



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:44 AM GMT

PDB ID : 3PNG
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((2-fluoro-2-(3-fluorophenyl)ethyl)amino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.; Poulos, T.L.
Deposited on : 2010-11-18
Resolution : 1.88 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

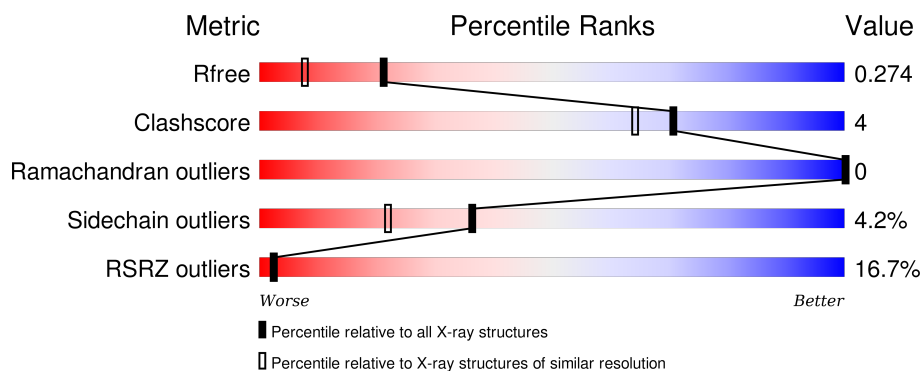
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	<div> <div>21%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
1	B	422	<div> <div>12%</div> <div>90%</div> <div>7%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	860	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7240 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	409	Total	C	N	O	S	0	2	0
			3340	2138	571	609	22			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2147	575	613	22			

- 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: $C_9H_{15}N_5O_3$).



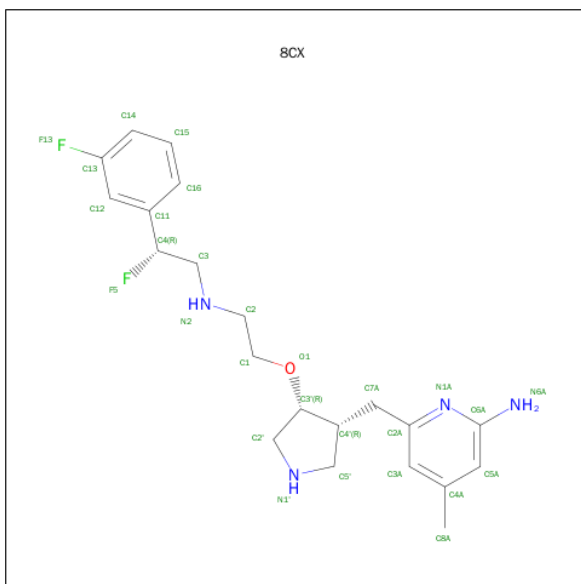
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 5 is 6-{{[(3R,4R)-4-(2-{{[(2R)-2-FLUORO-2-(3-FLUOROPHENYL)ETHYL]AMINO}ETHOXY)PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: 8CX) (formula: C₂₁H₂₈F₂N₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			28	21	2	4	1		
5	B	1	Total	C	F	N	O	0	0
			28	21	2	4	1		

