



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2014 – 03:46 PM EDT

PDB ID : 4CX3  
Title : Structure of rat neuronal nitric oxide synthase M336V D597N mutant heme domain in complex with 4-METHYL-6-(((3R,4R)-4-((5-(PYRIDIN-2-YL)PENTYL)OXY)PYRROLIDIN-3-YL)METHYL)PYRIDIN-2-AMINE  
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Deposited on : 2014-04-03  
Resolution : 1.97 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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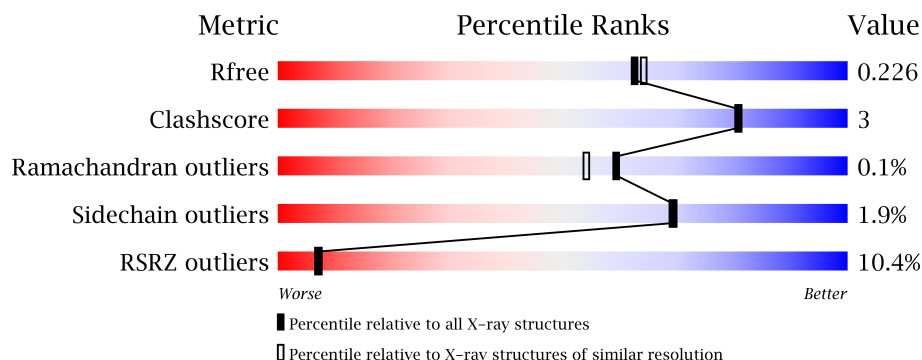
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 1.97 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))
$R_{free}$	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	HW8	A	800	-	X
4	HW8	B	800	-	X
5	ACT	A	860	-	X
6	GOL	A	880	-	X
6	GOL	B	880	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7310 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

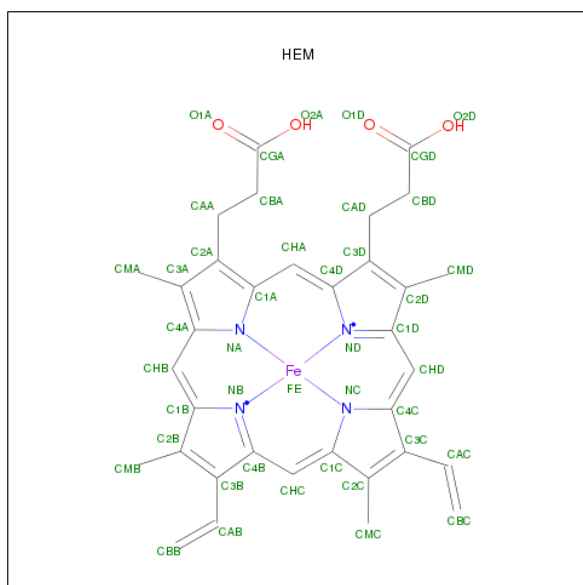
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	3	1
			3330	2132	570	608	20			
1	B	411	Total	C	N	O	S	0	4	0
			3359	2150	575	613	21			

There are 4 discrepancies between the modelled and reference sequences:

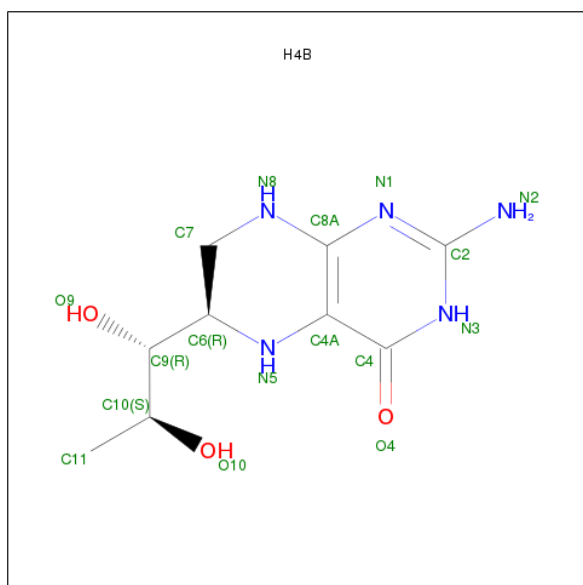
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

