



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:31 PM GMT

PDB ID : 5AD4  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with  
7-((3-(2-(Dimethylamino)ethyl)phenoxy)methyl)quinolin-2- amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2015-08-20  
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

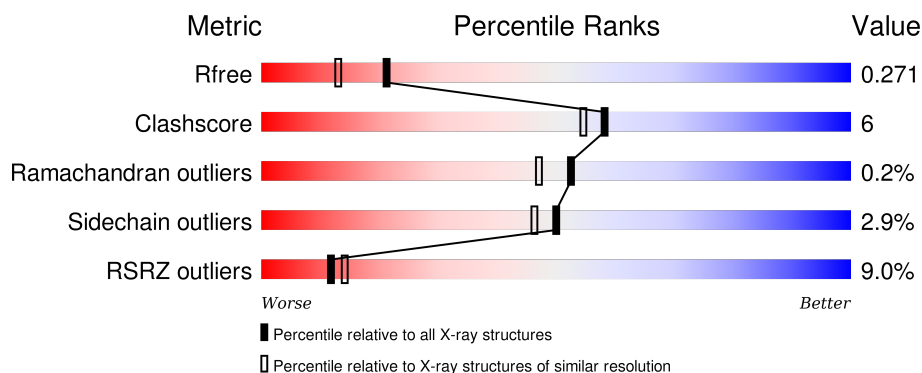
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (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. 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	
1	B	422	

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	H4B	A	760	-	-	-	X
3	H4B	B	760	-	-	-	X
4	6M8	B	800	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7148 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	408	Total	C	N	O	S	0	3	1
			3326	2129	567	608	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	574	614	21			

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



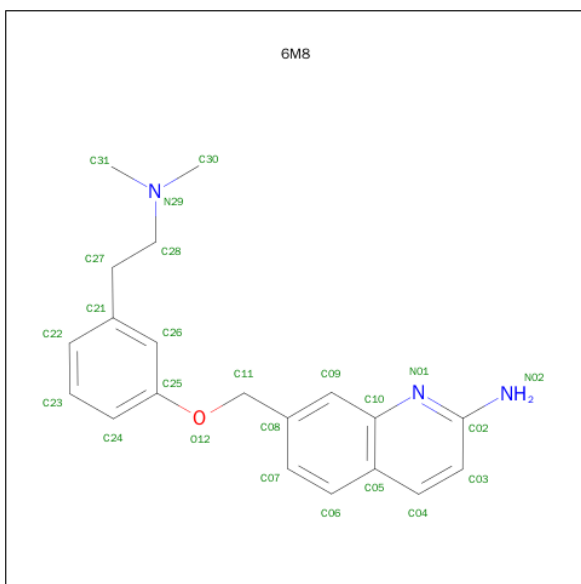
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 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 7-[[3-[2-(DIMETHYLAMINO)ETHYL]PHENOXY]METHYL]QUINOLIN-2-AMINE (three-letter code: 6M8) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			24	20	3	1		

- 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	B	1	Total	Zn	0	0
			1	1		

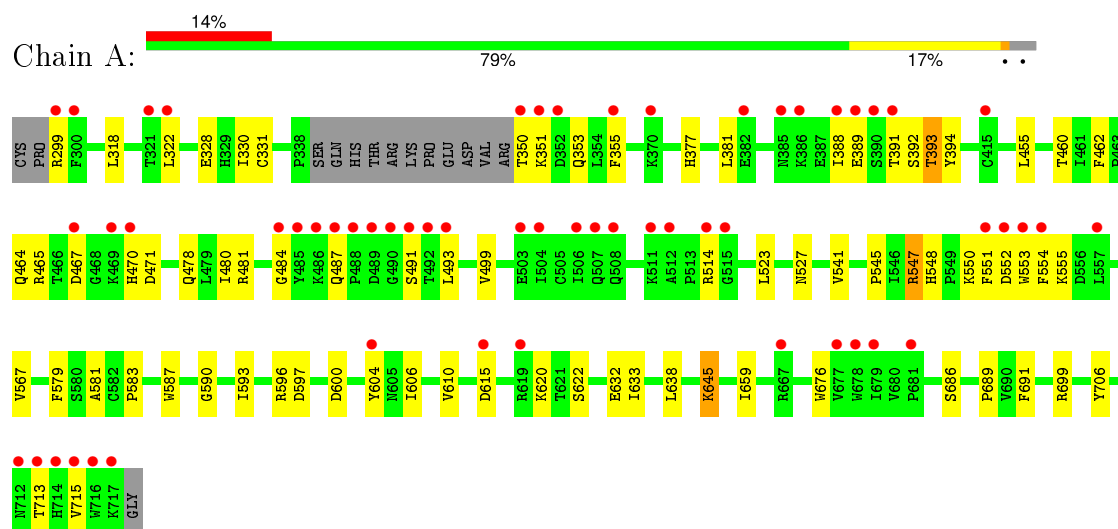
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	129	Total	O	0	0
			129	129		
7	B	159	Total	O	0	0
			159	159		