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

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

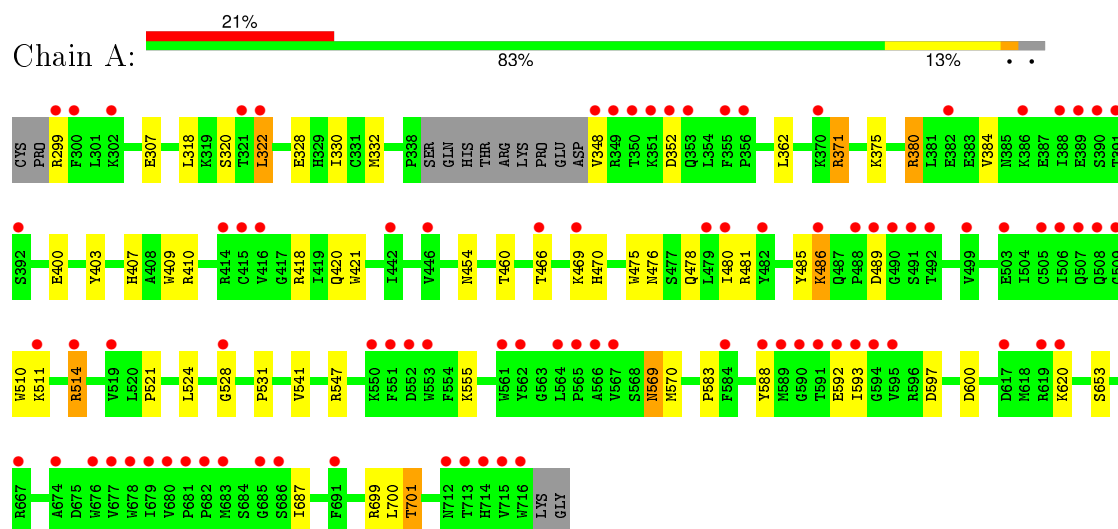
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	151	Total	O	0	0
			151	151		
7	B	207	Total	O	0	0
			207	207		

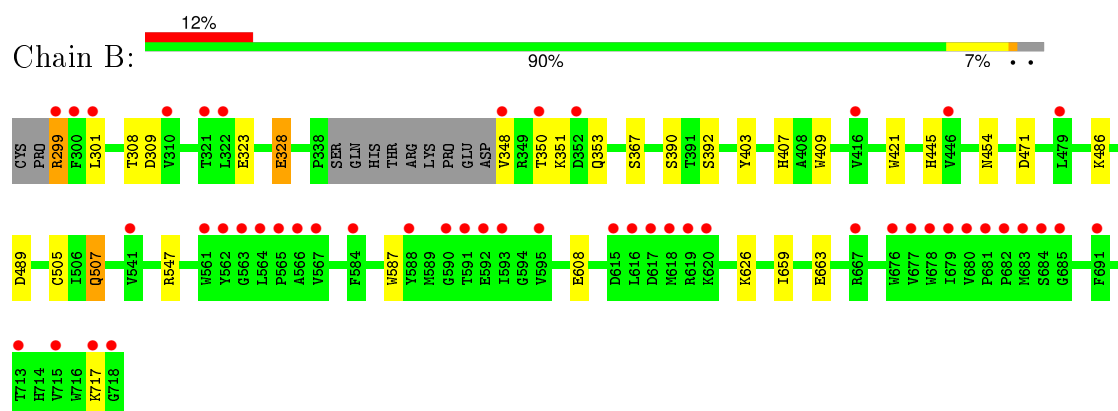
3 Residue-property plots

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, α , β , γ	51.81Å 110.75Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.89 – 1.88 38.89 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.89-1.88) 99.8 (38.89-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.193 , 0.235 0.233 , 0.274	Depositor DCC
R_{free} test set	3840 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 77461 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8CX, HEM, ZN, H4B, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/3439	0.75	4/4665 (0.1%)
1	B	0.81	0/3453	0.82	5/4681 (0.1%)
All	All	0.77	0/6892	0.78	9/9346 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASP	CB-CG-OD2	9.08	126.47	118.30
1	B	471	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	570	MET	CA-CB-CG	-6.57	102.13	113.30
1	A	600	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	471	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	505	CYS	CA-CB-SG	-5.96	103.28	114.00
1	A	570	MET	CG-SD-CE	5.55	109.08	100.20
1	A	410	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	489	ASP	CB-CG-OD1	-5.24	113.58	118.30

