



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:37 PM GMT

PDB ID : 4CTV
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(3-amino-2-(6-(2-(6-amino-4-methylpyridin-2-yl)ethyl) pyridin-2-yl)propyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-03-15
Resolution : 1.78 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

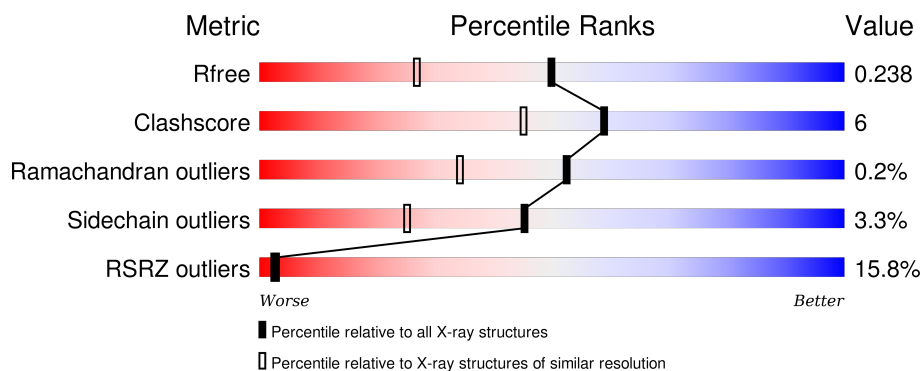
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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>81%</div> <div>15%</div> <div>..</div> </div>
1	B	422	<div> <div>9%</div> <div>85%</div> <div>12%</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
5	ACT	A	1720	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7192 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	4	0
			3365	2156	574	613	22			

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



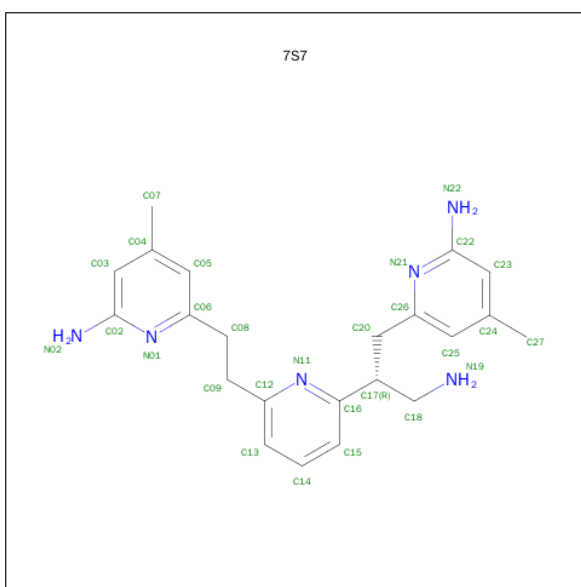
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	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 6-(3-AMINO-2-(6-(2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL)PYRIDIN-2-YL)PROPYL)-4-METHYLPYRIDIN-2-AMINE (three-letter code: 7S7) (formula: C₂₂H₂₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	22	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			28	22	6		

