



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 10:09 AM EDT

PDB ID : 3NLZ
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-(2,2-Difluoro-2-phenylethylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : unknown
Resolution : 1.92 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

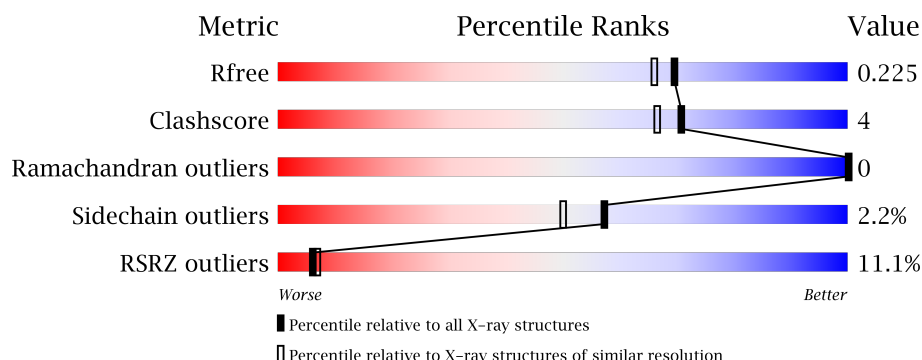
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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	ACT	A	860	-	-	-	X
4	ACT	B	860	-	-	-	X
7	GOL	B	883	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7342 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	4	0
			3346	2142	571	611	22			
1	B	411	Total	C	N	O	S	0	4	0
			3360	2150	574	614	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: $C_9H_{15}N_5O_3$).



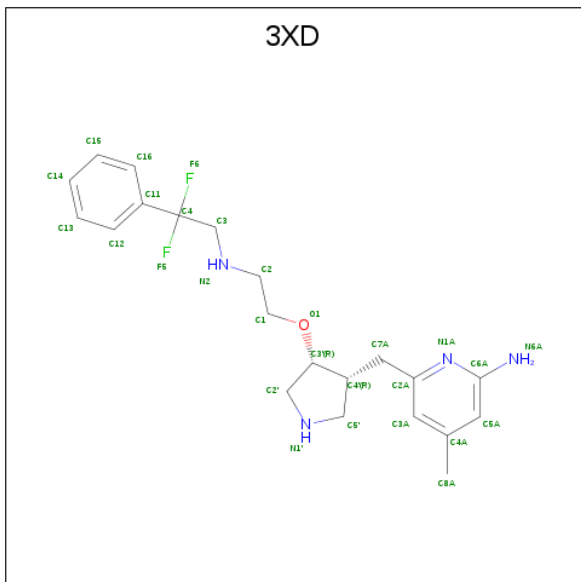
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 6-{[(3R,4R)-4-{2-[(2,2-difluoro-2-phenylethyl)amino]ethoxy}pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: 3XD) (formula: C₂₁H₂₈F₂N₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	1
			42	31	4	5	2		
5	B	1	Total	C	F	N	O	0	1
			42	31	4	5	2		

- 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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

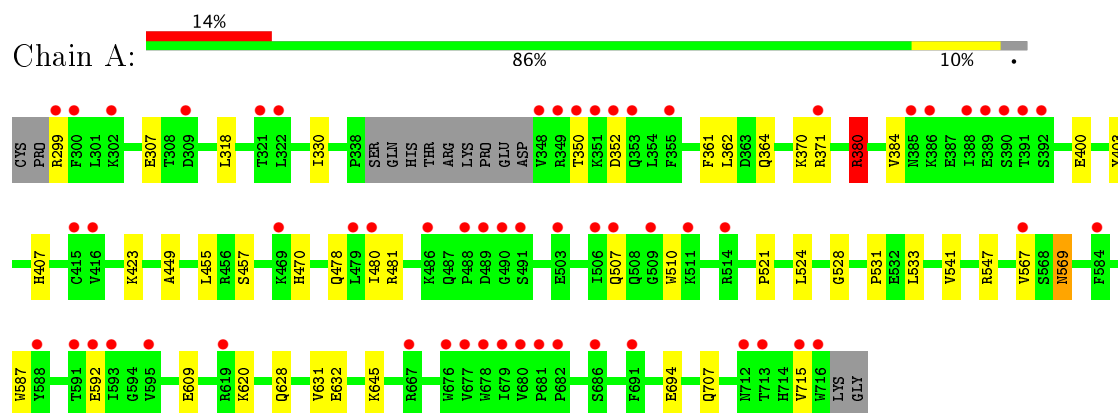
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	180	Total	O	0	0
			180	180		
8	B	237	Total	O	0	0
			237	237		

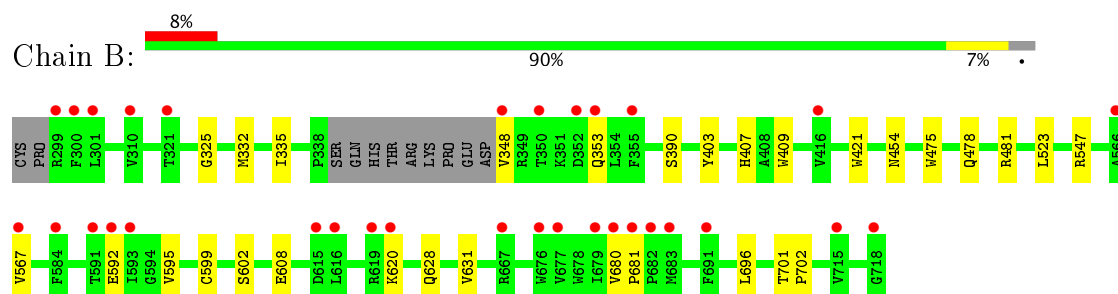
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- 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 110.43Å 163.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.92 37.82 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.64-1.92) 99.7 (37.82-1.92)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.210 0.189 , 0.225	Depositor DCC
R_{free} test set	3613 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, ZN, 3XD, H4B, 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	0.62	0/3451	0.66	1/4681 (0.0%)
1	B	0.67	0/3465	0.66	0/4697
All	All	0.64	0/6916	0.66	1/9378 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3346	0	3264	32	0
1	B	3360	0	3280	16	0
2	A	43	0	30	6	0
2	B	43	0	30	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	42	0	26	8	0
5	B	42	0	26	6	0
6	A	1	0	0	0	0
7	B	6	0	8	0	0
8	A	180	0	0	2	0
8	B	237	0	0	3	0
All	All	7342	0	6700	56	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 (56) 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)
2:A:750:HEM:HBA2	5:A:800[B]:3XD:F5	1.51	0.98
