



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4IMU
Title : Structure of rat neuronal nitric oxide synthase in complex with 6,6'-((5-(aminomethyl)-1,3-phenylene)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-01-03
Resolution : 2.03 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

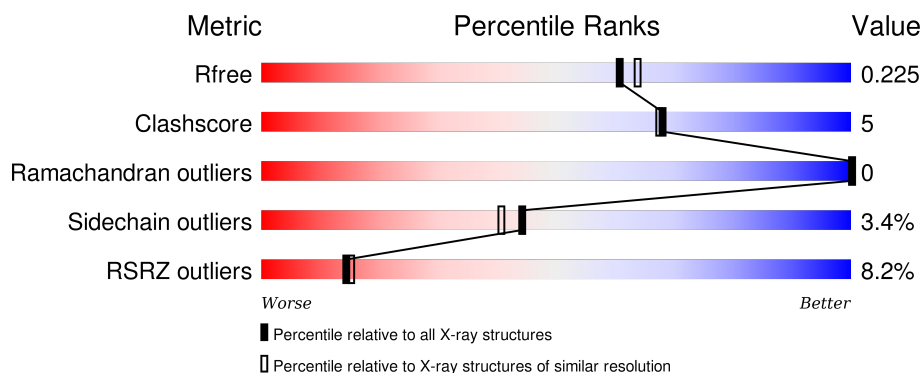
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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 ≥ 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
4	1ET	A	803	-	-	-	X
4	1ET	B	802	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7226 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	3	0
			3327	2130	567	608	22			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2148	574	614	21			

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



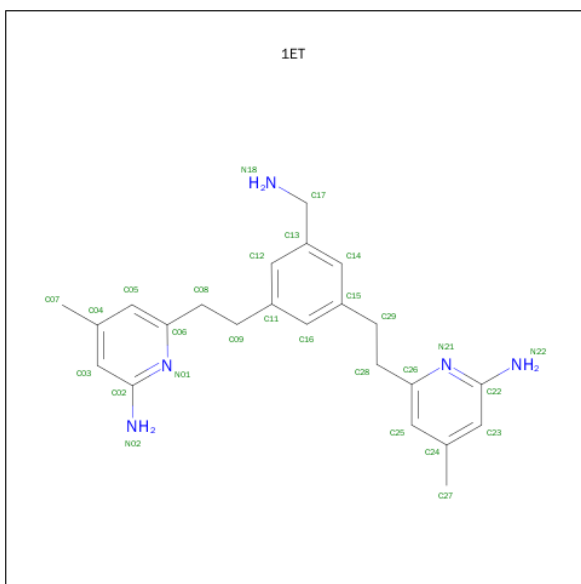
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17	C 9	N 5	O 3	0	0
3	A	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is 6,6'-{[5-(AMINOMETHYL)BENZENE-1,3-DIYL]DIETHANE-2,1-DIYL}BIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: 1ET) (formula: C₂₃H₂₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	23	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			28	23	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	B	1	Total	Zn	0	0
			1	1		
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

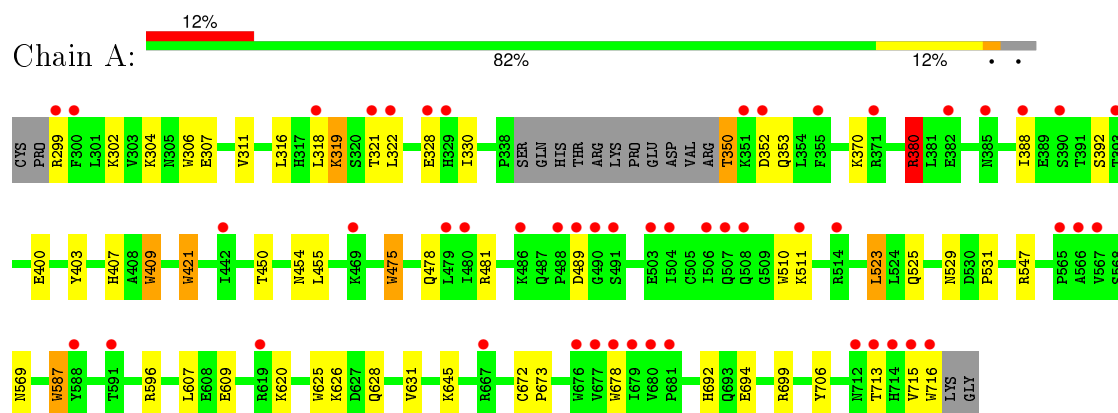
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	147	Total 147	O 147	0	0
8	B	204	Total 204	O 204	0	0

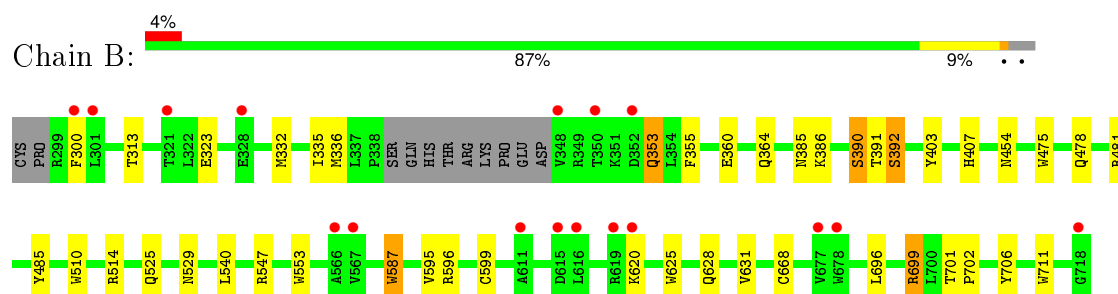