- 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	A	1	Total	Zn	0	0
			1	1		

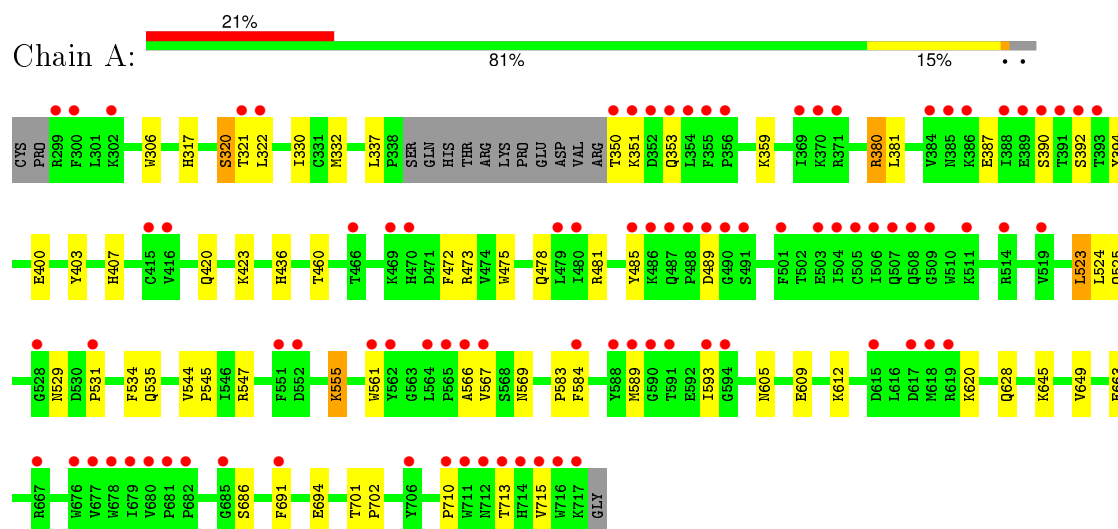
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	140	Total	O	0	0
			140	140		
7	B	176	Total	O	0	0
			176	176		

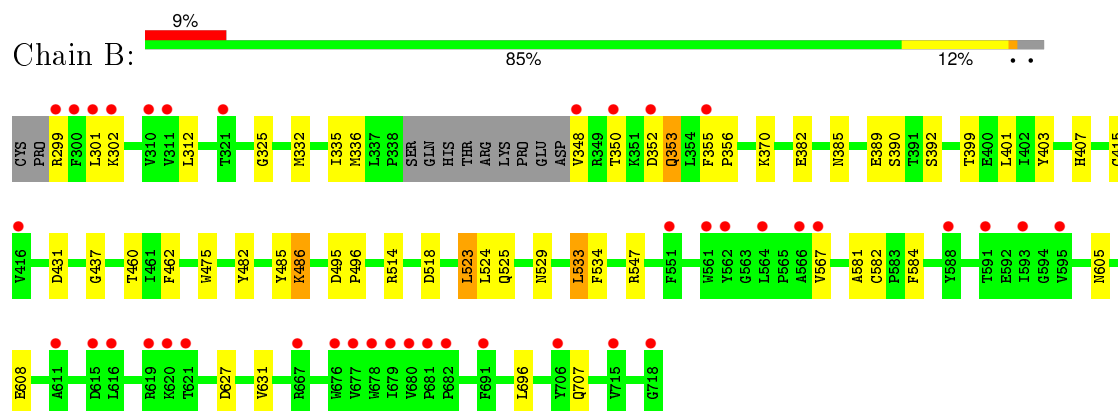
3 Residue-property plots

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	51.92Å 111.06Å 164.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.78 39.01 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.04-1.78) 99.4 (39.01-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.239 0.200 , 0.238	Depositor DCC
R_{free} test set	4551 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 91167 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: HEM, ZN, H4B, 7S7, 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	0.67	0/3428	0.76	0/4651
1	B	0.82	1/3471 (0.0%)	0.94	8/4706 (0.2%)
All	All	0.75	1/6899 (0.0%)	0.85	8/9357 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	GLY	N-CA	5.26	1.53	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	LEU	CB-CG-CD2	7.42	123.61	111.00
1	B	533	LEU	CB-CG-CD1	-6.92	99.23	111.00
1	B	401	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	B	399	THR	CA-CB-CG2	-5.85	104.21	112.40
1	B	401	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	431	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	523	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	486	LYS	N-CA-C	-5.01	97.47	111.00

