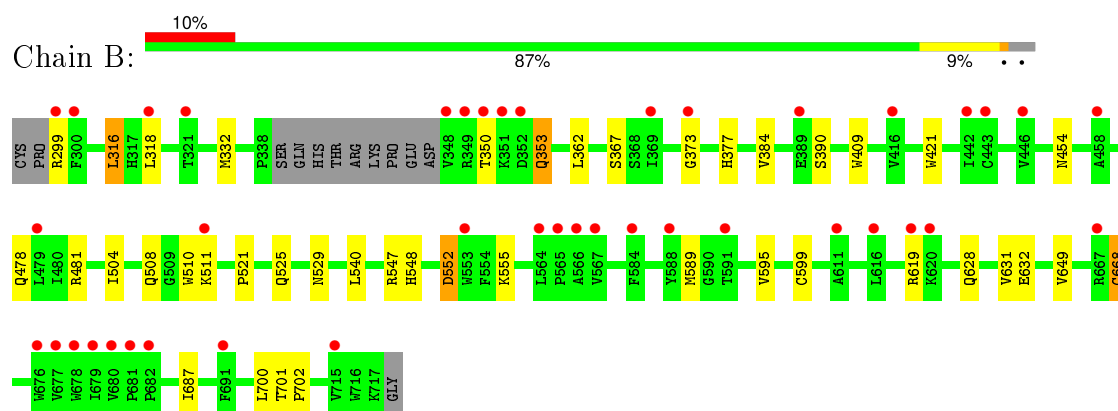
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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, brain



- Molecule 1: Nitric oxide synthase, brain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.02Å 110.88Å 164.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.27 – 2.00 45.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (45.27-2.00) 92.3 (45.27-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.178 , 0.216 0.227 , 0.255	Depositor DCC
$R_{free}$ test set	2986 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.9	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 60178 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: HEM, ZN, JI5, H4B, ACT

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	0/3406	0.65	0/4621
1	B	0.65	1/3433 (0.0%)	0.65	0/4656
All	All	0.62	1/6839 (0.0%)	0.65	0/9277

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	668	CYS	CB-SG	5.01	1.90	1.82

There are no bond angle outliers.

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	3313	0	3223	21	0
1	B	3340	0	3258	23	0
2	A	43	0	30	4	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	1	0
4	B	27	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	165	0	0	1	0
7	B	214	0	0	3	0
All	All	7215	0	6637	51	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 (51) 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:668:CYS:HB2	7:B:1015:HOH:O	1.52	1.08
1:B:373:GLY:H	1:B:377:HIS:HD2	0.96	0.95
1:B:373:GLY:H	1:B:377:HIS:CD2	1.88	0.90
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.57	0.86
1:A:307:GLU:HG3	7:B:1029:HOH:O	1.82	0.80
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.71	0.71
1:B:373:GLY:N	1:B:377:HIS:HD2	1.81	0.69
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.23	0.67
1:A:299:ARG:HG2	1:A:318:LEU:HD21	1.77	0.67
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.78	0.66
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.82	0.61
1:A:302:LYS:HD3	1:A:311:VAL:HG11	1.85	0.58
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.35	0.56
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.90	0.53
1:B:299:ARG:HG2	1:B:318:LEU:HD21	1.91	0.53
1:A:299:ARG:HA	7:A:1005:HOH:O	2.08	0.53
1:B:525:GLN:HG3	1:B:529:ASN:O	2.09	0.53
2:B:750:HEM:HMC1	2:B:750:HEM:HBC2	1.93	0.51
1:A:569:ASN:O	1:A:707:GLN:HG2	2.12	0.50
1:A:391:THR:O	1:A:392:SER:OG	2.28	0.49
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.01	0.49
1:A:502:THR:O	1:A:506:ILE:HG12	2.12	0.49
1:B:552:ASP:OD2	1:B:555:LYS:NZ	2.47	0.48
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.93	0.48
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.95	0.48
1:A:299:ARG:HG2	1:A:318:LEU:CD2	2.44	0.47
1:B:504:ILE:O	1:B:508:GLN:HG2	2.15	0.47
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLN:NE2	1:A:562:TYR:OH	2.48	0.46
1:B:701:THR:HA	1:B:702:PRO:C	2.36	0.46
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.52	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.45
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.52	0.45
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.57	0.45
1:B:595:VAL:O	1:B:599:CYS:HB2	2.18	0.43
1:B:511:LYS:HG2	7:B:1153:HOH:O	2.18	0.43
1:A:302:LYS:HD3	1:A:311:VAL:CG1	2.47	0.43
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	2.00	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.43
1:A:316:LEU:HD13	1:A:700:LEU:HD11	2.01	0.42
1:A:504:ILE:O	1:A:508:GLN:HG2	2.19	0.42
1:B:316:LEU:HD13	1:B:700:LEU:HD11	2.00	0.42
2:A:750:HEM:HBA1	4:A:800:JI5:H4	2.00	0.42
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.42
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.42	0.41
1:A:460:THR:O	1:A:583:PRO:HD2	2.21	0.41
1:B:619:ARG:HE	1:B:619:ARG:HB2	1.65	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.02	0.41
1:B:589:MET:HA	1:B:649:VAL:O	2.21	0.40
2:B:750:HEM:HMC1	2:B:750:HEM:CBC	2.51	0.40
2:B:750:HEM:HBA1	4:B:800:JI5:H4	2.03	0.40