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, 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, α , β , γ	51.91Å 110.22Å 163.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.03 40.74 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.03) 98.8 (40.74-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.184 , 0.225 0.183 , 0.225	Depositor DCC
R_{free} test set	3008 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 60693 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, H4B, CL, 1ET, 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	0.69	9/3429 (0.3%)	0.69	2/4652 (0.0%)
1	B	0.71	6/3456 (0.2%)	0.70	0/4685
All	All	0.70	15/6885 (0.2%)	0.69	2/9337 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TRP	CD2-CE2	6.32	1.49	1.41
1	A	716	TRP	CD2-CE2	5.66	1.48	1.41
1	A	510	TRP	CD2-CE2	5.59	1.48	1.41
1	B	587	TRP	CD2-CE2	5.58	1.48	1.41
1	B	625	TRP	CD2-CE2	5.52	1.48	1.41
1	A	421	TRP	CD2-CE2	5.47	1.48	1.41
1	B	553	TRP	CD2-CE2	5.45	1.47	1.41
1	B	510	TRP	CD2-CE2	5.35	1.47	1.41
1	A	587	TRP	CD2-CE2	5.30	1.47	1.41
1	A	678	TRP	CD2-CE2	5.28	1.47	1.41
1	A	475	TRP	CD2-CE2	5.23	1.47	1.41
1	A	625	TRP	CD2-CE2	5.18	1.47	1.41
1	A	306	TRP	CD2-CE2	5.13	1.47	1.41
1	B	711	TRP	CD2-CE2	5.03	1.47	1.41
1	B	475	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	380	ARG	NE-CZ-NH2	-6.05	117.27	120.30

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	3327	0	3238	31	0
1	B	3357	0	3271	24	0
2	A	43	0	30	9	0
2	B	43	0	30	8	0
3	A	34	0	30	2	0
4	A	28	0	29	3	0
4	B	28	0	29	6	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	147	0	0	2	0
8	B	204	0	0	3	0
All	All	7226	0	6663	64	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 5.

