

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 28, 2023 - 06:57 AM EDT

PDB ID	:	3JX5
Title	:	Structure of rat neuronal nitric oxide synthase $D597N/M336V$ mutant heme
		domain in complex with N1-{(3'S,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	:	2.15 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.15 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	$1560 \ (2.16-2.16)$
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	422	8%	14%	•••			
1	В	422	80%	16%	••			



## 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7024 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	А	407	Total 3312	C 2121	N 567	O 604	S 20	0	0	0
1	В	411	Total 3344	C 2140	N 575	O 609	S 20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	336	VAL	MET	engineered mutation	UNP P29476
А	597	ASN	ASP	engineered mutation	UNP P29476
В	336	VAL	MET	engineered mutation	UNP P29476
В	597	ASN	ASP	engineered mutation	UNP P29476

• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
0	Λ	1	Total	С	Fe	Ν	Ο	0	0	
	2 A	L	43	34	1	4	4	0	0	
0	В	1	Total	С	Fe	Ν	Ο	0	0	
	D	L	43	34	1	4	4	0	0	

• 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	А	1	Total         C         N         O           17         9         5         3	0	0
3	В	1	Total         C         N         O           17         9         5         3	0	0

• Molecule 4 is N-{(3S,4R)-4-[(6-amino-4-methylpyridin-2-yl)methyl]pyrrolidin-3-yl}-N'-[2-(3-fluorophenyl)ethyl]ethane-1,2-diamine (three-letter code: J14) (formula:  $C_{21}H_{30}FN_5$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Λ	1	Total	С	F	Ν	0	0
4	A	L	27	21	1	5	0	0
4	Р	1	Total	С	F	Ν	0	0
4	D	L	27	21	1	5	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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

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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	77	Total O 77 77	0	0
7	В	108	Total         O           108         108	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	51.74Å 111.38Å 164.69Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	49.39 - 2.15	Depositor
	49.36 - 2.15	EDS
% Data completeness	98.2 (49.39-2.15)	Depositor
(in resolution range)	98.2 (49.36-2.15)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	$2.31 (at 2.16 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.5.0089$ , CNS	Depositor
B B.	0.195 , $0.241$	Depositor
II, II, <i>free</i>	0.229 , $0.266$	DCC
$R_{free}$ test set	2556 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	43.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $52.0$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: H4B, J14, ZN, 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		Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.84	9/3405~(0.3%)	0.70	1/4621~(0.0%)	
1	В	0.78	2/3437~(0.1%)	0.76	3/4661~(0.1%)	
All	All	0.81	11/6842~(0.2%)	0.73	4/9282~(0.0%)	

All (11) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	382	GLU	CG-CD	8.82	1.65	1.51
1	А	375	LYS	CE-NZ	7.88	1.68	1.49
1	В	582	CYS	CB-SG	7.64	1.95	1.82
1	А	382	GLU	CD-OE1	7.52	1.33	1.25
1	А	556	ASP	CG-OD2	6.58	1.40	1.25
1	А	556	ASP	CG-OD1	6.42	1.40	1.25
1	А	379	ASP	C-O	6.07	1.34	1.23
1	А	547	ARG	CZ-NH2	5.92	1.40	1.33
1	В	432	CYS	CB-SG	-5.83	1.72	1.81
1	А	383	GLU	CG-CD	5.19	1.59	1.51
1	A	387	GLU	CB-CG	5.08	1.61	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	А	547	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	В	410	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	В	438	MET	CG-SD-CE	5.80	109.48	100.20
1	В	489	ASP	CB-CG-OD2	5.47	123.22	118.30

