



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 PM GMT

PDB ID : 4V3V
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with N-(2-(1H-imidazol-1-yl)-4-pyrimidylmethyl)-3-(3- fluorophenyl)propan-1-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-10-20
Resolution : 2.06 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

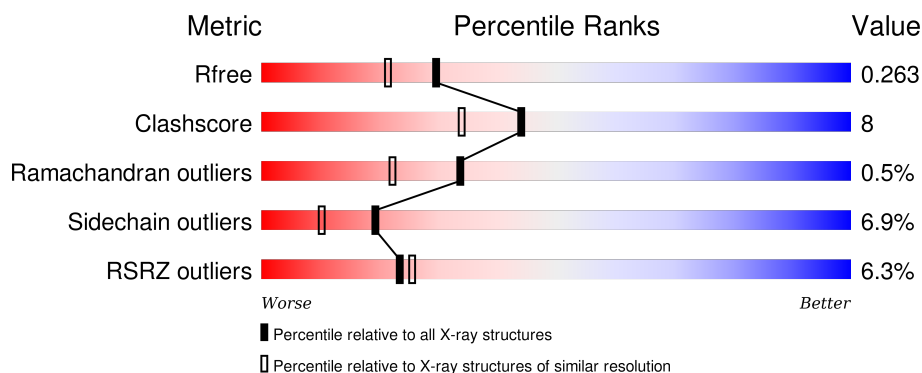
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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>9%</div> <div>73%</div> <div>20%</div> <div>• •</div> </div>
1	B	422	<div> <div>3%</div> <div>81%</div> <div>15%</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	860	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7025 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	0	1
			3314	2121	567	605	21			
1	B	411	Total	C	N	O	S	0	2	0
			3354	2146	574	612	22			

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



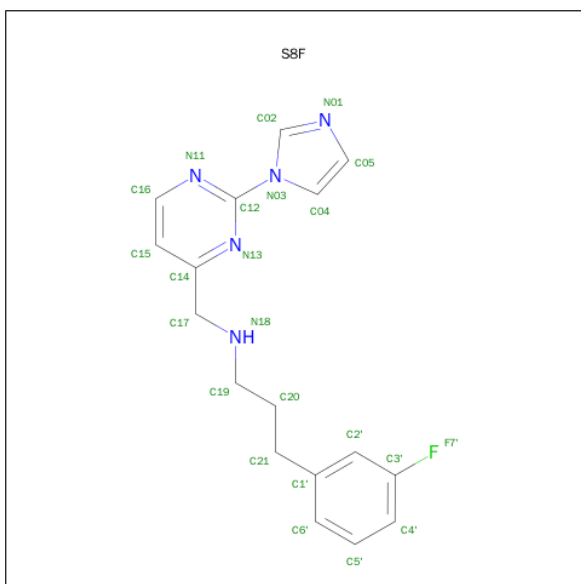
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 3-(3-FLUOROPHENYL)-N-{[2-(1H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL]METHYL}PROPAN-1-AMINE (three-letter code: S8F) (formula: C₁₇H₁₈FN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	17	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			23	17	1	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	A	1	Total	Zn	0	0
			1	1		