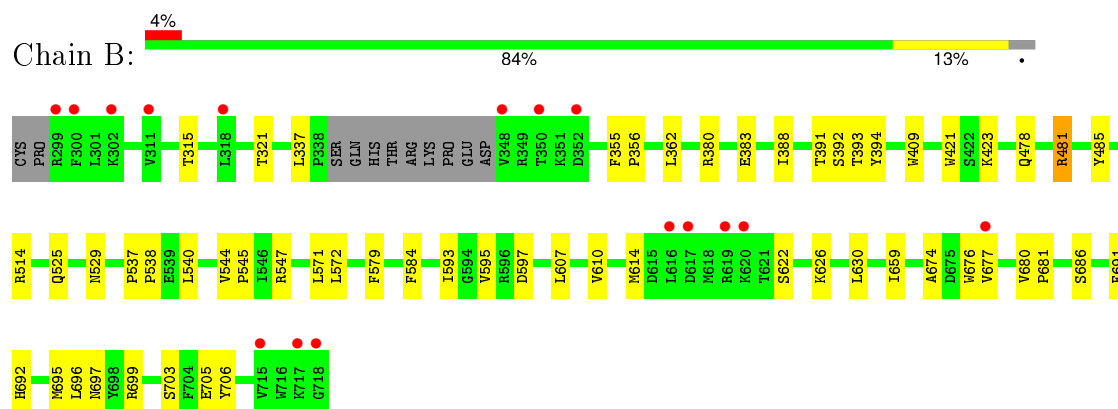
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	51.71Å 111.76Å 164.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 1.98 39.12 – 1.98	Depositor EDS
% Data completeness (in resolution range)	72.2 (39.12-1.98) 72.2 (39.12-1.98)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.202 , 0.266 0.210 , 0.271	Depositor DCC
$R_{free}$ test set	2376 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 48516 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, H4B, 6M8, 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	0.39	0/3428	0.57	0/4651
1	B	0.41	0/3459	0.57	0/4689
All	All	0.40	0/6887	0.57	0/9340

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	3326	0	3237	40	0
1	B	3357	0	3275	32	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	24	0	23	3	0
4	B	24	0	23	5	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	129	0	0	2	1
7	B	159	0	0	2	1
All	All	7148	0	6654	79	1

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 6.