2:A:750:HEM:CBA	5:A:800[B]:3XD:F5	2.11	0.89
2:B:750:HEM:CBA	5:B:800[B]:3XD:F5	2.17	0.83
2:B:750:HEM:HBA2	5:B:800[B]:3XD:F5	1.68	0.83
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.68	0.75
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.50	0.75
1:A:307:GLU:HG3	8:B:1024:HOH:O	1.86	0.74
1:A:609:GLU:HG3	8:A:1103:HOH:O	1.90	0.69
2:B:750:HEM:HBA1	5:B:800[B]:3XD:F5	1.86	0.64
1:A:567:VAL:HG23	5:A:800[A]:3XD:H12	1.82	0.61
1:A:592[A]:GLU:OE1	5:A:800[A]:3XD:H16	2.02	0.59
5:B:800[A]:3XD:H1	8:B:1158:HOH:O	2.02	0.59
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.17	0.55
5:A:800[A]:3XD:H1	8:A:1147:HOH:O	2.08	0.54
2:A:750:HEM:HBA1	5:A:800[B]:3XD:F5	1.94	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.90	0.54
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.90	0.53
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.90	0.53
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.09	0.52
1:B:325:GLY:O	1:B:332:MET:HG3	2.10	0.52
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.43	0.52
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.92	0.52
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.92	0.51
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.47	0.50
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.75	0.49
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.94	0.49
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:VAL:HG23	5:B:800[A]:3XD:H12	1.95	0.48
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.47
1:A:592[B]:GLU:OE1	5:A:800[B]:3XD:H3A	2.14	0.47
1:A:510:TRP:HB2	1:A:533:LEU:HD11	1.98	0.46
1:A:569:ASN:O	1:A:707:GLN:HG2	2.15	0.46
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.96	0.46
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.98	0.45
1:B:608:GLU:HG3	8:B:1011:HOH:O	2.17	0.45
1:A:449:ALA:O	1:A:455:LEU:HA	2.18	0.44
1:A:569:ASN:H	1:A:569:ASN:HD22	1.65	0.43
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.99	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG3	2.01	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.42
1:A:380:ARG:CD	1:A:400:GLU:OE1	2.67	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.20	0.42
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.41
1:A:423:LYS:O	1:A:457[B]:SER:OG	2.37	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.93	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.02	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:361:PHE:O	1:A:364:GLN:HG2	2.20	0.41