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	А	3312	0	3223	41	0
1	В	3344	0	3261	47	0
2	А	43	0	30	6	0
2	В	43	0	30	9	0
3	А	17	0	15	0	0
3	В	17	0	15	1	0
4	А	27	0	30	6	0
4	В	27	0	30	5	0
5	А	4	0	3	0	0
5	В	4	0	3	0	0
6	А	1	0	0	0	0
7	А	77	0	0	2	0
7	В	108	0	0	1	0
All	All	7024	0	6640	97	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 (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:375:LYS:NZ	1:A:375:LYS:CE	1.68	1.53
1:B:567:VAL:HG21	4:B:800:J14:H5'A	1.46	0.97
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.90	0.87
1:B:500:GLN:HA	1:B:503:GLU:OE2	1.74	0.86
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.39	0.85
1:A:567:VAL:HG21	4:A:800:J14:H5'A	1.60	0.83
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.64	0.80
1:A:317:HIS:O	1:A:320:SER:HB3	1.82	0.80
4:A:800:J14:H2'A	4:A:800:J14:H4	1.65	0.79
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.99	0.76
1:B:659:ILE:O	1:B:663:GLU:HG3	1.90	0.71
1:B:501:PHE:CE2	1:B:505:CYS:SG	2.84	0.69
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.57	0.69
2:B:750:HEM:HBA2	2:B:750:HEM:CMA	2.21	0.69



	A h	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.76	0.67	
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.25	0.67	
1:A:567:VAL:CG2	4:A:800:J14:H5'A	2.25	0.66	
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.13	0.66	
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.30	0.65	
2:B:750:HEM:HBA1	3:B:760:H4B:HN22	1.64	0.63	
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.81	0.61	
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.63	0.59	
1:B:350:THR:HG22	1:B:352:ASP:H	1.67	0.59	
1:B:567:VAL:HG21	4:B:800:J14:C5'	2.28	0.59	
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.51	0.58	
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.29	0.58	
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.35	0.56	
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.89	0.56	
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.88	0.54	
1:A:525:GLN:HG3	1:A:529:ASN:O	2.07	0.54	
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.22	0.54	
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.90	0.53	
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.43	0.53	
4:A:800:J14:H4	4:A:800:J14:C2'	2.38	0.52	
1:A:306:TRP:CZ3	4:B:800:J14:H15	2.45	0.52	
1:A:299:ARG:O	1:A:317:HIS:CE1	2.64	0.50	
1:A:352:ASP:OD2	1:A:352:ASP:N	2.44	0.50	
1:A:299:ARG:O	1:A:317:HIS:NE2	2.45	0.50	
1:A:554:PHE:HB3	7:A:1009:HOH:O	2.12	0.49	
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.95	0.49	
1:B:494:GLY:O	1:B:496:PRO:HD3	2.12	0.49	
2:B:750:HEM:O2A	4:B:800:J14:H3'	2.13	0.49	
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.48	0.48	
1:B:501:PHE:CZ	1:B:505:CYS:SG	3.07	0.48	
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.95	0.48	
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.48	0.48	
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.96	0.48	
1:B:520:LEU:HB3	1:B:521:PRO:HD2	1.95	0.48	
2:A:750:HEM:HBC2	2:A:750:HEM:HMC1	1.96	0.47	
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.50	0.47	
1:B:624:LEU:O	1:B:628:GLN:HG3	2.15	0.47	
1:A:460:THR:O	1:A:583:PRO:HD2	2.15	0.47	
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.03	0.47	
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.78	0.47	
1:B:505:CYS:O	1:B:506:ILE:C	2.53	0.47	