All (64) 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:299:ARG:HA	1:A:318:LEU:HD21	1.54	0.87
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.60	0.83
2:A:801:HEM:O1D	4:A:803:1ET:H11	1.77	0.83
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.64	0.79
1:B:668:CYS:HB3	8:B:929:HOH:O	1.82	0.78
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.64	0.77
1:B:699:ARG:HH11	1:B:699:ARG:HB2	1.51	0.75
1:A:307[B]:GLU:HG2	1:A:692:HIS:CG	2.23	0.73
1:A:489:ASP:HB2	8:A:1019:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:809:H4B:HN22	2:B:801:HEM:CGA	2.06	0.69
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.95	0.66
2:A:801:HEM:CGA	3:A:802:H4B:HN22	2.13	0.62
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.84	0.58
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.83	0.58
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.86	0.58
1:A:609:GLU:HG3	8:A:983:HOH:O	2.03	0.58
1:A:350:THR:N	1:A:353:GLN:HE21	2.02	0.57
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.35	0.56
1:B:364:GLN:NE2	8:B:1088:HOH:O	2.37	0.56
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.88	0.55
1:A:403:TYR:CE1	1:A:407:HIS:CE1	2.95	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.72	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.53
1:A:304:LYS:O	1:A:694:GLU:HG3	2.09	0.53
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.43	0.53
4:B:802:1ET:H12	4:B:802:1ET:H7	1.91	0.52
1:B:596:ARG:HE	4:B:802:1ET:H15	1.59	0.50
1:B:525:GLN:HG3	1:B:529:ASN:O	2.12	0.49
2:A:801:HEM:C1C	4:A:803:1ET:H30	2.47	0.49
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.49	0.48
1:A:607:LEU:HD13	1:A:626:LYS:HG2	1.95	0.48
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.95	0.48
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.60	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.48
1:B:699:ARG:HH11	1:B:699:ARG:CB	2.23	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.15	0.47
1:A:321:THR:HG23	1:A:322:LEU:HG	1.97	0.47
1:B:386:LYS:O	1:B:390:SER:HB3	2.15	0.47
1:B:587:TRP:H	2:B:801:HEM:HAB	1.80	0.47
2:A:801:HEM:HMB3	5:A:804:ACT:H2	1.97	0.46
1:B:454:ASN:ND2	8:B:926:HOH:O	2.49	0.45
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.45
1:A:525:GLN:HG3	1:A:529:ASN:O	2.16	0.45
1:A:321:THR:HG23	1:A:322:LEU:H	1.82	0.44
1:B:300:PHE:HB3	1:B:313:THR:CG2	2.47	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.44
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:A:388:ILE:O	1:A:392:SER:HA	2.18	0.43
1:A:302:LYS:HE3	1:A:311:VAL:HG11	2.01	0.43
2:B:801:HEM:C1C	4:B:802:1ET:H30	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:TRP:H	2:A:801:HEM:HAB	1.84	0.42