1:A:470:HIS:HA	1:A:528:GLY:HA3	2.03	0.41
1:B:592[A]:GLU:OE1	5:B:800[A]:3XD:H16	2.21	0.41
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.80	0.40
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.57	0.40
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.41	0.40
1:A:299:ARG:HG3	1:A:318:LEU:HD21	2.03	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	409/422 (97%)	399 (98%)	10 (2%)	0	100	100
1	B	411/422 (97%)	408 (99%)	3 (1%)	0	100	100
All	All	820/844 (97%)	807 (98%)	13 (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	369/377 (98%)	360 (98%)	9 (2%)	54	46
1	B	370/377 (98%)	363 (98%)	7 (2%)	62	56
All	All	739/754 (98%)	723 (98%)	16 (2%)	57	50

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	352	ASP
1	A	380	ARG
1	A	507	GLN
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	348	VAL
1	B	353	GLN
1	B	390	SER
1	B	454	ASN
1	B	547	ARG
1	B	602	SER
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	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	28,50,50	2.17	9 (32%)	17,82,82	2.69	4 (23%)
3	H4B	A	760	-	14,18,18	0.95	1 (7%)	12,26,26	2.35	4 (33%)
5	3XD	A	800[A]	-	26,30,30	0.86	2 (7%)	30,41,41	1.78	6 (20%)
5	3XD	A	800[B]	-	26,30,30	1.01	2 (7%)	30,41,41	1.80	6 (20%)
4	ACT	A	860	-	1,3,3	1.55	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.11	8 (28%)	17,82,82	2.56	3 (17%)
3	H4B	B	760	-	14,18,18	1.05	1 (7%)	12,26,26	2.15	5 (41%)
5	3XD	B	800[A]	-	26,30,30	0.84	2 (7%)	30,41,41	1.68	5 (16%)
5	3XD	B	800[B]	-	26,30,30	0.90	2 (7%)	30,41,41	1.67	5 (16%)
4	ACT	B	860	-	1,3,3	1.74	0	0,3,3	0.00	-
7	GOL	B	883	-	5,5,5	0.18	0	5,5,5	0.61	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	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	3XD	A	800[A]	-	-	0/18/29/29	0/3/3/3
5	3XD	A	800[B]	-	-	0/18/29/29	0/3/3/3
4	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
5	3XD	B	800[A]	-	-	0/18/29/29	0/3/3/3
5	3XD	B	800[B]	-	-	0/18/29/29	0/3/3/3
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0
7	GOL	B	883	-	-	0/4/4/4	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-C2B	-5.50	1.33	1.40
2	B	750	HEM	C3B-C2B	-4.33	1.34	1.40
2	B	750	HEM	C3C-C2C	-4.11	1.34	1.40
2	A	750	HEM	C3C-C2C	-3.94	1.35	1.40
5	A	800[B]	3XD	F5-C4	-3.06	1.30	1.37
5	B	800[B]	3XD	F5-C4	-2.81	1.31	1.37
5	A	800[B]	3XD	F6-C4	-2.52	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800[B]	3XD	F6-C4	-2.42	1.32	1.37
5	A	800[A]	3XD	F6-C4	-2.11	1.32	1.37
5	B	800[A]	3XD	F6-C4	-2.10	1.32	1.37
5	B	800[A]	3XD	F5-C4	-2.08	1.32	1.37
5	A	800[A]	3XD	F5-C4	-2.06	1.33	1.37