There are no symmetry-related clashes.

## 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	403/422 (96%)	392 (97%)	11 (3%)	0	100	100
1	B	406/422 (96%)	397 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	809/844 (96%)	789 (98%)	20 (2%)	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	363/377 (96%)	347 (96%)	16 (4%)	35	30
1	B	366/377 (97%)	356 (97%)	10 (3%)	52	52
All	All	729/754 (97%)	703 (96%)	26 (4%)	42	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	321	THR
1	A	328	GLU
1	A	350	THR
1	A	396	LEU
1	A	487	GLN
1	A	493	LEU
1	A	514	ARG
1	A	516	ARG
1	A	527	ASN
1	A	547	ARG
1	A	550	LYS
1	A	555	LYS
1	A	620	LYS
1	A	662	MET
1	A	713	THR
1	B	316	LEU
1	B	332	MET
1	B	350	THR
1	B	353	GLN

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Mol	Chain	Res	Type
1	B	367	SER
1	B	390	SER
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	HIS
1	A	451	ASN
1	A	454	ASN
1	A	478	GLN
1	A	500	GLN
1	A	634	ASN
1	A	697	ASN
1	B	377	HIS
1	B	451	ASN
1	B	454	ASN
1	B	478	GLN
1	B	507	GLN
1	B	508	GLN
1	B	535	GLN
1	B	634	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

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	30,50,50	2.23	9 (30%)	24,82,82	2.84	12 (50%)
3	H4B	A	760	-	13,18,18	0.85	0	11,26,26	2.79	5 (45%)
4	JI5	A	800	-	26,29,29	0.74	0	30,38,38	1.81	7 (23%)
5	ACT	A	860	-	1,3,3	1.49	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	1.95	7 (23%)	24,82,82	2.58	15 (62%)
3	H4B	B	760	-	13,18,18	1.00	0	11,26,26	2.38	5 (45%)
4	JI5	B	800	-	26,29,29	0.82	0	30,38,38	2.11	7 (23%)
5	ACT	B	860	-	1,3,3	1.38	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	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JI5	A	800	-	-	0/13/23/23	0/3/3/3
5	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	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	JI5	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-6.13	1.43	1.51
2	A	750	HEM	C3B-C4B	-6.08	1.46	1.51
2	B	750	HEM	C3B-C4B	-4.86	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C2C-C1C	-4.29	1.44	1.52
2	B	750	HEM	C3D-C4D	-4.16	1.46	1.51
2	B	750	HEM	C2C-C1C	-3.97	1.45	1.52
2	A	750	HEM	C2B-C1B	-2.23	1.44	1.51
2	A	750	HEM	C2D-C1D	-2.22	1.44	1.51
2	A	750	HEM	CAA-C2A	2.07	1.55	1.52
2	B	750	HEM	FE-NB	2.11	2.08	1.97
2	A	750	HEM	FE-NB	2.20	2.09	1.97
2	B	750	HEM	C1C-NC	2.48	1.39	1.36
2	A	750	HEM	FE-NC	2.73	2.06	1.95
2	A	750	HEM	FE-ND	2.74	2.12	1.97
2	B	750	HEM	FE-NC	2.77	2.06	1.95
2	B	750	HEM	FE-ND	2.94	2.13	1.97