All (79) 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:A:596:ARG:NH2	1:A:600:ASP:OD2	2.19	0.76
1:B:584:PHE:HE1	4:B:800:6M8:H06	1.50	0.76
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.69	0.73
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.07	0.70
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.73	0.69
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.75	0.68
2:B:750:HEM:HBD1	4:B:800:6M8:H111	1.76	0.67
1:B:593:ILE:HA	1:B:597:ASP:HB2	1.77	0.66
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.78	0.66
1:A:393:THR:OG1	1:A:394:TYR:N	2.30	0.63
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.80	0.62
1:A:487:GLN:HE21	1:A:493:LEU:HB2	1.65	0.62
1:A:351:LYS:NZ	1:A:389:GLU:O	2.35	0.60
2:B:750:HEM:O2A	4:B:800:6M8:H24	2.01	0.59
7:A:2100:HOH:O	1:B:692:HIS:ND1	2.30	0.58
1:B:393:THR:OG1	1:B:394:TYR:N	2.37	0.58
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.18	0.57
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.87	0.57
1:A:567:VAL:HG21	4:A:800:6M8:C07	2.33	0.57
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.70	0.56
1:A:593:ILE:HA	1:A:597:ASP:HB2	1.88	0.55
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.89	0.55
1:B:699:ARG:NH2	1:B:705:GLU:OE1	2.42	0.52
1:A:465:ARG:NH2	1:A:471:ASP:OD2	2.35	0.52
1:B:572:LEU:HB3	1:B:579:PHE:HB2	1.92	0.52
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.47	0.49
1:B:610:VAL:O	1:B:614:MET:HG3	2.11	0.49
1:A:686:SER:HA	1:A:691:PHE:CG	2.47	0.49
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.93	0.49
1:A:484:GLY:O	1:A:499:VAL:HA	2.14	0.48
1:A:350:THR:N	1:A:353:GLN:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ALA:HB3	1:B:695:MET:HB3	1.96	0.47
1:A:377:HIS:CD2	1:A:381:LEU:HD13	2.50	0.46
1:B:595:VAL:HG13	1:B:630:LEU:HD11	1.98	0.46
1:B:686:SER:HA	1:B:691:PHE:CG	2.51	0.46
1:B:391:THR:HG22	7:B:2027:HOH:O	2.15	0.46
1:A:462:PHE:HB2	1:A:581:ALA:HB3	1.97	0.46
1:A:659:ILE:HG13	1:A:689:PRO:HB2	1.97	0.46
1:A:470:HIS:HB3	1:A:527:ASN:OD1	2.16	0.46
1:A:596:ARG:O	1:A:600:ASP:HB2	2.16	0.45
1:A:590:GLY:HA3	1:A:638:LEU:HD21	1.98	0.45
4:B:800:6M8:H282	4:B:800:6M8:H22	1.60	0.45
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.52	0.45
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.98	0.45
1:A:391:THR:O	1:A:392:SER:OG	2.29	0.45
1:A:331:CYS:HB3	1:B:697:ASN:HB3	1.99	0.45
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.32	0.44
1:A:467:ASP:OD1	1:A:470:HIS:ND1	2.51	0.44
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.53	0.44
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.99	0.44
1:A:554:PHE:HB3	7:A:2086:HOH:O	2.17	0.44
1:A:464:GLN:HB3	1:A:579:PHE:CE1	2.53	0.43
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.48	0.43
1:A:548:HIS:NE2	1:A:632:GLU:OE1	2.51	0.43
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.34	0.43
2:A:750:HEM:HBD1	4:A:800:6M8:H111	2.00	0.42
1:A:606:ILE:O	1:A:610:VAL:HG23	2.19	0.42
1:A:480:ILE:HD13	1:A:541:VAL:HG13	2.01	0.42
1:A:604:TYR:O	1:A:606:ILE:HG23	2.19	0.42
2:A:750:HEM:O2A	4:A:800:6M8:H24	2.19	0.42
1:B:380:ARG:NH1	1:B:383:GLU:OE1	2.51	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.42
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.90	0.41
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.83	0.41
1:B:659:ILE:HD13	1:B:659:ILE:HA	1.88	0.41
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	2.02	0.41
1:B:388:ILE:O	1:B:392:SER:N	2.48	0.41
1:A:299:ARG:HG3	1:A:318:LEU:HD21	2.03	0.41
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.51	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.86	0.41
1:B:676:TRP:CE2	1:B:680:VAL:HG21	2.56	0.41
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:PHE:CE1	4:B:800:6M8:H06	2.41	0.41
1:B:703:SER:HB2	7:B:2035:HOH:O	2.20	0.41
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.89	0.41
1:A:460:THR:O	1:A:583:PRO:HD2	2.21	0.40
1:B:544:VAL:HA	1:B:545:PRO:HD3	1.93	0.40
1:B:525:GLN:HG3	1:B:529:ASN:O	2.21	0.40
1:B:355:PHE:N	1:B:356:PRO:HD2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2055:HOH:O	7:B:2056:HOH:O[2_554]	2.15	0.05