2:B:801:HEM:O1D	4:B:802:1ET:H8	2.19	0.42
2:B:801:HEM:O1D	4:B:802:1ET:H11	2.20	0.42
2:B:801:HEM:CBA	4:B:802:1ET:H22	2.49	0.42
1:A:596:ARG:NH1	2:A:801:HEM:O2A	2.53	0.41
1:A:481:ARG:NH2	4:A:803:1ET:H13	2.36	0.41
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.70	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.41
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.20	0.40
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.56	0.40
1:A:672:CYS:HA	1:A:673:PRO:HD2	1.96	0.40
1:A:450:THR:HA	1:A:455:LEU:HD22	2.04	0.40
1:A:316:LEU:HD12	1:A:319:LYS:HD3	2.03	0.40
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.34	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	406/422 (96%)	392 (97%)	14 (3%)	0	100	100
1	B	409/422 (97%)	402 (98%)	7 (2%)	0	100	100
All	All	815/844 (97%)	794 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	Percentiles	
1	A	366/377 (97%)	352 (96%)	14 (4%)	40	35
1	B	368/377 (98%)	357 (97%)	11 (3%)	48	46
All	All	734/754 (97%)	709 (97%)	25 (3%)	44	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	328	GLU
1	A	350	THR
1	A	352	ASP
1	A	380	ARG
1	A	454	ASN
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	323	GLU
1	B	332	MET
1	B	336	MET
1	B	353	GLN
1	B	360	GLU
1	B	390	SER
1	B	392	SER
1	B	540	LEU
1	B	547	ARG
1	B	620	LYS
1	B	699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	601	ASN
1	B	605	ASN
1	B	692	HIS
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are 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	801	1	30,50,50	2.83	14 (46%)	24,82,82	2.64	8 (33%)
3	H4B	A	802	-	13,18,18	0.79	0	11,26,26	2.57	6 (54%)
4	1ET	A	803	-	30,30,30	0.69	0	40,41,41	1.61	7 (17%)
5	ACT	A	804	-	1,3,3	1.45	0	0,3,3	0.00	-
3	H4B	A	809	-	13,18,18	0.94	0	11,26,26	2.67	6 (54%)
2	HEM	B	801	1	30,50,50	2.57	15 (50%)	24,82,82	2.98	10 (41%)
4	1ET	B	802	-	30,30,30	0.64	0	40,41,41	1.82	8 (20%)
5	ACT	B	803	-	1,3,3	1.28	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	801	1	-	0/10/54/54	0/0/8/8
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	1ET	A	803	-	-	0/12/12/12	0/3/3/3
5	ACT	A	804	-	-	0/0/0/0	0/0/0/0
3	H4B	A	809	-	-	0/8/17/17	0/2/2/2
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
4	1ET	B	802	-	-	0/12/12/12	0/3/3/3
5	ACT	B	803	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C4B	-3.97	1.48	1.51
2	B	801	HEM	C3B-C4B	-3.24	1.49	1.51
2	A	801	HEM	C3D-C4D	-3.05	1.47	1.51
2	A	801	HEM	C2D-C3D	-2.85	1.46	1.54
2	B	801	HEM	C2D-C3D	-2.81	1.46	1.54
2	B	801	HEM	C3D-C4D	-2.39	1.48	1.51
2	A	801	HEM	C2C-C1C	-2.21	1.48	1.52
2	B	801	HEM	C2C-C1C	-2.08	1.48	1.52
2	B	801	HEM	C2D-C1D	-2.05	1.45	1.51