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	42	0
1	B	3365	0	3284	35	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	28	0	28	6	0
4	B	28	0	28	6	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	140	0	0	3	0
7	B	176	0	0	4	0
All	All	7192	0	6673	79	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 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)
2:B:1719:HEM:HBD1	4:B:1721:7S7:C14	2.16	0.76
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.69	0.73
1:B:382:GLU:HG3	7:B:2020:HOH:O	1.89	0.72
1:A:420:GLN:OE1	1:A:423:LYS:HE2	1.94	0.68
1:B:608:GLU:HG3	7:B:2146:HOH:O	1.96	0.65
2:A:1717:HEM:HBD1	4:A:1719:7S7:H14	1.80	0.64
1:A:567:VAL:HG21	4:A:1719:7S7:C14	2.27	0.64
2:B:1719:HEM:HBA2	4:B:1721:7S7:H17	1.80	0.64
2:B:1719:HEM:O2D	7:B:2174:HOH:O	2.15	0.63
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.35	0.62
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.81	0.61
1:B:325:GLY:O	1:B:332:MET:HG3	2.01	0.60
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.38	0.58
1:B:355[B]:PHE:HB2	1:B:356:PRO:CD	2.33	0.58
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.06	0.56
1:B:605:ASN:ND2	7:B:2144:HOH:O	2.37	0.56
1:A:350:THR:N	1:A:353:GLN:NE2	2.53	0.55
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.54
1:A:686:SER:HA	1:A:691:PHE:CG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.91	0.53
1:A:525:GLN:HG3	1:A:529:ASN:O	2.09	0.53
1:B:370:LYS:N	1:B:370:LYS:HD3	2.24	0.53
1:B:524:LEU:HD12	1:B:534:PHE:CD2	2.46	0.51
1:B:355[A]:PHE:CE1	1:B:385:ASN:HB2	2.46	0.51
2:B:1719:HEM:HBD1	4:B:1721:7S7:C13	2.40	0.50
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.92	0.50
1:B:350:THR:O	1:B:353:GLN:HG2	2.12	0.50
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.94	0.50
1:B:567:VAL:HG21	4:B:1721:7S7:C14	2.42	0.49
1:A:460:THR:O	1:A:583:PRO:HD2	2.11	0.49
1:A:609:GLU:HG3	7:A:2108:HOH:O	2.12	0.49
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.48	0.49
1:A:420:GLN:OE1	1:A:423:LYS:CE	2.61	0.48
1:B:403:TYR:CE2	1:B:407:HIS:CE1	3.01	0.48
2:A:1717:HEM:HBD1	4:A:1719:7S7:C14	2.44	0.47
1:A:605:ASN:ND2	7:A:2105:HOH:O	2.41	0.47
1:B:460:THR:O	1:B:582:CYS:HA	2.15	0.47
1:A:472:PHE:HA	1:A:525:GLN:O	2.15	0.47
1:A:359:LYS:HE2	1:A:381:LEU:HD21	1.96	0.47
1:A:567:VAL:HG23	4:A:1719:7S7:H25	1.96	0.47
1:A:524:LEU:O	1:A:531:PRO:HA	2.15	0.46