## 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	407/422 (96%)	387 (95%)	18 (4%)	2 (0%)	34	25
1	B	410/422 (97%)	394 (96%)	16 (4%)	0	100	100
All	All	817/844 (97%)	781 (96%)	34 (4%)	2 (0%)	52	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	491	SER

### 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%)	354 (97%)	12 (3%)	45	40
1	B	369/377 (98%)	360 (98%)	9 (2%)	57	55
All	All	735/754 (98%)	714 (97%)	21 (3%)	50	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	393	THR
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	552	ASP
1	A	555	LYS
1	A	615	ASP
1	A	622	SER
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	315	THR
1	B	321	THR
1	B	337	LEU
1	B	423	LYS
1	B	481	ARG
1	B	540	LEU
1	B	547	ARG
1	B	571	LEU
1	B	622	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 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	24,50,50	2.33	7 (29%)	16,82,82	1.83	4 (25%)
3	H4B	A	760	-	15,18,18	0.84	0	12,26,26	2.34	6 (50%)
4	6M8	A	800	-	26,26,26	0.98	1 (3%)	35,35,35	1.06	1 (2%)
5	ACT	A	860	-	0,3,3	0.00	-	0,3,3	0.00	-
2	HEM	B	750	1	24,50,50	2.40	6 (25%)	16,82,82	1.76	4 (25%)
3	H4B	B	760	-	15,18,18	0.86	0	12,26,26	2.37	6 (50%)
4	6M8	B	800	-	26,26,26	0.82	1 (3%)	35,35,35	1.10	2 (5%)
5	ACT	B	860	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	750	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	6M8	A	800	-	-	0/10/10/10	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	6M8	B	800	-	-	0/10/10/10	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-5.22	1.33	1.40
2	A	750	HEM	C3B-C2B	-4.94	1.34	1.40
2	B	750	HEM	C3C-C2C	-4.75	1.34	1.40
2	A	750	HEM	C3C-C2C	-4.28	1.34	1.40
2	A	750	HEM	CMA-C3A	2.01	1.55	1.51
2	A	750	HEM	C4D-ND	2.39	1.40	1.36
4	B	800	6M8	C02-N01	2.68	1.36	1.33
2	B	750	HEM	C4D-ND	2.72	1.40	1.36
4	A	800	6M8	C02-N01	3.23	1.36	1.33
2	B	750	HEM	C3B-CAB	3.39	1.55	1.47
2	A	750	HEM	C3C-CAC	3.48	1.55	1.47
2	B	750	HEM	C3C-CAC	3.49	1.55	1.47
2	A	750	HEM	C3B-CAB	3.65	1.55	1.47
2	B	750	HEM	C3D-C2D	5.08	1.52	1.37
2	A	750	HEM	C3D-C2D	5.48	1.53	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBD-CAD-C3D	-4.25	105.01	112.47
2	A	750	HEM	CBA-CAA-C2A	-3.52	106.30	112.49
2	B	750	HEM	CBA-CAA-C2A	-3.38	106.55	112.49
3	A	760	H4B	N3-C2-N1	-3.32	120.09	125.51
3	B	760	H4B	N3-C2-N1	-3.12	120.42	125.51
2	B	750	HEM	CAA-CBA-CGA	-3.05	106.85	112.78
2	B	750	HEM	CBD-CAD-C3D	-2.99	107.22	112.47
2	A	750	HEM	CAD-CBD-CGD	-2.27	108.37	112.78
2	A	750	HEM	C3C-CAC-CBC	-2.11	122.15	126.40
2	B	750	HEM	CAD-CBD-CGD	-2.02	108.84	112.78
3	B	760	H4B	N2-C2-N3	2.41	121.18	117.20
3	A	760	H4B	C4A-C8A-N8	2.69	121.10	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	H4B	C4A-C8A-N8	2.70	121.12	118.26
3	B	760	H4B	C2-N1-C8A	2.71	120.73	114.63
3	A	760	H4B	N2-C2-N3	2.74	121.73	117.20
4	B	800	6M8	C02-N01-C10	2.78	121.01	117.60
3	A	760	H4B	C2-N1-C8A	3.02	121.42	114.63
4	B	800	6M8	N02-C02-N01	3.22	120.02	118.03
3	A	760	H4B	C4-N3-C2	3.40	119.87	115.88
4	A	800	6M8	C02-N01-C10	3.55	121.95	117.60
3	B	760	H4B	C4-N3-C2	3.61	120.11	115.88
3	A	760	H4B	C4-C4A-C8A	4.31	118.40	114.61
3	B	760	H4B	C4-C4A-C8A	4.77	118.81	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
4	A	800	6M8	3	0
2	B	750	HEM	6	0
4	B	800	6M8	5	0