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	3340	0	3254	41	0
1	B	3357	0	3269	17	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	28	0	28	3	0
5	B	28	0	28	2	0
6	A	1	0	0	0	0
7	A	151	0	0	1	0
7	B	207	0	0	3	0
All	All	7240	0	6675	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (59) 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:307:GLU:HG3	7:B:11:HOH:O	1.83	0.77
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.66	0.77
1:B:299:ARG:HG3	1:B:299:ARG:HH11	1.51	0.76
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.87	0.74
1:A:687:ILE:HD12	1:B:626:LYS:HB3	1.77	0.66
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.79	0.65
2:A:750:HEM:HBA1	5:A:800:8CX:H4	1.79	0.64
1:A:469:LYS:O	1:A:470:HIS:HD2	1.82	0.63
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.12	0.62
1:A:514:ARG:HG3	1:A:514:ARG:HH21	1.65	0.60
1:A:332:MET:CE	1:B:301:LEU:HD22	2.32	0.59
1:A:514:ARG:HH21	1:A:514:ARG:CG	2.16	0.58
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.85	0.58
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.16	0.56
1:B:507:GLN:NE2	7:B:95:HOH:O	2.38	0.56
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.20	0.55
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.88	0.55
1:A:701:THR:HG23	7:A:228:HOH:O	2.07	0.53
1:A:569:ASN:H	1:A:569:ASN:HD22	1.54	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.90	0.52
1:A:322:LEU:HD12	1:A:699:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.92	0.50
1:B:328:GLU:CD	1:B:328:GLU:H	2.15	0.50
1:B:308:THR:O	1:B:309:ASP:HB2	2.11	0.49
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.77	0.49
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.01	0.49
1:A:332:MET:HE2	1:B:301:LEU:HD22	1.95	0.48
1:B:608:GLU:HG3	7:B:41:HOH:O	2.13	0.48
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.48	0.47
1:A:469:LYS:O	1:A:470:HIS:CD2	2.65	0.47
1:A:592[A]:GLU:OE1	5:A:800:8CX:H16	2.15	0.47
1:A:330:ILE:CG2	1:A:330:ILE:O	2.63	0.46
1:B:299:ARG:CG	1:B:299:ARG:NH1	2.74	0.46
2:A:750:HEM:CBA	5:A:800:8CX:H4	2.45	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45
1:A:330:ILE:HG23	1:A:330:ILE:O	2.16	0.45
1:A:514:ARG:NH2	1:A:514:ARG:CG	2.78	0.45
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.47	0.45
1:B:659:ILE:O	1:B:663:GLU:HG3	2.17	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:A:460:THR:O	1:A:583:PRO:HD2	2.17	0.44
1:A:328:GLU:HB3	1:B:323:GLU:HG2	1.99	0.44
1:A:348:VAL:HG21	1:A:466:THR:O	2.18	0.43
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.39	0.42
1:A:470:HIS:HA	1:A:528:GLY:HA3	2.00	0.42
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.50	0.42
1:B:587:TRP:O	5:B:800:8CX:H15	2.20	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.42
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.42
1:A:510:TRP:CD1	1:A:521:PRO:HG3	2.55	0.42
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.35	0.41
2:B:750:HEM:CBA	5:B:800:8CX:H4	2.50	0.41
1:A:418:ARG:C	1:A:420:GLN:N	2.73	0.41
1:A:524:LEU:O	1:A:531:PRO:HA	2.20	0.41
1:A:320:SER:HA	1:A:700:LEU:HD23	2.01	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.03	0.41
1:A:593:ILE:HA	1:A:597:ASP:OD2	2.21	0.41
1:A:486:LYS:HG2	1:A:486:LYS:H	1.69	0.40
1:B:445:HIS:C	1:B:445:HIS:CD2	2.94	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%)	396 (97%)	11 (3%)	0	100	100
1	B	409/422 (97%)	402 (98%)	7 (2%)	0	100	100
All	All	816/844 (97%)	798 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/377 (97%)	350 (95%)	17 (5%)	33	19
1	B	368/377 (98%)	354 (96%)	14 (4%)	40	25
All	All	735/754 (98%)	704 (96%)	31 (4%)	36	22

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	352	ASP
1	A	371	ARG
1	A	375	LYS
1	A	380	ARG
1	A	454	ASN
1	A	476	ASN
1	A	485	TYR

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Mol	Chain	Res	Type
1	A	486	LYS
1	A	489	ASP
1	A	511	LYS
1	A	514	ARG
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	653	SER
1	A	701	THR
1	B	299	ARG
1	B	328	GLU
1	B	348	VAL
1	B	350	THR
1	B	351	LYS
1	B	353	GLN
1	B	367	SER
1	B	390	SER
1	B	392	SER
1	B	454	ASN
1	B	486	LYS
1	B	507	GLN
1	B	547	ARG
1	B	717	LYS