2	A	750	HEM	CMD-C2D	2.01	1.55	1.51
2	A	750	HEM	C1D-ND	2.02	1.40	1.36
2	B	750	HEM	CMC-C2C	2.06	1.56	1.51
2	B	750	HEM	CMB-C2B	2.06	1.56	1.51
2	B	750	HEM	C1C-NC	2.11	1.39	1.36
3	A	760	H4B	C4-N3	2.24	1.37	1.33
3	B	760	H4B	C4-N3	2.27	1.37	1.33
2	A	750	HEM	CMC-C2C	2.31	1.56	1.51
2	A	750	HEM	CMA-C3A	2.47	1.56	1.51
2	B	750	HEM	C3B-CAB	3.34	1.54	1.47
2	A	750	HEM	C3B-CAB	3.44	1.54	1.47
2	A	750	HEM	C3C-CAC	3.74	1.55	1.47
2	B	750	HEM	C3C-CAC	4.14	1.56	1.47
2	B	750	HEM	C3D-C2D	4.33	1.50	1.37
2	A	750	HEM	C3D-C2D	4.96	1.52	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-7.23	98.66	112.48
2	A	750	HEM	CBD-CAD-C3D	-6.93	99.24	112.47
2	A	750	HEM	CBA-CAA-C2A	-6.43	100.20	112.48
2	B	750	HEM	CBD-CAD-C3D	-6.26	100.53	112.47
2	A	750	HEM	C1D-C2D-C3D	-3.61	104.49	107.00
3	A	760	H4B	N3-C2-N1	-3.40	119.93	125.45
5	B	800[B]	3XD	F5-C4-C11	-3.03	106.96	110.47
3	B	760	H4B	N3-C2-N1	-2.78	120.95	125.45
5	A	800[B]	3XD	C4A-C3A-C2A	-2.67	118.59	120.26
5	A	800[A]	3XD	C4A-C3A-C2A	-2.67	118.59	120.26
5	B	800[A]	3XD	C3A-C2A-N1A	-2.65	120.03	122.91
5	B	800[B]	3XD	C3A-C2A-N1A	-2.65	120.03	122.91
3	B	760	H4B	C6-C7-N8	-2.50	107.04	111.01
5	A	800[B]	3XD	C3A-C2A-N1A	-2.16	120.57	122.91
5	A	800[A]	3XD	C3A-C2A-N1A	-2.16	120.57	122.91
2	A	750	HEM	CMC-C2C-C3C	2.08	128.74	124.89
2	B	750	HEM	C4C-C3C-C2C	2.26	108.48	106.90
3	B	760	H4B	C2-N1-C8A	2.40	119.92	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800[B]	3XD	N6A-C6A-N1A	2.57	120.97	116.64
5	A	800[A]	3XD	N6A-C6A-N1A	2.57	120.97	116.64
5	B	800[A]	3XD	C5'-N1'-C2'	2.58	111.40	105.40
5	B	800[B]	3XD	C5'-N1'-C2'	2.58	111.40	105.40
5	A	800[B]	3XD	C2-N2-C3	2.86	119.14	113.35
3	B	760	H4B	C4-N3-C2	2.86	120.17	116.06
5	B	800[A]	3XD	N6A-C6A-N1A	2.86	121.46	116.64
5	B	800[B]	3XD	N6A-C6A-N1A	2.86	121.46	116.64
3	A	760	H4B	C2-N1-C8A	3.10	121.49	114.51
5	A	800[A]	3XD	C2-N2-C3	3.27	119.97	113.35
3	A	760	H4B	C4-N3-C2	3.30	120.81	116.06
5	A	800[B]	3XD	C5'-N1'-C2'	3.43	113.37	105.40
5	A	800[A]	3XD	C5'-N1'-C2'	3.43	113.37	105.40
5	B	800[A]	3XD	C2-N2-C3	3.54	120.52	113.35
3	B	760	H4B	C4-C4A-C8A	4.22	118.38	114.56
3	A	760	H4B	C4-C4A-C8A	4.53	118.66	114.56
5	B	800[A]	3XD	C6A-N1A-C2A	5.30	121.92	118.17
5	B	800[B]	3XD	C6A-N1A-C2A	5.30	121.92	118.17
5	A	800[B]	3XD	C6A-N1A-C2A	5.67	122.18	118.17
5	A	800[A]	3XD	C6A-N1A-C2A	5.67	122.18	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	6	0
5	A	800[A]	3XD	3	0
5	A	800[B]	3XD	5	0
2	B	750	HEM	4	0
5	B	800[A]	3XD	3	0