## 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 ⓘ

### 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	58 (14%) 4 4	12, 35, 76, 104	0
1	B	411/422 (97%)	0.21	16 (3%) 43 47	9, 27, 58, 83	0
All	All	819/844 (97%)	0.53	74 (9%) 12 14	9, 31, 72, 104	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	7.8
1	A	715	VAL	7.5
1	A	488	PRO	7.4
1	A	716	TRP	6.8
1	A	490	GLY	6.4
1	A	486	LYS	6.3
1	B	348	VAL	5.9
1	B	300	PHE	5.5
1	B	620	LYS	5.4
1	A	551	PHE	5.1
1	A	352	ASP	4.9
1	A	508	GLN	4.9
1	A	351	LYS	4.7
1	A	713	THR	4.6
1	A	507	GLN	4.6
1	B	619	ARG	4.3
1	A	355	PHE	4.2
1	A	714	HIS	4.2
1	A	493	LEU	4.2
1	A	506	ILE	4.0
1	A	388	ILE	4.0
1	B	718	GLY	3.9
1	A	712	ASN	3.6
1	A	504	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	515	GLY	3.5
1	A	484	GLY	3.5
1	A	485	TYR	3.3
1	A	489	ASP	3.3
1	A	390	SER	3.3
1	A	470	HIS	3.2
1	A	514	ARG	3.2
1	B	350	THR	3.2
1	A	503	GLU	3.1
1	A	619	ARG	3.0
1	A	389	GLU	2.9
1	A	552	ASP	2.9
1	A	321	THR	2.9
1	A	300	PHE	2.9
1	A	553	TRP	2.8
1	B	352	ASP	2.8
1	A	511	LYS	2.8
1	A	491	SER	2.8
1	B	299	ARG	2.8
1	A	391	THR	2.7
1	A	382	GLU	2.6
1	B	302	LYS	2.6
1	B	677	VAL	2.6
1	A	385	ASN	2.6
1	A	467	ASP	2.6
1	B	617	ASP	2.6
1	A	386	LYS	2.5
1	B	717	LYS	2.5
1	A	554	PHE	2.5
1	A	487	GLN	2.5
1	A	677	VAL	2.5
1	A	469	LYS	2.5
1	B	616	LEU	2.5
1	A	415	CYS	2.4
1	A	667	ARG	2.4
1	B	318	LEU	2.3
1	A	678	TRP	2.3
1	B	715	VAL	2.3
1	B	311	VAL	2.3
1	A	350	THR	2.3
1	A	322	LEU	2.2
1	A	681	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	2.1
1	A	370	LYS	2.1
1	A	557	LEU	2.1
1	A	512	ALA	2.1
1	A	492	THR	2.1
1	A	615	ASP	2.0
1	A	604	TYR	2.0
1	A	679	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
4	6M8	B	800	24/24	0.94	0.22	3.10	9,52,99,102	0
3	H4B	B	760	17/17	0.87	0.24	2.79	26,54,67,70	0
3	H4B	A	760	17/17	0.88	0.23	2.21	36,55,79,80	0
5	ACT	B	860	4/4	0.97	0.11	1.77	37,43,47,56	0
2	HEM	B	750	43/43	0.98	0.15	1.53	4,16,39,74	0
4	6M8	A	800	24/24	0.94	0.18	1.14	11,23,67,78	0
5	ACT	A	860	4/4	0.96	0.13	1.01	26,36,39,39	0
2	HEM	A	750	43/43	0.98	0.17	0.96	6,18,42,71	0
6	ZN	B	900	1/1	1.00	0.08	-1.37	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.