1:B:302:LYS:HA	1:B:312:LEU:O	2.15	0.46
1:A:436:HIS:CD2	1:A:534:PHE:HE2	2.34	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.96	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.16	0.46
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.51	0.45
1:A:403:TYR:CE2	1:A:407:HIS:CE1	3.04	0.45
1:A:317:HIS:O	1:A:320:SER:HB3	2.16	0.45
1:B:567:VAL:HG23	4:B:1721:7S7:H25	1.99	0.45
1:A:321:THR:HG22	7:A:2005:HOH:O	2.16	0.45
1:A:332:MET:CE	1:B:301:LEU:HD22	2.47	0.45
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.44
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.70	0.44
1:B:523:LEU:HD13	1:B:533:LEU:HG	1.99	0.44
1:A:321:THR:HG23	1:A:322:LEU:HG	2.00	0.44
2:B:1719:HEM:HBD1	4:B:1721:7S7:H14	1.97	0.43
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.32	0.43
1:B:350:THR:OG1	1:B:353:GLN:NE2	2.51	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.53	0.43
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:TRP:CD1	1:A:593:ILE:HG12	2.53	0.42
1:A:584:PHE:CD1	2:A:1717:HEM:CAC	3.03	0.42
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.54	0.42
2:A:1717:HEM:HBA1	4:A:1719:7S7:H17	2.02	0.42
1:B:482:TYR:HA	1:B:518:ASP:O	2.20	0.42
1:B:567:VAL:N	1:B:584:PHE:O	2.53	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.41
1:A:337:LEU:HD21	4:A:1719:7S7:H03	2.02	0.41
1:B:355[B]:PHE:HB2	1:B:356:PRO:HD3	2.03	0.41
1:B:525:GLN:HG3	1:B:529:ASN:O	2.21	0.41
1:B:495:ASP:HA	1:B:496:PRO:HD3	1.87	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.41
1:A:478:GLN:HA	1:A:566:ALA:O	2.20	0.40
2:B:1719:HEM:HBA1	2:B:1719:HEM:HMA2	2.02	0.40
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.93	0.40
1:A:332:MET:HE3	1:B:301:LEU:HD22	2.04	0.40
1:B:415:CYS:HB2	2:B:1719:HEM:ND	2.37	0.40
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.95	0.40
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.36	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	407/422 (96%)	394 (97%)	12 (3%)	1 (0%)	52	34
1	B	411/422 (97%)	400 (97%)	10 (2%)	1 (0%)	52	34
All	All	818/844 (97%)	794 (97%)	22 (3%)	2 (0%)	52	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASP
1	A	489	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/377 (97%)	351 (96%)	15 (4%)	37	17
1	B	370/377 (98%)	361 (98%)	9 (2%)	57	38
All	All	736/754 (98%)	712 (97%)	24 (3%)	45	25