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBD-CAD-C3D	-5.19	98.45	113.55
2	A	750	HEM	CBA-CAA-C2A	-4.67	104.16	112.53
4	A	800	JI5	C3-C4-C11	-3.93	104.67	112.83
3	A	760	H4B	N3-C2-N1	-3.68	119.50	125.53
2	B	750	HEM	CBD-CAD-C3D	-3.65	102.92	113.55
2	B	750	HEM	CAA-C2A-C1A	-3.32	123.41	127.01
4	B	800	JI5	C3-C4-C11	-3.28	106.03	112.83
2	A	750	HEM	C3C-CAC-CBC	-3.27	119.44	124.46
3	B	760	H4B	N3-C2-N1	-3.20	120.28	125.53
4	A	800	JI5	C31-C21-N11	-2.79	119.81	122.96
4	B	800	JI5	C31-C21-N11	-2.75	119.86	122.96
2	B	750	HEM	CAA-CBA-CGA	-2.68	107.84	112.75
4	B	800	JI5	C2'-C3'-N1	-2.56	106.54	111.90
4	A	800	JI5	C2'-C3'-N1	-2.55	106.56	111.90
2	B	750	HEM	CBA-CAA-C2A	-2.54	107.98	112.53
2	A	750	HEM	CAA-C2A-C1A	-2.43	124.37	127.01
2	A	750	HEM	CMA-C3A-C4A	-2.37	124.44	128.36
2	B	750	HEM	C3B-C4B-NB	-2.26	107.30	111.63
2	B	750	HEM	C3C-CAC-CBC	-2.22	121.05	124.46
4	B	800	JI5	C41-C31-C21	-2.12	118.95	120.28
2	B	750	HEM	C3B-CAB-CBB	-2.03	121.34	124.46
4	A	800	JI5	C1-C2-N2	2.02	117.33	111.55
3	B	760	H4B	C4A-C8A-N8	2.06	120.86	118.43
4	B	800	JI5	C11-C12-C13	2.10	120.58	118.84
4	A	800	JI5	N61-C61-N11	2.19	120.49	116.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C2D-C3D-C4D	2.40	105.56	101.50
2	B	750	HEM	C2C-C1C-CHC	2.47	127.43	123.68
2	B	750	HEM	C3B-C4B-CHC	2.59	126.81	123.16
3	B	760	H4B	C2-N1-C8A	2.68	120.57	114.54
2	A	750	HEM	CMD-C2D-C3D	2.76	126.56	114.35
2	B	750	HEM	CMD-C2D-C3D	2.76	126.56	114.35
2	A	750	HEM	C2D-C3D-C4D	3.45	107.34	101.50
2	A	750	HEM	C3B-C4B-CHC	3.62	128.27	123.16
3	A	760	H4B	C2-N1-C8A	3.66	122.77	114.54
3	A	760	H4B	C4-N3-C2	3.67	121.03	115.94
2	A	750	HEM	CAD-C3D-C4D	3.68	125.45	112.47
3	B	760	H4B	C4-N3-C2	3.73	121.11	115.94
2	B	750	HEM	CMC-C2C-C3C	3.85	126.14	116.53
4	A	800	JI5	C2-C1-N1	3.90	116.26	110.67
3	A	760	H4B	C4A-C8A-N8	4.02	123.16	118.43
2	A	750	HEM	CMB-C2B-C3B	4.10	126.76	116.53
2	B	750	HEM	CMB-C2B-C3B	4.32	127.31	116.53
2	B	750	HEM	CAD-C3D-C4D	4.43	128.09	112.47
2	B	750	HEM	CAD-C3D-C2D	4.55	126.29	113.22
3	A	760	H4B	C4-C4A-C8A	4.55	118.68	114.56
3	B	760	H4B	C4-C4A-C8A	4.60	118.72	114.56
4	A	800	JI5	C61-N11-C21	4.78	121.62	118.23
2	A	750	HEM	CAD-C3D-C2D	4.83	127.09	113.22
2	A	750	HEM	CMC-C2C-C3C	5.01	129.04	116.53
4	B	800	JI5	C61-N11-C21	6.34	122.73	118.23
4	B	800	JI5	C1-N1-C3'	6.35	123.46	113.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	4	0
4	A	800	JI5	1	0
2	B	750	HEM	6	0
4	B	800	JI5	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%)	1.12	82 (20%) 1 2	29, 56, 104, 128	0
1	B	410/422 (97%)	0.73	41 (10%) 9 10	28, 44, 71, 98	0
All	All	817/844 (96%)	0.93	123 (15%) 3 3	28, 49, 96, 128	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	7.6