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

Mol	Chain	Res	Type
1	A	454	ASN
1	A	470	HIS
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	697	ASN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN

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Mol	Chain	Res	Type
1	B	697	ASN

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	30,50,50	2.34	10 (33%)	24,82,82	3.13	12 (50%)
3	H4B	A	760	-	13,18,18	1.57	3 (23%)	11,26,26	2.87	6 (54%)
5	8CX	A	800	-	26,30,30	1.18	4 (15%)	26,40,40	2.51	7 (26%)
4	ACT	A	860	-	1,3,3	1.81	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.18	8 (26%)	24,82,82	3.15	11 (45%)
3	H4B	B	760	-	13,18,18	1.25	1 (7%)	11,26,26	2.62	2 (18%)
5	8CX	B	800	-	26,30,30	0.81	1 (3%)	26,40,40	1.83	5 (19%)
4	ACT	B	860	-	1,3,3	1.69	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	750	1	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	8CX	A	800	-	-	0/15/26/26	0/3/3/3
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	8CX	B	800	-	-	0/15/26/26	0/3/3/3
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-6.52	1.46	1.51
2	B	750	HEM	C3D-C4D	-5.68	1.44	1.51
2	A	750	HEM	C3D-C4D	-5.54	1.44	1.51
2	B	750	HEM	C3B-C4B	-5.53	1.46	1.51
2	B	750	HEM	C2C-C1C	-4.09	1.44	1.52
2	A	750	HEM	C2C-C1C	-3.56	1.45	1.52
2	A	750	HEM	C2D-C1D	-2.94	1.42	1.51
5	A	800	8CX	C11-C4	-2.84	1.47	1.50
2	B	750	HEM	C2D-C1D	-2.38	1.44	1.51
5	B	800	8CX	C3-N2	-2.22	1.43	1.47
3	A	760	H4B	C4A-C8A	-2.20	1.37	1.41
5	A	800	8CX	C3-N2	-2.19	1.43	1.47
2	A	750	HEM	C2B-C1B	-2.10	1.45	1.51
3	B	760	H4B	C8A-N1	2.02	1.38	1.34
5	A	800	8CX	C6A-N6A	2.08	1.41	1.35
2	A	750	HEM	C3C-CAC	2.10	1.55	1.51
2	B	750	HEM	C3C-CAC	2.11	1.55	1.51
2	A	750	HEM	FE-NB	2.34	2.09	1.97
2	A	750	HEM	CHC-C1C	2.38	1.42	1.36
2	B	750	HEM	FE-NB	2.40	2.10	1.97
3	A	760	H4B	C8A-N1	2.46	1.39	1.34
2	B	750	HEM	C1C-NC	2.58	1.39	1.36
5	A	800	8CX	C5A-C4A	2.64	1.43	1.38
2	B	750	HEM	FE-NC	2.97	2.07	1.95
2	A	750	HEM	FE-ND	3.26	2.14	1.97
3	A	760	H4B	C2-N2	3.53	1.41	1.34
2	A	750	HEM	C1C-NC	4.20	1.41	1.36