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	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:320:SER:HA	1:A:700:LEU:HD23	1.98	0.46
2:A:750:HEM:HBA2	4:A:800:J14:H71	1.98	0.46
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.51	0.45
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.32	0.45
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.16	0.45
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.46	0.45
1:A:375:LYS:NZ	1:A:375:LYS:CD	2.72	0.45
2:B:750:HEM:CMA	2:B:750:HEM:CBA	2.94	0.45
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.82	0.45
1:B:567:VAL:CG2	4:B:800:J14:H5'A	2.32	0.44
1:B:303:VAL:HG23	1:B:312:LEU:HB2	2.00	0.44
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.53	0.44
1:B:525:GLN:HG3	1:B:529:ASN:O	2.18	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.43
1:B:388:ILE:O	1:B:392:SER:N	2.46	0.43
1:A:321:THR:HG23	1:A:322:LEU:HG	2.00	0.43
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.54	0.43
1:A:492:THR:HG21	1:A:496:PRO:HG3	2.01	0.42
1:B:519:VAL:HG21	1:B:541:VAL:HG11	2.01	0.42
1:B:588:TYR:CD1	1:B:593:ILE:HD11	2.53	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.02	0.42
1:B:447:LYS:HD2	1:B:540:LEU:HD11	2.00	0.42
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.54	0.42
2:A:750:HEM:O2A	4:A:800:J14:H3'	2.19	0.42
1:B:512:ALA:HA	1:B:513:PRO:HD3	1.89	0.42
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.01	0.42
1:B:659:ILE:HD13	1:B:659:ILE:HA	1.91	0.42
1:A:605:ASN:ND2	7:A:1032:HOH:O	2.45	0.42
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.69	0.41
1:A:402:ILE:CG2	1:A:406:LYS:HE3	2.50	0.41
1:B:316:LEU:HD21	1:B:700:LEU:HD11	2.02	0.41
1:B:302:LYS:HB2	1:B:302:LYS:HE3	1.79	0.41
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.56	0.41
1:B:300:PHE:HD2	1:B:315:THR:CG2	2.21	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.89	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.04	0.40
1:B:507:GLN:O	1:B:507:GLN:HG2	2.19	0.40
1:B:572:LEU:HB3	1:B:579:PHE:HB2	2.02	0.40
1:A:369:ILE:HG13	1:A:371:ARG:HB2	2.03	0.40
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.10	0.40
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.96	0.40

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Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)	
1:B:449:ALA:HB1	7:B:1026:HOH:O	2.21	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	А	403/422~(96%)	388~(96%)	15~(4%)	0	100 100
1	В	407/422~(96%)	396~(97%)	9~(2%)	2~(0%)	29 22
All	All	810/844~(96%)	784 (97%)	24 (3%)	2 (0%)	47 46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	402	ILE
1	В	685	GLY

#### 5.3.2 Protein sidechains (i)

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	Perce	$\mathbf{ntiles}$
1	А	363/377~(96%)	347~(96%)	16 (4%)	28	25
1	В	366/377~(97%)	355~(97%)	11 (3%)	41	40
All	All	729/754~(97%)	702~(96%)	27~(4%)	34	32



Mol	Chain	Res	Type
1	А	320	SER
1	А	350	THR
1	А	352	ASP
1	А	371	ARG
1	А	380	ARG
1	А	454	ASN
1	А	489	ASP
1	А	507	GLN
1	А	527	ASN
1	А	547	ARG
1	А	555	LYS
1	А	601	ASN
1	А	615	ASP
1	А	620	LYS
1	А	645	LYS
1	А	662	MET
1	В	303	VAL
1	В	321	THR
1	В	352	ASP
1	В	353	GLN
1	В	369	ILE
1	В	454	ASN
1	В	481	ARG
1	В	486	LYS
1	В	507	GLN
1	В	540	LEU
1	В	547	ARG

All (27) residues with a non-rotameric sidechain are listed below:

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

Mol	Chain	Res	Type
1	А	353	GLN
1	А	364	GLN
1	А	454	ASN
1	А	507	GLN
1	А	601	ASN
1	А	605	ASN
1	А	642	GLN
1	А	697	ASN
1	А	712	ASN
1	В	364	GLN



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Mol	Chain	Res	Type
1	В	454	ASN
1	В	508	GLN
1	В	535	GLN
1	В	605	ASN
1	В	642	GLN
1	В	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 monosaccharides in this entry.