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



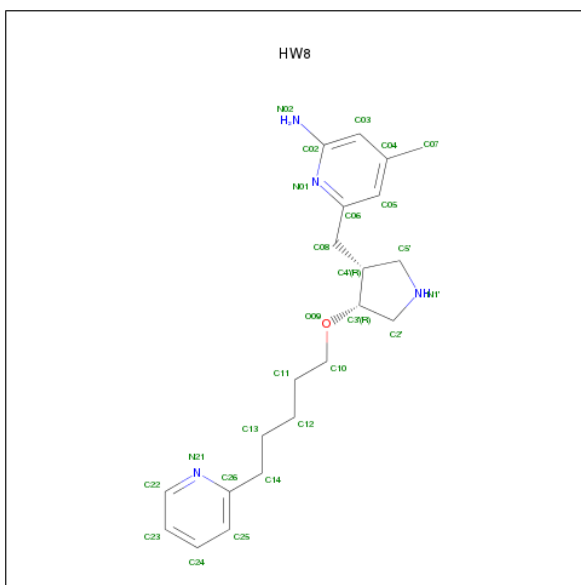
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



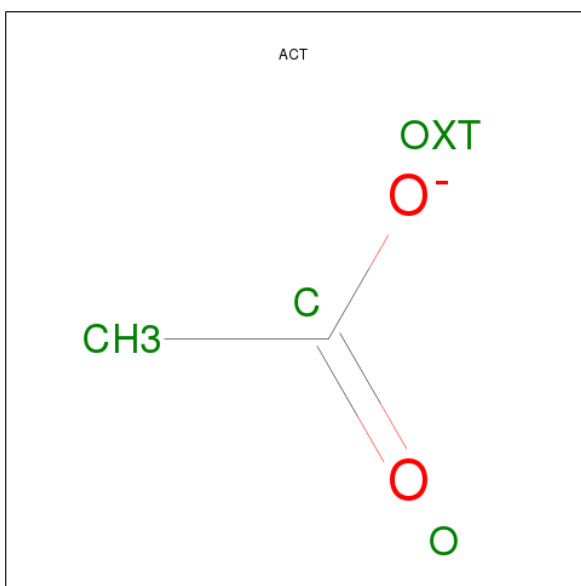
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-METHYL-6-{[(3R,4R)-4-{[5-(PYRIDIN-2-YL)PENTYL]OXY}PYRROLIDIN-3-YL]METHYL}PYRIDIN-2-AMINE (three-letter code: HW8) (formula:  $C_{21}H_{30}N_4O$ ).



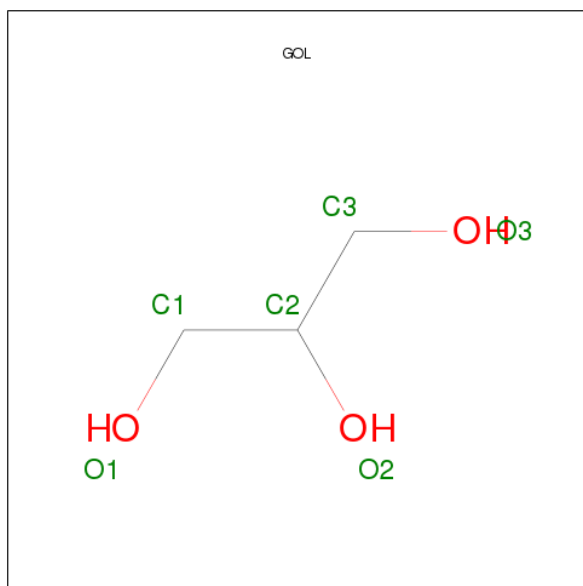
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 26	C 21	N 4	O 1	0	0
4	B	1	Total 26	C 21	N 4	O 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		