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	380	ARG
1	A	390	SER
1	A	485	TYR
1	A	523	LEU
1	A	535	GLN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	612	LYS
1	A	620	LYS
1	A	645	LYS
1	A	663	GLU
1	A	713	THR
1	A	715	VAL
1	B	348	VAL
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	392	SER
1	B	486	LYS
1	B	547	ARG

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Mol	Chain	Res	Type
1	B	627	ASP
1	B	707	GLN

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	353	GLN
1	A	436	HIS
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	454	ASN
1	B	507	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 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	1717	1	30,50,50	2.03	7 (23%)	24,82,82	2.45	9 (37%)
3	H4B	A	1718	-	13,18,18	2.03	2 (15%)	11,26,26	3.76	6 (54%)
4	7S7	A	1719	-	30,30,30	1.41	3 (10%)	37,41,41	2.45	12 (32%)
5	ACT	A	1720	-	1,3,3	1.99	0	0,3,3	0.00	-
2	HEM	B	1719	1	30,50,50	2.18	5 (16%)	24,82,82	2.59	9 (37%)
3	H4B	B	1720	-	13,18,18	1.74	2 (15%)	11,26,26	2.77	5 (45%)
4	7S7	B	1721	-	30,30,30	1.23	3 (10%)	37,41,41	2.21	13 (35%)
5	ACT	B	1722	-	1,3,3	1.12	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	1717	1	-	0/10/54/54	0/0/8/8
3	H4B	A	1718	-	-	0/8/17/17	0/2/2/2
4	7S7	A	1719	-	-	0/15/15/15	0/3/3/3
5	ACT	A	1720	-	-	0/0/0/0	0/0/0/0
2	HEM	B	1719	1	-	0/10/54/54	0/0/8/8
3	H4B	B	1720	-	-	0/8/17/17	0/2/2/2
4	7S7	B	1721	-	-	0/15/15/15	0/3/3/3
5	ACT	B	1722	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1719	HEM	C2C-C1C	-7.72	1.37	1.52
2	A	1717	HEM	C2C-C1C	-6.32	1.40	1.52
2	A	1717	HEM	C2D-C3D	-6.07	1.36	1.54
2	B	1719	HEM	C2D-C3D	-6.07	1.36	1.54
4	A	1719	7S7	C20-C17	-4.22	1.49	1.54
4	B	1721	7S7	C20-C17	-3.51	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1719	HEM	C2B-C1B	-2.64	1.43	1.51
2	A	1717	HEM	C3D-C4D	-2.41	1.48	1.51
2	B	1719	HEM	C3D-C4D	-2.15	1.48	1.51
2	A	1717	HEM	C2B-C1B	-2.12	1.44	1.51
2	A	1717	HEM	C3B-CAB	-2.10	1.47	1.51
4	B	1721	7S7	C25-C24	2.01	1.42	1.38
4	B	1721	7S7	C22-N21	2.26	1.39	1.35
4	A	1719	7S7	C23-C24	2.40	1.43	1.38
2	A	1717	HEM	FE-NB	2.41	2.10	1.97
2	A	1717	HEM	FE-NC	2.59	2.06	1.95
2	B	1719	HEM	FE-NC	2.60	2.06	1.95
3	B	1720	H4B	C8A-N1	2.97	1.40	1.34
3	B	1720	H4B	C7-N8	3.33	1.50	1.46
3	A	1718	H4B	C2-N2	3.37	1.40	1.34
4	A	1719	7S7	C16-N11	3.78	1.39	1.34
3	A	1718	H4B	C7-N8	5.72	1.53	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1717	HEM	CBA-CAA-C2A	-5.12	103.34	112.53
4	A	1719	7S7	C27-C24-C25	-4.56	114.02	120.95
2	B	1719	HEM	CBA-CAA-C2A	-4.08	105.22	112.53
4	A	1719	7S7	C05-C06-N01	-3.71	118.77	122.96
2	A	1717	HEM	C1D-CHD-C4C	-3.63	119.75	125.82
3	B	1720	H4B	N3-C2-N1	-3.51	119.78	125.53
4	B	1721	7S7	C15-C16-N11	-3.48	118.84	122.50