#### 5.6 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).

Mal	Turne	Chain	Dec	Timle	Bo	ond leng	$_{\rm sths}$	E	ond ang	gles
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	HEM	А	750	1	41,50,50	1.87	8 (19%)	45,82,82	2.34	10 (22%)
5	ACT	В	860	-	3,3,3	0.72	0	3,3,3	0.86	0
3	H4B	В	760	-	16,18,18	1.10	2 (12%)	11,26,26	2.93	8 (72%)
4	J14	В	800	-	27,29,29	0.73	0	30,38,38	2.21	7 (23%)
4	J14	А	800	-	27,29,29	0.78	0	30,38,38	2.31	9 (30%)
2	HEM	В	750	1	41,50,50	1.93	9 (21%)	45,82,82	1.80	12 (26%)
5	ACT	А	860	-	3,3,3	0.77	0	3,3,3	0.76	0



Mal	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
IVIOI	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	H4B	А	760	-	16,18,18	0.86	0	11,26,26	<mark>3.19</mark>	6 (54%)

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	А	750	1	-	2/12/54/54	-
3	H4B	В	760	-	-	1/8/17/17	0/2/2/2
4	J14	В	800	-	-	8/13/23/23	0/3/3/3
4	J14	А	800	-	-	8/13/23/23	0/3/3/3
2	HEM	В	750	1	-	6/12/54/54	-
3	H4B	А	760	-	-	0/8/17/17	0/2/2/2

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	750	HEM	C3D-C2D	7.48	1.52	1.36
2	В	750	HEM	C3D-C2D	7.15	1.51	1.36
2	В	750	HEM	C3C-C2C	-5.28	1.33	1.40
2	А	750	HEM	C3C-C2C	-3.87	1.35	1.40
2	В	750	HEM	C3C-CAC	3.38	1.54	1.47
2	А	750	HEM	CAB-C3B	2.82	1.55	1.47
2	А	750	HEM	CAA-C2A	2.76	1.56	1.52
2	А	750	HEM	CMC-C2C	2.72	1.58	1.51
2	В	750	HEM	CMB-C2B	2.65	1.56	1.50
3	В	760	H4B	C7-C6	2.57	1.54	1.52
2	В	750	HEM	CAB-C3B	2.51	1.54	1.47
2	А	750	HEM	CMB-C2B	2.49	1.56	1.50
2	В	750	HEM	CMD-C2D	2.44	1.56	1.50
2	А	750	HEM	C3C-CAC	2.35	1.52	1.47
2	В	750	HEM	C3B-C2B	-2.25	1.32	1.37
3	В	760	H4B	C7-N8	2.21	1.48	1.44
2	В	750	HEM	CMC-C2C	2.12	1.56	1.51
2	A	750	HEM	CMD-C2D	2.10	1.55	1.50
2	В	750	HEM	CMA-C3A	2.04	1.55	1.51

All (19) bond length outliers are listed below:

All (52) bond angle outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	750	HEM	CBA-CAA-C2A	-9.28	96.78	112.62
4	А	800	J14	C61-N11-C21	7.25	123.60	118.10
3	А	760	H4B	C4-C4A-N5	6.71	124.75	119.12
4	В	800	J14	C61-N11-C21	6.49	123.02	118.10
3	В	760	H4B	C8A-C4A-C4	6.29	120.16	114.57
2	А	750	HEM	C4D-ND-C1D	5.54	110.79	105.07
4	А	800	J14	C31-C21-N11	-5.21	117.38	122.90
4	В	800	J14	C31-C21-N11	-4.92	117.68	122.90
2	А	750	HEM	C2C-C3C-C4C	4.83	110.27	106.90
4	А	800	J14	C1-N1-C3'	4.41	120.44	114.20
4	В	800	J14	C2'-C3'-N1	-4.36	105.97	113.73
2	В	750	HEM	C4D-ND-C1D	4.02	109.23	105.07
3	А	760	H4B	C8A-C4A-C4	4.01	118.13	114.57
3	В	760	H4B	C2-N3-C4	3.83	122.02	115.93
2	В	750	HEM	CBA-CAA-C2A	-3.75	106.22	112.62
3	А	760	H4B	C2-N3-C4	3.70	121.80	115.93
3	А	760	H4B	N1-C2-N3	-3.64	119.71	125.42
2	В	750	HEM	CMA-C3A-C4A	-3.53	123.05	128.46
4	В	800	J14	C5'-N1'-C2'	3.51	113.72	105.42
2	А	750	HEM	CHA-C4D-ND	3.47	128.67	124.38
4	В	800	J14	C1-N1-C3'	3.46	119.09	114.20
3	А	760	H4B	C2-N1-C8A	3.40	122.16	114.54
2	А	750	HEM	CMC-C2C-C3C	3.28	130.82	124.68
4	А	800	J14	C5'-N1'-C2'	3.24	113.08	105.42
3	В	760	H4B	N1-C2-N3	-3.07	120.60	125.42
2	В	750	HEM	C2C-C3C-C4C	2.95	108.96	106.90
2	А	750	HEM	CMD-C2D-C1D	2.91	129.47	125.04
2	А	750	HEM	C4C-CHD-C1D	2.81	126.26	122.56
2	А	750	HEM	CAD-CBD-CGD	-2.76	107.66	113.60
3	В	760	H4B	C4-C4A-N5	2.75	121.43	119.12
2	В	750	HEM	CAA-CBA-CGA	-2.75	106.06	113.76
2	В	750	HEM	CMA-C3A-C2A	2.74	130.10	124.94
3	В	760	H4B	N2-C2-N3	2.71	$1\overline{21.47}$	117.25
2	В	750	HEM	C1D-C2D-C3D	-2.63	104.19	106.96
3	A	760	H4B	N2-C2-N3	2.62	121.32	117.25
4	A	800	J14	C14-C13-C12	-2.57	119.95	123.29
3	В	760	H4B	C2-N1-C8A	2.54	120.23	114.54
2	В	750	HEM	C4B-CHC-C1C	2.49	125.85	122.56
2	В	750	HEM	CHB-C1B-NB	2.45	127.41	124.38
4	A	800	J14	C71-C21-C31	2.42	126.19	121.04
2	A	750	HEM	CHB-C1B-NB	2.37	127.31	124.38
4	В	800	J14	C14-C13-C12	-2.34	120.25	123.29
2	A	750	HEM	C3C-C4C-NC	-2.28	106.64	110.94



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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	750	HEM	CHD-C1D-ND	2.26	126.88	124.43
3	В	760	H4B	C4A-C4-N3	-2.24	117.64	124.01
4	А	800	J14	C2-C1-N1	2.24	114.70	111.06
2	В	750	HEM	CMD-C2D-C1D	2.14	128.30	125.04
2	В	750	HEM	C4C-CHD-C1D	2.14	125.38	122.56
4	А	800	J14	C2'-C3'-N1	-2.12	109.96	113.73
4	В	800	J14	C71-C21-C31	2.11	125.53	121.04
3	В	760	H4B	C4A-N5-C6	-2.09	115.46	121.16
4	А	800	J14	C21-C71-C4'	2.07	122.36	115.55

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There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	750	HEM	C1A-C2A-CAA-CBA
2	В	750	HEM	C3A-C2A-CAA-CBA
2	В	750	HEM	C2A-CAA-CBA-CGA
4	А	800	J14	N11-C21-C71-C4'
4	А	800	J14	C31-C21-C71-C4'
4	А	800	J14	C3'-C4'-C71-C21
4	А	800	J14	C5'-C4'-C71-C21
4	В	800	J14	N11-C21-C71-C4'
4	В	800	J14	C31-C21-C71-C4'
4	В	800	J14	C3'-C4'-C71-C21
4	В	800	J14	C5'-C4'-C71-C21
4	А	800	J14	N2-C3-C4-C11
4	В	800	J14	N2-C3-C4-C11
4	А	800	J14	N1-C1-C2-N2
4	В	800	J14	N1-C1-C2-N2
4	А	800	J14	C2-C1-N1-C3'
4	В	800	J14	C2-C1-N1-C3'
4	В	800	J14	C1-C2-N2-C3
2	В	750	HEM	C4B-C3B-CAB-CBB
2	А	750	HEM	CAA-CBA-CGA-O2A
2	В	750	HEM	CAA-CBA-CGA-O2A
2	В	750	HEM	CAA-CBA-CGA-O1A
2	А	750	HEM	CAA-CBA-CGA-O1A
4	A	800	J14	C4-C3-N2-C2
3	В	760	H4B	N5-C6-C9-O9