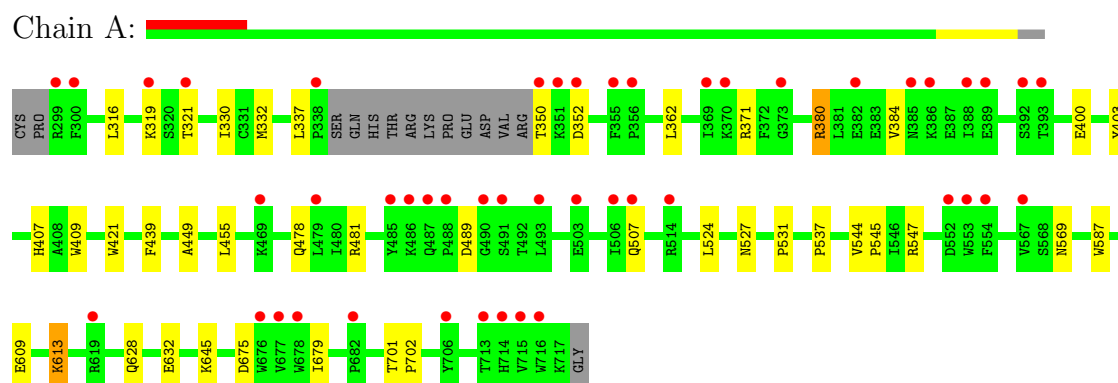
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	196	Total	O	0	0
			196	196		
8	B	232	Total	O	0	0
			232	232		

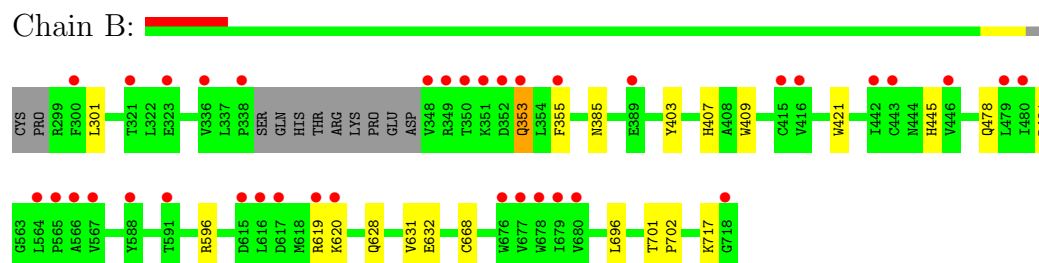
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	51.92Å 110.68Å 164.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.89 – 1.97 43.89 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.89-1.97) 98.6 (43.89-1.97)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.175 , 0.209 0.192 , 0.226	Depositor DCC
$R_{free}$ test set	3318 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67034 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, HW8, 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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.64	0/3432	0.65	0/4658
1	B	0.69	0/3464	0.66	0/4697
All	All	0.67	0/6896	0.66	0/9355

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3243	25	0
1	B	3359	0	3282	17	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	26	0	30	4	0
4	B	26	0	30	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	8	0	0
6	B	6	0	8	4	0
7	B	1	0	0	0	0
8	A	196	0	0	2	0
8	B	232	0	0	4	0
All	All	7310	0	6697	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:717:LYS:NZ	8:B:2161:HOH:O	2.14	0.80
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.64	0.77
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.84	0.60
1:B:596:ARG:HH22	6:B:880:GOL:H11	1.66	0.60
2:B:750:HEM:HBB2	2:B:750:HEM:HHC	1.84	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.04	0.57
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.43	0.51
1:A:337:LEU:CD2	4:A:800:HW8:H3	2.40	0.51
1:A:609:GLU:O	1:A:613:LYS:HG2	2.11	0.51
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.94	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.94	0.48
2:A:750:HEM:HHC	2:A:750:HEM:HBB2	1.95	0.47
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.03	0.47
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.47
1:A:609:GLU:HG3	8:A:2153:HOH:O	2.16	0.46
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.96	0.46
1:A:337:LEU:HD21	4:A:800:HW8:H3	1.98	0.46
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.96	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.97	0.46
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.39	0.45
1:A:319:LYS:HE3	8:A:2005:HOH:O	2.17	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.05	0.45
1:B:596:ARG:HH22	6:B:880:GOL:C1	2.30	0.45
4:B:800:HW8:H13	6:B:880:GOL:H32	1.82	0.45
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.50	0.45
4:B:800:HW8:C2'	8:B:2230:HOH:O	2.67	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.43
4:B:800:HW8:H17	8:B:2230:HOH:O	2.19	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:619:ARG:HE	1:B:619:ARG:HB2	1.52	0.42
1:B:353:GLN:HG2	1:B:353:GLN:H	1.66	0.42
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.54	0.42
1:A:439:PHE:HZ	1:A:537:PRO:HD3	1.84	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.42
1:B:668[B]:CYS:SG	8:B:2218:HOH:O	2.27	0.42
3:B:760:H4B:O4	6:B:880:GOL:H12	2.20	0.41
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.95	0.41
1:A:337:LEU:HD23	4:A:800:HW8:H3	2.02	0.41
1:A:675:ASP:O	1:A:679:ILE:HG12	2.21	0.41
1:A:337:LEU:HD21	4:A:800:HW8:H5	2.02	0.41
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.03	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.40
1:A:449:ALA:O	1:A:455:LEU:HA	2.21	0.40
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.40