2	B	1719	HEM	CAA-C2A-C1A	-3.42	123.29	127.01
4	B	1721	7S7	C27-C24-C25	-2.90	116.55	120.95
4	B	1721	7S7	C04-C05-C06	-2.83	118.51	120.28
4	B	1721	7S7	C05-C06-N01	-2.82	119.78	122.96
4	A	1719	7S7	C13-C12-N11	-2.66	119.16	122.41
4	B	1721	7S7	C13-C12-N11	-2.58	119.25	122.41
3	A	1718	H4B	N3-C2-N1	-2.49	121.45	125.53
2	A	1717	HEM	CBD-CAD-C3D	-2.47	106.36	113.55
4	B	1721	7S7	C20-C17-C16	-2.40	106.48	111.10
4	A	1719	7S7	N22-C22-N21	-2.38	112.16	116.50
4	A	1719	7S7	C04-C05-C06	-2.24	118.88	120.28
4	A	1719	7S7	C15-C16-C17	-2.06	118.36	121.27
4	A	1719	7S7	C20-C26-C25	-2.05	115.64	120.88
3	A	1718	H4B	C4A-C8A-N1	-2.03	114.55	118.76
4	B	1721	7S7	C05-C04-C03	2.03	120.67	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1719	7S7	C16-N11-C12	2.11	121.34	118.72
2	A	1717	HEM	C2D-C3D-C4D	2.25	105.32	101.50
2	B	1719	HEM	C2D-C3D-C4D	2.48	105.70	101.50
2	B	1719	HEM	C3C-CAC-CBC	2.72	128.63	124.46
3	B	1720	H4B	C2-N1-C8A	2.95	121.17	114.54
3	B	1720	H4B	C4-N3-C2	3.05	120.17	115.94
3	A	1718	H4B	C7-C6-N5	3.07	116.82	110.45
4	B	1721	7S7	C27-C24-C23	3.08	125.63	120.95
2	A	1717	HEM	CMD-C2D-C3D	3.14	128.25	114.35
2	B	1719	HEM	CMD-C2D-C3D	3.15	128.29	114.35
4	B	1721	7S7	C09-C12-N11	3.19	120.40	115.69
4	B	1721	7S7	C22-N21-C26	3.19	120.50	118.23
4	A	1719	7S7	C17-C16-N11	3.35	120.81	116.05
4	B	1721	7S7	C17-C16-N11	3.37	120.83	116.05
2	A	1717	HEM	CMB-C2B-C3B	3.39	125.00	116.53
2	A	1717	HEM	CMC-C2C-C3C	3.70	125.76	116.53
4	B	1721	7S7	C16-N11-C12	3.79	123.42	118.72
3	A	1718	H4B	C2-N1-C8A	3.85	123.20	114.54
2	B	1719	HEM	CMC-C2C-C3C	4.06	126.68	116.53
2	B	1719	HEM	CAD-C3D-C4D	4.08	126.88	112.47
2	A	1717	HEM	CAD-C3D-C4D	4.13	127.04	112.47
4	A	1719	7S7	C09-C12-N11	4.22	121.92	115.69
3	B	1720	H4B	N2-C2-N1	4.34	124.38	117.20
4	A	1719	7S7	C27-C24-C23	4.71	128.10	120.95
2	B	1719	HEM	CAD-C3D-C2D	4.94	127.42	113.22
2	A	1717	HEM	CAD-C3D-C2D	5.01	127.63	113.22
2	B	1719	HEM	CMB-C2B-C3B	5.03	129.09	116.53
3	B	1720	H4B	C4-C4A-C8A	5.66	119.69	114.56
3	A	1718	H4B	C4A-C8A-N8	6.45	126.03	118.43
4	B	1721	7S7	C02-N01-C06	7.21	123.35	118.23
3	A	1718	H4B	C4-C4A-C8A	8.40	122.16	114.56
4	A	1719	7S7	C02-N01-C06	8.89	124.55	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1717	HEM	4	0
4	A	1719	7S7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1719	HEM	7	0
4	B	1721	7S7	6	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	408/422 (96%)	1.13	89 (21%) 1 1	25, 49, 85, 104	0
1	B	411/422 (97%)	0.61	40 (9%) 10 9	21, 38, 66, 88	0
All	All	819/844 (97%)	0.87	129 (15%) 3 2	21, 43, 80, 104	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	9.6
1	A	488	PRO	8.5
1	B	300	PHE	8.5
1	A	715	VAL	7.8
1	B	348	VAL	7.8
1	A	355	PHE	7.4
1	A	713	THR	5.7
1	A	300	PHE	5.4