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-8.53	97.24	112.53
5	A	800	8CX	C4A-C3A-C2A	-7.51	115.58	120.28
2	A	750	HEM	CBA-CAA-C2A	-7.50	99.08	112.53
3	A	760	H4B	N3-C2-N1	-4.31	118.46	125.53
2	A	750	HEM	CBD-CAD-C3D	-4.29	101.08	113.55
2	B	750	HEM	CAA-C2A-C1A	-3.90	122.78	127.01
2	B	750	HEM	CBD-CAD-C3D	-3.52	103.31	113.55
2	A	750	HEM	CAA-C2A-C1A	-3.42	123.30	127.01
5	B	800	8CX	C3A-C2A-N1A	-3.08	119.48	122.96
5	A	800	8CX	C14-C13-C12	-2.65	119.93	123.35
2	B	750	HEM	C3C-CAC-CBC	-2.35	120.84	124.46
5	B	800	8CX	C14-C13-C12	-2.33	120.35	123.35
5	A	800	8CX	F5-C4-C11	-2.16	106.81	109.80
2	A	750	HEM	C3C-CAC-CBC	-2.09	121.25	124.46
2	A	750	HEM	C3B-C4B-NB	-2.02	107.76	111.63
2	B	750	HEM	C3B-C4B-NB	-2.01	107.78	111.63
5	A	800	8CX	N6A-C6A-N1A	2.14	120.40	116.50
5	B	800	8CX	N6A-C6A-N1A	2.28	120.65	116.50
2	B	750	HEM	CMD-C2D-C3D	2.48	125.33	114.35
3	A	760	H4B	C2-N1-C8A	2.50	120.16	114.54
5	A	800	8CX	F13-C13-C14	2.52	122.72	118.52
3	A	760	H4B	N2-C2-N3	2.61	121.53	117.20
2	A	750	HEM	C2D-C3D-C4D	2.72	106.11	101.50
5	A	800	8CX	C16-C11-C12	2.72	122.06	118.79
5	B	800	8CX	F13-C13-C14	2.79	123.17	118.52
3	B	760	H4B	C4-N3-C2	2.90	119.96	115.94
3	A	760	H4B	C4A-C8A-N8	3.44	122.48	118.43
3	A	760	H4B	C4-C4A-C8A	3.51	117.75	114.56
2	A	750	HEM	CMD-C2D-C3D	3.64	130.44	114.35
2	B	750	HEM	C3B-C4B-CHC	3.78	128.49	123.16
2	A	750	HEM	CAD-C3D-C4D	3.99	126.53	112.47
2	B	750	HEM	CAD-C3D-C2D	4.32	125.64	113.22
2	B	750	HEM	CMB-C2B-C3B	4.52	127.81	116.53
2	A	750	HEM	CMC-C2C-C3C	4.83	128.59	116.53
2	A	750	HEM	C3B-C4B-CHC	4.86	130.01	123.16
2	A	750	HEM	CMB-C2B-C3B	4.87	128.68	116.53
2	A	750	HEM	CAD-C3D-C2D	4.91	127.33	113.22
3	A	760	H4B	C4-N3-C2	4.98	122.85	115.94
2	B	750	HEM	CAD-C3D-C4D	4.98	130.05	112.47
2	B	750	HEM	CMC-C2C-C3C	5.25	129.65	116.53
5	B	800	8CX	C6A-N1A-C2A	6.36	122.75	118.23
5	A	800	8CX	C6A-N1A-C2A	7.23	123.37	118.23
3	B	760	H4B	C4-C4A-C8A	7.65	121.49	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	4	0
5	A	800	8CX	3	0
2	B	750	HEM	2	0
5	B	800	8CX	2	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, 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	409/422 (96%)	1.20	88 (21%) 1 1	27, 52, 87, 115	0
1	B	411/422 (97%)	0.65	49 (11%) 6 6	28, 41, 66, 81	0
All	All	820/844 (97%)	0.92	137 (16%) 2 2	27, 46, 82, 115	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	10.0
1	A	488	PRO	8.1
1	A	713	THR	7.3
1	A	716	TRP	6.9
1	A	351	LYS	6.7
1	A	348	VAL	6.4
1	A	300	PHE	6.2
1	A	352	ASP	5.9
1	A	355	PHE	5.8
1	A	715	VAL	5.2
1	B	677	VAL	5.1
1	A	592[A]	GLU	5.1
1	A	322	LEU	4.8
1	A	486	LYS	4.7
1	B	619	ARG	4.7
1	A	677	VAL	4.5
1	B	616	LEU	4.4
1	A	506	ILE	4.3
1	A	567	VAL	4.3