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	407/422 (96%)	398 (98%)	8 (2%)	1 (0%)	56	50
1	B	411/422 (97%)	404 (98%)	7 (2%)	0	100	100
All	All	818/844 (97%)	802 (98%)	15 (2%)	1 (0%)	59	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

### 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	366/377 (97%)	355 (97%)	11 (3%)	53	48
1	B	370/377 (98%)	367 (99%)	3 (1%)	89	91
All	All	736/754 (98%)	722 (98%)	14 (2%)	69	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	350	THR
1	A	352	ASP
1	A	371	ARG
1	A	380	ARG
1	A	507	GLN
1	A	527	ASN
1	A	547	ARG
1	A	569	ASN
1	A	613	LYS
1	A	645	LYS
1	B	353	GLN
1	B	547	ARG
1	B	620	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	454	ASN

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Mol	Chain	Res	Type
1	B	507	GLN
1	B	601	ASN
1	B	605	ASN
1	B	628	GLN
1	B	697	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	42,50,50	3.76	14 (33%)	27,82,82	1.67	3 (11%)
3	H4B	A	760	-	18,18,18	1.29	2 (11%)	24,26,26	1.69	5 (20%)
4	HW8	A	800	-	28,28,28	0.55	0	36,36,36	1.90	9 (25%)
5	ACT	A	860	-	1,3,3	1.49	0	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.38	0	5,5,5	0.62	0
2	HEM	B	750	1	42,50,50	3.81	14 (33%)	27,82,82	1.82	3 (11%)
3	H4B	B	760	-	18,18,18	1.41	3 (16%)	24,26,26	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HW8	B	800	-	28,28,28	0.64	0	36,36,36	1.94	7 (19%)
5	ACT	B	860	-	1,3,3	1.47	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.37	0	5,5,5	0.49	0