2	B	801	HEM	C1A-CHA	2.16	1.45	1.39
2	B	801	HEM	FE-NB	2.16	2.08	1.97
2	B	801	HEM	C4A-CHB	2.34	1.46	1.39
2	A	801	HEM	C4A-CHB	2.38	1.46	1.39
2	A	801	HEM	FE-ND	2.52	2.10	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-ND	2.52	2.10	1.97
2	A	801	HEM	CHD-C1D	2.57	1.46	1.38
2	A	801	HEM	FE-NB	2.63	2.11	1.97
2	B	801	HEM	CHC-C4B	2.71	1.46	1.38
2	A	801	HEM	CHC-C4B	2.88	1.46	1.38
2	B	801	HEM	C2A-C3A	3.39	1.47	1.37
2	A	801	HEM	C2A-C3A	3.51	1.48	1.37
2	B	801	HEM	CHC-C1C	3.74	1.45	1.36
2	B	801	HEM	CHD-C4C	3.76	1.45	1.36
2	A	801	HEM	CHC-C1C	3.95	1.45	1.36
2	A	801	HEM	CHD-C4C	4.72	1.47	1.36
2	B	801	HEM	C4C-NC	5.45	1.42	1.36
2	A	801	HEM	C4C-NC	6.71	1.44	1.36
2	B	801	HEM	C1C-NC	7.46	1.45	1.36
2	A	801	HEM	C1C-NC	7.76	1.45	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-5.71	102.29	112.53
4	A	803	1ET	C05-C06-N01	-4.11	118.32	122.96
4	B	802	1ET	C05-C06-N01	-3.79	118.68	122.96
3	A	802	H4B	N3-C2-N1	-3.38	120.00	125.53
3	A	809	H4B	N3-C2-N1	-3.35	120.04	125.53
4	B	802	1ET	C29-C28-C26	-3.12	106.53	112.53
2	B	801	HEM	CAA-CBA-CGA	-2.97	107.31	112.75
2	A	801	HEM	CBA-CAA-C2A	-2.89	107.35	112.53
4	A	803	1ET	C25-C26-N21	-2.66	119.95	122.96
2	B	801	HEM	C3B-CAB-CBB	-2.53	120.58	124.46
4	A	803	1ET	C09-C08-C06	-2.23	108.23	112.53
2	B	801	HEM	CAA-C2A-C1A	-2.14	124.69	127.01
4	B	802	1ET	C07-C04-C05	-2.12	117.73	120.95
4	B	802	1ET	C09-C08-C06	-2.08	108.51	112.53
2	A	801	HEM	C3B-C4B-NB	2.08	115.60	111.63
4	B	802	1ET	N22-C22-N21	2.10	120.32	116.50
3	A	809	H4B	C2-N1-C8A	2.16	119.40	114.54
4	A	803	1ET	C28-C26-N21	2.28	119.05	115.69
2	B	801	HEM	C2C-C1C-NC	2.32	114.12	110.21
2	A	801	HEM	C2C-C1C-NC	2.35	114.17	110.21
3	A	802	H4B	C2-N1-C8A	2.42	119.97	114.54
3	A	809	H4B	N2-C2-N3	2.78	121.81	117.20
3	A	809	H4B	C4A-C8A-N8	2.81	121.74	118.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	N2-C2-N3	2.87	121.95	117.20
4	B	802	1ET	C28-C26-N21	2.96	120.07	115.69
2	A	801	HEM	CMD-C2D-C3D	2.98	127.55	114.35
3	A	802	H4B	C4A-C8A-N8	3.24	122.25	118.43
4	A	803	1ET	C08-C06-N01	3.27	120.52	115.69
4	A	803	1ET	C02-N01-C06	3.90	121.00	118.23
3	A	802	H4B	C4-C4A-C8A	3.92	118.11	114.56
2	B	801	HEM	CMD-C2D-C3D	3.95	131.82	114.35
4	B	802	1ET	C08-C06-N01	4.02	121.62	115.69
4	A	803	1ET	C22-N21-C26	4.03	121.09	118.23
2	A	801	HEM	CAD-C3D-C4D	4.12	127.01	112.47
3	A	809	H4B	C4-N3-C2	4.29	121.90	115.94
3	A	802	H4B	C4-N3-C2	4.30	121.91	115.94
2	B	801	HEM	CAD-C3D-C4D	4.55	128.51	112.47
2	B	801	HEM	CMC-C2C-C3C	4.92	128.82	116.53
3	A	809	H4B	C4-C4A-C8A	5.07	119.15	114.56
2	A	801	HEM	CMC-C2C-C3C	5.30	129.77	116.53
2	A	801	HEM	CAD-C3D-C2D	5.45	128.88	113.22
2	B	801	HEM	CAD-C3D-C2D	5.56	129.20	113.22