1	A	352	ASP	5.1
1	A	717	LYS	4.8
1	B	619	ARG	4.7
1	A	507	GLN	4.6
1	B	616	LEU	4.6
1	B	350	THR	4.6
1	B	718	GLY	4.5
1	B	677	VAL	4.5
1	A	551	PHE	4.5
1	A	619	ARG	4.4
1	A	390	SER	4.4
1	A	486	LYS	4.4
1	A	506	ILE	4.4
1	A	491	SER	4.4
1	A	676	TRP	4.2
1	B	680	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	706	TYR	4.2
1	A	392	SER	4.1
1	A	351	LYS	4.1
1	A	469	LYS	4.0
1	B	355[A]	PHE	4.0
1	A	389	GLU	3.9
1	A	480	ILE	3.9
1	A	386	LYS	3.8
1	A	503	GLU	3.8
1	A	353	GLN	3.8
1	B	615	ASP	3.8
1	A	588	TYR	3.8
1	A	714	HIS	3.6
1	A	388	ILE	3.6
1	A	711	TRP	3.6
1	A	712	ASN	3.6
1	B	706	TYR	3.6
1	A	593	ILE	3.6
1	B	299	ARG	3.5
1	A	489	ASP	3.5
1	A	678	TRP	3.5
1	A	677	VAL	3.5
1	B	678	TRP	3.5
1	B	561	TRP	3.4
1	A	680	VAL	3.4
1	A	321	THR	3.4
1	A	391	THR	3.3
1	A	511	LYS	3.3
1	B	310	VAL	3.3
1	A	385	ASN	3.3
1	A	528	GLY	3.2
1	A	504	ILE	3.2
1	A	350	THR	3.2
1	A	561	TRP	3.2
1	B	676	TRP	3.2
1	A	508	GLN	3.2
1	A	490	GLY	3.2
1	B	591	THR	3.1
1	A	509	GLY	3.1
1	A	679	ILE	3.1
1	A	591	THR	3.1
1	B	321	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	620	LYS	3.0
1	B	562	TYR	3.0
1	B	679	ILE	3.0
1	B	691	PHE	3.0
1	A	617	ASP	2.9
1	A	487	GLN	2.9
1	B	301	LEU	2.9
1	A	567	VAL	2.9
1	B	595	VAL	2.9
1	A	479	LEU	2.8
1	B	588	TYR	2.8
1	A	384	VAL	2.8
1	B	302	LYS	2.8
1	A	505	CYS	2.8
1	A	691	PHE	2.7
1	B	567	VAL	2.7
1	A	710	PRO	2.7
1	B	682	PRO	2.7
1	A	393	THR	2.7
1	A	370	LYS	2.7
1	A	514	ARG	2.6
1	A	416	VAL	2.6
1	A	466	THR	2.6
1	B	352	ASP	2.6
1	A	299	ARG	2.6
1	B	667	ARG	2.6
1	B	311	VAL	2.5
1	B	611	ALA	2.5
1	A	501	PHE	2.5
1	A	302	LYS	2.5
1	A	552	ASP	2.5
1	A	564	LEU	2.5
1	A	681	PRO	2.5
1	A	682	PRO	2.5
1	A	562	TYR	2.5
1	A	565	PRO	2.5
1	A	685	GLY	2.5
1	A	519	VAL	2.5
1	A	322	LEU	2.5
1	A	470	HIS	2.4
1	B	564	LEU	2.4
1	A	584	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	354	LEU	2.4
1	B	593	ILE	2.3
1	B	416	VAL	2.3
1	A	594	GLY	2.2
1	B	566	ALA	2.2
1	A	356	PRO	2.2
1	A	667	ARG	2.2
1	A	531	PRO	2.2
1	A	615	ASP	2.2
1	B	681	PRO	2.2
1	A	415	CYS	2.1
1	A	566	ALA	2.1
1	B	715	VAL	2.1
1	A	371	ARG	2.1
1	A	590	GLY	2.0
1	B	551	PHE	2.0
1	A	589	MET	2.0
1	B	621	THR	2.0
1	A	369	ILE	2.0
1	A	485	TYR	2.0
1	A	618	MET	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
5	ACT	A	1720	4/4	0.91	0.22	5.44	65,69,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	7S7	B	1721	28/28	0.90	0.19	0.88	26,51,63,64	0
2	HEM	A	1717	43/43	0.97	0.18	0.68	28,32,39,45	0
2	HEM	B	1719	43/43	0.97	0.16	0.65	21,29,47,57	0
5	ACT	B	1722	4/4	0.94	0.12	0.40	57,62,63,63	0
3	H4B	B	1720	17/17	0.95	0.17	0.35	29,32,36,38	0
4	7S7	A	1719	28/28	0.87	0.17	0.02	16,43,50,52	0
3	H4B	A	1718	17/17	0.97	0.12	-0.38	25,28,31,33	0
6	ZN	A	1721	1/1	1.00	0.09	-0.78	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.