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	-	0/14/114/114	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	HW8	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	GOL	A	880	-	-	0/4/4/4	0/0/0/0
2	HEM	B	750	1	-	0/14/114/114	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	HW8	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3C-C2C	-15.85	1.33	1.45
2	A	750	HEM	C3B-C2B	-13.27	1.32	1.45
2	A	750	HEM	C3C-C2C	-13.07	1.35	1.45
2	B	750	HEM	C3B-C2B	-11.13	1.34	1.45
2	B	750	HEM	CMD-C2D	6.79	1.56	1.45
2	A	750	HEM	CMB-C2B	6.65	1.56	1.45
2	A	750	HEM	CMD-C2D	6.56	1.56	1.45
2	B	750	HEM	CMC-C2C	6.40	1.55	1.45
2	A	750	HEM	CMC-C2C	6.22	1.55	1.45
2	B	750	HEM	CMB-C2B	5.78	1.54	1.45
2	A	750	HEM	C3C-CAC	4.56	1.55	1.40
2	B	750	HEM	C3C-CAC	4.52	1.55	1.40
2	A	750	HEM	C3B-CAB	4.39	1.54	1.40
2	B	750	HEM	C3B-CAB	4.33	1.54	1.40
3	A	760	H4B	C2-N2	3.58	1.37	1.32
2	A	750	HEM	C3D-C2D	3.30	1.52	1.43
2	A	750	HEM	FE-NB	3.16	2.06	1.95
2	A	750	HEM	FE-ND	3.10	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	760	H4B	C7-C6	3.05	1.55	1.52
3	A	760	H4B	C2-N1	2.91	1.37	1.33
2	B	750	HEM	FE-ND	2.82	2.07	1.95
3	B	760	H4B	C2-N1	2.79	1.37	1.33
2	B	750	HEM	FE-NB	2.60	2.04	1.95
2	B	750	HEM	C1C-NC	2.52	1.40	1.33
2	B	750	HEM	C4D-ND	2.45	1.39	1.33
2	A	750	HEM	C1D-ND	2.39	1.39	1.33
3	B	760	H4B	C2-N2	2.22	1.35	1.32
2	A	750	HEM	C4D-ND	2.18	1.39	1.33
2	B	750	HEM	C3D-C2D	2.18	1.49	1.43
2	A	750	HEM	CMA-C3A	2.11	1.56	1.51
2	A	750	HEM	FE-NC	2.10	2.04	1.95
2	B	750	HEM	CMA-C3A	2.09	1.56	1.51
2	B	750	HEM	CAD-C3D	2.00	1.56	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	HW8	C02-N01-C06	8.04	123.88	118.24
4	A	800	HW8	C02-N01-C06	6.13	122.54	118.24
2	A	750	HEM	CBD-CAD-C3D	-5.89	101.73	114.51
2	B	750	HEM	CBA-CAA-C2A	-5.82	102.94	112.63
3	B	760	H4B	C4-C4A-C8A	5.50	119.54	114.56
2	B	750	HEM	CBD-CAD-C3D	-4.89	103.89	114.51
2	A	750	HEM	CBA-CAA-C2A	-4.26	105.54	112.63
3	A	760	H4B	C4-C4A-C8A	4.19	118.35	114.56
2	B	750	HEM	CAD-C3D-C4D	3.20	130.11	125.60
4	A	800	HW8	C5'-N1'-C2'	3.10	113.73	105.92
3	B	760	H4B	N8-C8A-N1	3.07	120.32	115.82
3	A	760	H4B	C4-N3-C2	3.07	121.93	120.20
4	A	800	HW8	C23-C22-N21	-2.97	118.42	123.42
4	A	800	HW8	C07-C04-C05	-2.97	116.50	120.94
3	A	760	H4B	C4A-C8A-N8	2.96	121.91	118.43
4	B	800	HW8	C5'-N1'-C2'	2.94	113.31	105.92
4	A	800	HW8	C22-N21-C26	2.84	121.35	117.37
4	B	800	HW8	C05-C06-N01	-2.70	119.95	122.96
4	B	800	HW8	C04-C05-C06	-2.67	118.53	120.28
2	A	750	HEM	CMC-C2C-C3C	2.46	130.08	124.26
4	A	800	HW8	C12-C13-C14	-2.41	103.99	113.95
4	B	800	HW8	C22-N21-C26	2.35	120.67	117.37
4	A	800	HW8	C07-C04-C03	2.28	124.34	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	H4B	N2-C2-N3	2.26	120.24	117.82