1	B	300	PHE	7.1
1	B	348	VAL	6.2
1	A	300	PHE	4.8
1	B	352	ASP	4.8
1	A	373	GLY	4.7
1	B	350	THR	4.6
1	A	551	PHE	4.6
1	A	299	ARG	4.3
1	A	715	VAL	4.2
1	A	355	PHE	4.1
1	A	469	LYS	4.1
1	A	352	ASP	4.0
1	A	486	LYS	4.0
1	B	677	VAL	4.0
1	A	511	LYS	3.8
1	A	667	ARG	3.7
1	B	680	VAL	3.7
1	B	567	VAL	3.7
1	A	503	GLU	3.7
1	A	531	PRO	3.5
1	A	680	VAL	3.5
1	A	488	PRO	3.5
1	A	506	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	492	THR	3.4
1	A	676	TRP	3.4
1	B	616	LEU	3.4
1	A	711	TRP	3.4
1	B	566	ALA	3.3
1	A	508	GLN	3.3
1	A	416	VAL	3.3
1	A	677	VAL	3.3
1	B	416	VAL	3.2
1	A	370	LYS	3.2
1	A	321	THR	3.2
1	A	712	ASN	3.2
1	B	676	TRP	3.2
1	A	388	ILE	3.1
1	A	678	TRP	3.1
1	B	564	LEU	3.1
1	A	714	HIS	3.1
1	A	393	THR	3.0
1	B	565	PRO	3.0
1	B	591	THR	3.0
1	B	321	THR	3.0
1	A	322	LEU	2.9
1	B	588	TYR	2.9
1	A	619	ARG	2.9
1	B	691	PHE	2.9
1	A	384	VAL	2.9
1	A	382	GLU	2.9
1	B	667	ARG	2.8
1	B	349	ARG	2.8
1	A	679	ILE	2.8
1	A	351	LYS	2.8
1	B	584	PHE	2.8
1	A	487	GLN	2.8
1	A	391	THR	2.8
1	B	351	LYS	2.7
1	A	553	TRP	2.7
1	B	678	TRP	2.7
1	B	619	ARG	2.7
1	A	590	GLY	2.7
1	B	389	GLU	2.7
1	A	691	PHE	2.7
1	B	681	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	686	SER	2.6
1	B	553	TRP	2.6
1	A	470	HIS	2.6
1	A	371	ARG	2.6
1	B	715	VAL	2.6
1	A	505	CYS	2.6
1	A	591	THR	2.6
1	A	567	VAL	2.5
1	A	491	SER	2.5
1	B	369	ILE	2.5
1	B	679	ILE	2.5
1	B	682	PRO	2.5
1	A	507	GLN	2.5
1	A	361	PHE	2.4
1	A	354	LEU	2.4
1	A	330	ILE	2.4
1	B	446	VAL	2.4
1	A	681	PRO	2.4
1	A	350	THR	2.4
1	B	620	LYS	2.4
1	B	443	CYS	2.4
1	A	504	ILE	2.4
1	B	299	ARG	2.4
1	A	415	CYS	2.4
1	A	386	LYS	2.3
1	A	615	ASP	2.3
1	B	479	LEU	2.3
1	A	501	PHE	2.3
1	B	611	ALA	2.3
1	A	523	LEU	2.3
1	A	494	GLY	2.3
1	A	528	GLY	2.3
1	A	685	GLY	2.3
1	A	550	LYS	2.3
1	A	713	THR	2.3
1	B	442	ILE	2.3
1	A	683	MET	2.2
1	B	511	LYS	2.2
1	A	394	TYR	2.2
1	A	385	ASN	2.2
1	A	682	PRO	2.2
1	A	356	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	373	GLY	2.1
1	A	484	GLY	2.1
1	B	458	ALA	2.1
1	A	366	TYR	2.1
1	A	593	ILE	2.1
1	A	381	LEU	2.1
1	A	323	GLU	2.0
1	A	302	LYS	2.0
1	A	353	GLN	2.0
1	A	710	PRO	2.0
1	A	595	VAL	2.0
1	B	318	LEU	2.0
1	A	319	LYS	2.0
1	A	392	SER	2.0
1	A	369	ILE	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
5	ACT	A	860	4/4	0.95	0.24	3.34	60,61,62,66	0
3	H4B	B	760	17/17	0.94	0.25	1.08	30,32,36,38	0
2	HEM	A	750	43/43	0.97	0.21	0.64	25,31,42,46	0
2	HEM	B	750	43/43	0.97	0.23	0.55	27,30,42,47	0
4	JI5	A	800	27/27	0.88	0.20	0.30	39,45,49,51	0
5	ACT	B	860	4/4	0.93	0.17	0.25	53,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	JI5	B	800	27/27	0.93	0.22	0.10	35,39,40,42	0
3	H4B	A	760	17/17	0.94	0.19	0.02	32,36,40,41	0
6	ZN	A	900	1/1	0.98	0.13	-0.60	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.