5	B	800[B]	3XD	3	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	409/422 (96%)	0.75	59 (14%) 3 3	22, 41, 71, 88	0
1	B	411/422 (97%)	0.30	32 (7%) 14 16	22, 33, 56, 68	0
All	All	820/844 (97%)	0.52	91 (11%) 6 7	22, 37, 65, 88	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	8.9
1	B	300	PHE	7.4
1	A	348	VAL	7.1
1	A	355	PHE	5.9
1	A	486	LYS	5.2
1	A	352	ASP	4.9
1	A	715	VAL	4.9
1	A	716	TRP	4.8
1	B	619	ARG	4.2
1	A	351	LYS	4.2
1	A	299	ARG	4.1
1	A	713	THR	4.1
1	A	350	THR	4.0
1	A	507	GLN	3.9
1	B	616	LEU	3.7
1	A	321	THR	3.7
1	A	619	ARG	3.6
1	B	350	THR	3.6
1	A	680	VAL	3.6
1	A	386	LYS	3.5
1	A	300	PHE	3.5
1	A	392	SER	3.4
1	A	677	VAL	3.4
1	A	490	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	511	LYS	3.2
1	B	718	GLY	3.1
1	B	321	THR	3.1
1	B	620	LYS	3.1
1	B	667	ARG	3.1
1	A	491	SER	3.1
1	A	678	TRP	3.0
1	A	509	GLY	2.9
1	A	390	SER	2.9
1	A	469	LYS	2.9
1	A	349	ARG	2.9
1	B	691	PHE	2.9
1	B	299	ARG	2.8
1	A	391	THR	2.8
1	A	679	ILE	2.8
1	A	592[A]	GLU	2.8
1	A	681	PRO	2.7
1	A	588	TYR	2.7
1	A	514	ARG	2.7
1	A	567	VAL	2.7
1	A	595	VAL	2.7
1	A	353	GLN	2.6
1	A	667	ARG	2.6
1	A	385	ASN	2.6
1	B	352	ASP	2.6
1	A	389	GLU	2.6
1	A	503	GLU	2.6
1	B	680	VAL	2.6
1	A	712	ASN	2.5
1	A	591	THR	2.5
1	A	322	LEU	2.5
1	A	682	PRO	2.5
1	B	677	VAL	2.4
1	B	591	THR	2.4
1	A	691	PHE	2.4
1	B	715	VAL	2.4
1	A	480	ILE	2.4
1	B	566	ALA	2.4
1	A	371	ARG	2.4
1	A	676	TRP	2.4
1	A	388	ILE	2.3
1	A	479	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	567	VAL	2.3
1	A	309	ASP	2.3
1	B	615	ASP	2.3
1	B	681	PRO	2.2
1	A	415	CYS	2.2
1	B	592[A]	GLU	2.2
1	B	310	VAL	2.2
1	B	348	VAL	2.2
1	A	506	ILE	2.2
1	B	679	ILE	2.2
1	B	682	PRO	2.2
1	A	584	PHE	2.2
1	A	489	ASP	2.2
1	A	593	ILE	2.1
1	B	593	ILE	2.1
1	B	676	TRP	2.1
1	B	355	PHE	2.1
1	A	686	SER	2.1
1	B	301	LEU	2.1
1	A	302	LYS	2.1
1	B	683	MET	2.1
1	B	416	VAL	2.1
1	B	353	GLN	2.0
1	A	416	VAL	2.0
1	B	584	PHE	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(\AA^2)	Q<0.9
4	ACT	A	860	4/4	0.93	0.23	6.88	50,51,52,54	0
7	GOL	B	883	6/6	0.58	0.20	4.13	53,56,57,57	0
4	ACT	B	860	4/4	0.96	0.13	2.10	40,42,43,43	0
3	H4B	B	760	17/17	0.98	0.17	0.43	22,25,28,29	0
2	HEM	B	750	43/43	0.99	0.17	0.41	21,24,31,35	0
3	H4B	A	760	17/17	0.96	0.18	0.40	23,26,29,31	0
2	HEM	A	750	43/43	0.98	0.19	0.20	22,27,31,33	0
5	3XD	A	800[A]	28/28	0.91	0.18	0.13	21,25,27,27	14
5	3XD	B	800[A]	28/28	0.96	0.14	-0.32	22,24,25,26	14
5	3XD	B	800[B]	28/28	0.96	0.14	-0.32	22,26,31,33	14
5	3XD	A	800[B]	28/28	0.91	0.18	-0.49	23,26,36,38	14
6	ZN	A	900	1/1	0.99	0.07	-1.16	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.