4	B	802	1ET	C02-N01-C06	5.89	122.41	118.23
2	A	801	HEM	CMB-C2B-C3B	6.29	132.24	116.53
2	B	801	HEM	CMB-C2B-C3B	6.92	133.79	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	9	0
3	A	802	H4B	1	0
4	A	803	1ET	3	0
5	A	804	ACT	1	0
3	A	809	H4B	1	0
2	B	801	HEM	8	0
4	B	802	1ET	6	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, 95th 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	A	407/422 (96%)	0.57	50 (12%) 5 6	28, 44, 76, 99	0
1	B	411/422 (97%)	0.16	17 (4%) 41 43	26, 38, 62, 83	0
All	All	818/844 (96%)	0.37	67 (8%) 14 15	26, 41, 71, 99	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	7.1
1	A	716	TRP	6.1
1	A	715	VAL	5.4
1	A	300	PHE	5.3
1	A	488	PRO	4.7
1	A	486	LYS	4.5
1	A	299	ARG	4.4
1	A	355	PHE	4.4
1	A	507	GLN	4.2
1	B	718	GLY	4.2
1	A	713	THR	4.0
1	B	619	ARG	3.9
1	B	350	THR	3.7
1	B	616	LEU	3.5
1	A	567	VAL	3.5
1	A	352	ASP	3.4
1	A	678	TRP	3.4
1	A	318	LEU	3.2
1	B	352	ASP	3.1
1	B	348	VAL	2.9
1	A	390	SER	2.9
1	A	677	VAL	2.8
1	A	712	ASN	2.7
1	A	491	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	490	GLY	2.7
1	B	567	VAL	2.7
1	A	588	TYR	2.6
1	A	322	LEU	2.6
1	A	371	ARG	2.6
1	A	479	LEU	2.6
1	A	480	ILE	2.6
1	A	508	GLN	2.5
1	B	611	ALA	2.5
1	B	301	LEU	2.5
1	A	504	ILE	2.5
1	A	714	HIS	2.5
1	A	328	GLU	2.5
1	A	489	ASP	2.4
1	B	321	THR	2.4
1	A	382	GLU	2.4
1	A	566	ALA	2.4
1	A	321	THR	2.3
1	A	591	THR	2.3
1	B	615	ASP	2.3
1	A	514	ARG	2.3
1	A	676	TRP	2.3
1	A	511	LYS	2.3
1	A	388	ILE	2.2
1	A	442	ILE	2.2
1	A	385	ASN	2.2
1	B	328	GLU	2.2
1	A	619	ARG	2.2
1	B	620	LYS	2.2
1	A	329	HIS	2.2
1	B	677	VAL	2.2
1	B	678	TRP	2.1
1	A	565	PRO	2.1
1	A	667	ARG	2.1
1	B	566	ALA	2.1
1	A	503	GLU	2.1
1	A	679	ILE	2.1
1	A	351	LYS	2.1
1	A	680	VAL	2.1
1	A	469	LYS	2.1
1	A	506	ILE	2.0
1	A	681	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	393	THR	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, 95th 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 ²)	Q<0.9
4	1ET	B	802	28/28	0.90	0.28	3.26	33,63,90,92	0
4	1ET	A	803	28/28	0.91	0.33	2.98	33,70,110,111	0
5	ACT	A	804	4/4	0.98	0.16	1.88	53,55,58,61	0
3	H4B	A	809	17/17	0.86	0.21	1.48	50,55,59,60	0
2	HEM	B	801	43/43	0.98	0.18	1.37	28,31,51,61	0
2	HEM	A	801	43/43	0.98	0.21	1.04	29,32,57,68	0
3	H4B	A	802	17/17	0.87	0.21	0.91	51,55,61,63	0
5	ACT	B	803	4/4	0.98	0.11	0.59	48,50,50,51	0
7	CL	A	808	1/1	0.95	0.19	0.22	58,58,58,58	0
7	CL	B	806	1/1	0.97	0.14	-0.77	51,51,51,51	0
6	ZN	A	805	1/1	0.99	0.06	-3.17	39,39,39,39	0
6	ZN	A	806	1/1	0.98	0.12	-	40,40,40,40	1
7	CL	B	805	1/1	0.99	0.11	-	51,51,51,51	0
7	CL	A	807	1/1	0.98	0.11	-	50,50,50,50	0
6	ZN	B	804	1/1	0.99	0.08	-	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.