1	A	678	TRP	4.3
1	A	593	ILE	4.3
1	A	619	ARG	4.2
1	B	561	TRP	4.1
1	B	680	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	4.1
1	A	679	ILE	4.1
1	A	469	LYS	4.0
1	A	507	GLN	4.0
1	B	667	ARG	4.0
1	B	348	VAL	3.9
1	A	299	ARG	3.8
1	B	592[A]	GLU	3.8
1	A	551	PHE	3.8
1	A	386	LYS	3.8
1	A	388	ILE	3.7
1	A	561	TRP	3.7
1	B	679	ILE	3.7
1	A	415	CYS	3.7
1	A	479	LEU	3.7
1	B	350	THR	3.7
1	A	676	TRP	3.6
1	A	588	TYR	3.6
1	A	491	SER	3.5
1	A	591	THR	3.5
1	B	676	TRP	3.5
1	A	680	VAL	3.5
1	A	416	VAL	3.4
1	A	519	VAL	3.4
1	A	389	GLU	3.4
1	A	390	SER	3.4
1	B	299	ARG	3.4
1	B	620	LYS	3.3
1	A	682	PRO	3.3
1	A	566	ALA	3.3
1	A	565	PRO	3.3
1	B	718	GLY	3.2
1	A	349	ARG	3.2
1	B	691	PHE	3.2
1	A	490	GLY	3.1
1	B	566	ALA	3.1
1	A	356	PRO	3.1
1	B	310	VAL	3.1
1	A	714	HIS	3.0
1	B	715	VAL	3.0
1	A	480	ILE	3.0
1	B	322	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	391	THR	2.9
1	A	595	VAL	2.9
1	A	667	ARG	2.9
1	A	508	GLN	2.9
1	A	564	LEU	2.9
1	B	615	ASP	2.9
1	A	683	MET	2.8
1	A	528	GLY	2.8
1	B	681	PRO	2.8
1	A	712	ASN	2.8
1	A	446	VAL	2.8
1	B	567	VAL	2.8
1	A	681	PRO	2.8
1	A	482	TYR	2.7
1	A	562	TYR	2.7
1	A	511	LYS	2.7
1	A	674	ALA	2.7
1	B	682	PRO	2.7
1	A	503	GLU	2.7
1	A	489	ASP	2.7
1	B	416	VAL	2.6
1	B	617	ASP	2.6
1	B	588	TYR	2.6
1	B	591	THR	2.6
1	A	685	GLY	2.6
1	A	589	MET	2.5
1	A	392	SER	2.5
1	A	584	PHE	2.5
1	A	514	ARG	2.5
1	B	618	MET	2.5
1	A	353	GLN	2.5
1	B	479	LEU	2.5
1	A	550	LYS	2.5
1	A	350	THR	2.5
1	A	691	PHE	2.4
1	A	499	VAL	2.4
1	B	562	TYR	2.4
1	B	352	ASP	2.4
1	A	590	GLY	2.4
1	A	492	THR	2.4
1	A	382	GLU	2.4
1	A	594	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	565	PRO	2.4
1	A	505	CYS	2.4
1	A	617	ASP	2.4
1	B	685	GLY	2.3
1	A	442	ILE	2.3
1	B	564	LEU	2.3
1	B	593	ILE	2.3
1	B	717	LYS	2.3
1	A	686	SER	2.2
1	A	370	LYS	2.2
1	B	321	THR	2.2
1	B	301	LEU	2.2
1	B	684	SER	2.2
1	A	466	THR	2.2
1	B	678	TRP	2.2
1	B	713	THR	2.2
1	B	541	VAL	2.2
1	A	302	LYS	2.2
1	B	584	PHE	2.2
1	B	446	VAL	2.2
1	B	683	MET	2.2
1	A	414	ARG	2.1
1	B	595	VAL	2.1
1	A	509	GLY	2.1
1	A	552	ASP	2.1
1	A	620	LYS	2.0
1	B	590	GLY	2.0
1	A	553	TRP	2.0
1	B	563	GLY	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, 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	ACT	A	860	4/4	0.96	0.37	13.83	57,57,59,61	0
4	ACT	B	860	4/4	0.96	0.14	0.41	43,46,47,48	0
3	H4B	A	760	17/17	0.96	0.20	0.30	27,31,38,40	0
2	HEM	B	750	43/43	0.97	0.19	0.19	25,32,42,49	0
3	H4B	B	760	17/17	0.95	0.19	0.17	28,32,36,38	0
2	HEM	A	750	43/43	0.96	0.23	0.12	27,33,41,43	0
5	8CX	A	800	28/28	0.88	0.15	-0.77	13,24,38,41	0
6	ZN	A	900	1/1	0.99	0.09	-1.00	40,40,40,40	0
5	8CX	B	800	28/28	0.91	0.12	-1.00	15,26,33,34	0

6.5 Other polymers

There are no such residues in this entry.