There are no ring outliers.

5 monomers are involved in 23 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	750	HEM	6	0
3	В	760	H4B	1	0
4	В	800	J14	5	0
4	А	800	J14	6	0
2	В	750	HEM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.













## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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		$OWAB(Å^2)$	Q<0.9	
1	А	407/422~(96%)	0.61	34~(8%)	11	15	32, 64, 119, 150	0
1	В	411/422 (97%)	0.37	14(3%)	45	53	31, 51, 84, 105	0
All	All	818/844 (96%)	0.49	48 (5%)	22	30	31, 57, 108, 150	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	352	ASP	5.9	
1	В	300	PHE	5.1	
1	В	352	ASP	4.1	
1	В	338	PRO	4.0	
1	А	551	PHE	4.0	
1	А	355	PHE	3.9	
1	А	488	PRO	3.9	
1	В	321	THR	3.9	
1	А	366	TYR	3.8	
1	А	493	LEU	3.6	
1	А	299	ARG	3.5	
1	А	375	LYS	3.5	
1	А	716	TRP	3.4	
1	А	556	ASP	3.3	
1	В	389	GLU	3.1	
1	А	557	LEU	3.1	
1	А	511	LYS	3.0	
1	А	373	GLY	3.0	
1	А	706	TYR	2.9	
1	В	554	PHE	2.8	
1	А	371	ARG	2.8	
1	В	301	LEU	2.7	
1	A	715	VAL	2.6	
1	В	615	ASP	2.6	



21	$[\mathbf{V}5]$
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Mol	Chain	Res	Type	RSRZ
1	В	350	THR	2.6
1	А	494	GLY	2.6
1	А	517	PHE	2.5
1	А	389	GLU	2.5
1	А	503	GLU	2.5
1	А	372	PHE	2.5
1	А	469	LYS	2.5
1	В	375	LYS	2.5
1	А	300	PHE	2.4
1	А	533	LEU	2.3
1	А	528	GLY	2.3
1	В	492	THR	2.3
1	А	486	LYS	2.3
1	А	328	GLU	2.2
1	А	554	PHE	2.2
1	В	355	PHE	2.2
1	А	394	TYR	2.1
1	А	391	THR	2.1
1	В	718	GLY	2.1
1	А	485	TYR	2.1
1	А	713	THR	2.1
1	А	552	ASP	2.1
1	В	699	ARG	2.0
1	А	338	PRO	2.0

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#### 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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.



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	J14	В	800	27/27	0.81	0.31	$68,\!87,\!111,\!112$	0
4	J14	А	800	27/27	0.85	0.28	$68,\!89,\!125,\!126$	0
5	ACT	А	860	4/4	0.91	0.32	84,87,87,88	0
3	H4B	В	760	17/17	0.93	0.12	33,40,48,48	0
5	ACT	В	860	4/4	0.94	0.24	90,91,91,92	0
3	H4B	А	760	17/17	0.95	0.12	38,43,49,49	0
2	HEM	А	750	43/43	0.97	0.14	35,39,60,61	0
2	HEM	В	750	43/43	0.97	0.17	34,40,58,63	0
6	ZN	А	900	1/1	0.97	0.13	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











## 6.5 Other polymers (i)

There are no such residues in this entry.