4	A	800	HW8	C06-C08-C4'	-2.19	107.24	115.31
4	A	800	HW8	C4'-C5'-N1'	-2.07	101.42	105.66
4	B	800	HW8	C23-C22-N21	-2.06	119.95	123.42
3	A	760	H4B	C7-C6-N5	2.06	113.92	109.61
3	A	760	H4B	C9-C6-N5	2.04	114.27	111.10
4	B	800	HW8	O09-C3'-C4'	2.02	113.67	108.90
3	B	760	H4B	C4-N3-C2	2.02	121.34	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	408/422 (96%)	0.84	47 (11%) 5 5	21, 42, 75, 94	0
1	B	411/422 (97%)	0.56	38 (9%) 9 9	20, 33, 56, 78	0
All	All	819/844 (97%)	0.70	85 (10%) 7 7	20, 37, 70, 94	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	6.7
1	B	300	PHE	6.6
1	B	350	THR	6.4
1	A	715	VAL	6.4
1	A	716	TRP	6.1
1	A	352	ASP	5.8
1	A	355	PHE	5.6
1	A	351	LYS	5.2
1	B	321	THR	4.8
1	A	488	PRO	4.5
1	B	352	ASP	4.3
1	A	369	ILE	4.0
1	B	619	ARG	3.9
1	A	706	TYR	3.8
1	A	714	HIS	3.6
1	A	382	GLU	3.6
1	A	386	LYS	3.5
1	A	507	GLN	3.4
1	A	321	THR	3.4
1	A	552	ASP	3.4
1	A	385	ASN	3.3
1	B	718	GLY	3.2
1	A	503	GLU	3.2
1	A	514	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	677	VAL	3.1
1	A	392	SER	3.1
1	B	353	GLN	3.1
1	B	620	LYS	3.1
1	A	300	PHE	3.0
1	A	677	VAL	2.9
1	A	373	GLY	2.8
1	B	680	VAL	2.8
1	A	676	TRP	2.7
1	B	566	ALA	2.7
1	B	564	LEU	2.7
1	A	486	LYS	2.7
1	B	323	GLU	2.7
1	B	442	ILE	2.7
1	B	567	VAL	2.6
1	A	713	THR	2.5
1	A	370	LYS	2.5
1	A	619	ARG	2.5
1	A	491	SER	2.5
1	B	355	PHE	2.5
1	B	616	LEU	2.4
1	B	615	ASP	2.4
1	B	588	TYR	2.4
1	A	487	GLN	2.4
1	A	553	TRP	2.4
1	A	554	PHE	2.4
1	A	469	LYS	2.4
1	A	678	TRP	2.4
1	A	356	PRO	2.4
1	B	479	LEU	2.4
1	B	416	VAL	2.4
1	A	485	TYR	2.3
1	A	393	THR	2.3
1	B	389	GLU	2.3
1	A	338	PRO	2.3
1	B	351	LYS	2.3
1	B	679	ILE	2.3
1	A	389	GLU	2.3
1	A	350	THR	2.3
1	A	490	GLY	2.3
1	A	299	ARG	2.2
1	B	349	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	480	ILE	2.2
1	B	565	PRO	2.2
1	B	591	THR	2.2
1	A	493	LEU	2.2
1	B	617	ASP	2.2
1	A	506	ILE	2.1
1	A	567	VAL	2.1
1	A	682	PRO	2.1
1	A	388	ILE	2.1
1	B	336	VAL	2.1
1	B	562	TYR	2.1
1	B	676	TRP	2.1
1	B	338	PRO	2.1
1	B	443	CYS	2.1
1	B	678	TRP	2.0
1	A	479	LEU	2.0
1	A	319	LYS	2.0
1	B	446	VAL	2.0
1	B	415	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	B	880	6/6	0.34	5.56	66,68,68,69	0
6	GOL	A	880	6/6	0.25	2.87	63,66,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	A	860	4/4	0.18	2.75	47,47,49,49	0
4	HW8	A	800	26/26	0.26	2.27	32,59,65,66	0
4	HW8	B	800	26/26	0.26	2.23	32,49,59,61	0
5	ACT	B	860	4/4	0.14	1.09	39,39,39,41	0
3	H4B	B	760	17/17	0.21	0.72	21,24,31,31	0
3	H4B	A	760	17/17	0.19	0.69	22,24,29,30	0
2	HEM	B	750	43/43	0.18	0.61	22,24,34,40	0
2	HEM	A	750	43/43	0.16	0.48	22,26,33,36	0
7	ZN	B	900	1/1	0.09	-1.77	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.