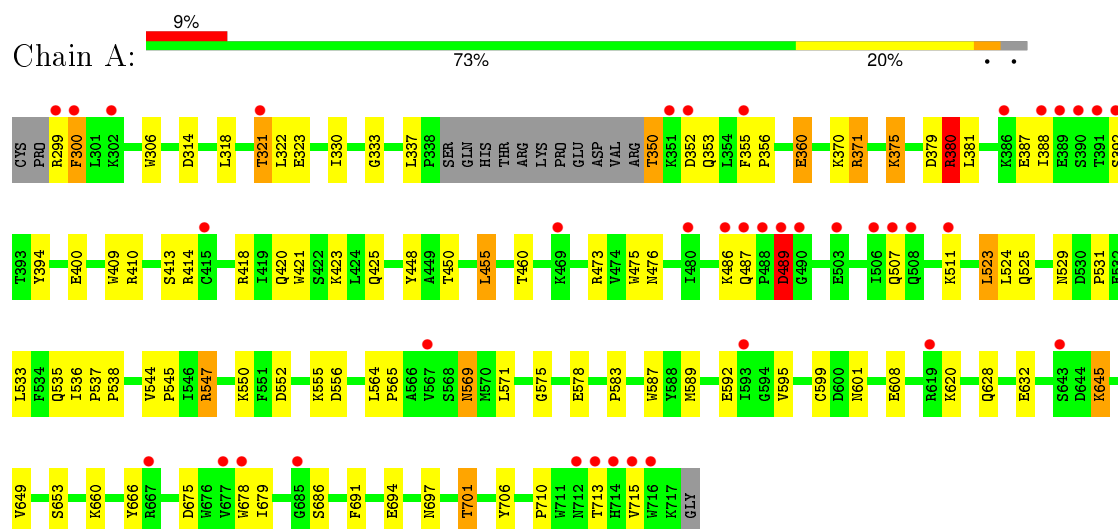
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	88	Total	O	0	0
			88	88		
7	B	94	Total	O	0	0
			94	94		

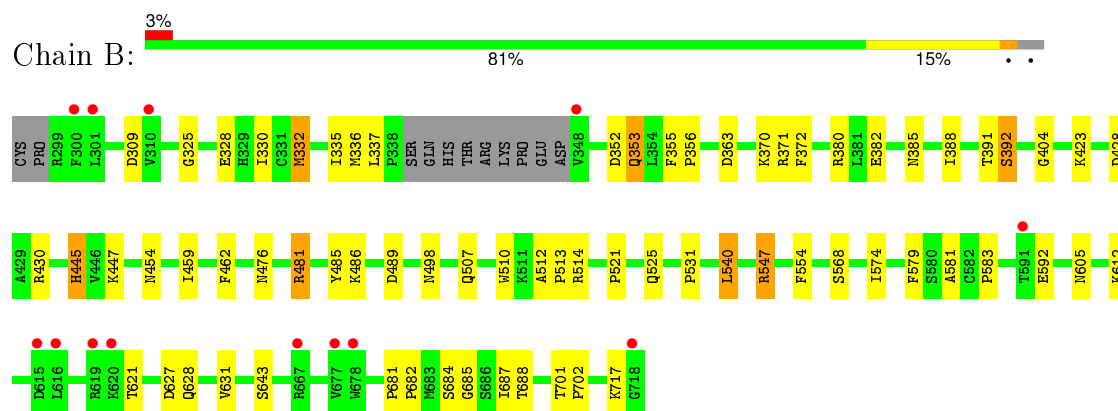
3 Residue-property plots

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	51.75Å 110.70Å 164.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.99 – 2.06 38.94 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.5 (91.99-2.06) 98.6 (38.94-2.06)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.207 , 0.263 0.207 , 0.263	Depositor DCC
R_{free} test set	2870 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 58108 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7025	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: HEM, ZN, H4B, S8F, 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	0.82	2/3407 (0.1%)	0.93	5/4623 (0.1%)
1	B	0.86	2/3453 (0.1%)	0.90	2/4681 (0.0%)
All	All	0.84	4/6860 (0.1%)	0.91	7/9304 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	GLU	CG-CD	8.20	1.64	1.51
1	B	592	GLU	CG-CD	5.84	1.60	1.51
1	A	360	GLU	CD-OE1	5.36	1.31	1.25
1	B	579	PHE	CG-CD1	5.13	1.46	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	592	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	380	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	380	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	410	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	547	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	489	ASP	CB-CG-OD1	5.13	122.92	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	3314	0	3221	68	0
1	B	3354	0	3270	37	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	23	0	18	3	0
4	B	23	0	18	2	0
5	A	4	0	3	2	0
5	B	4	0	3	1	0
6	A	1	0	0	0	0
7	A	88	0	0	1	0
7	B	94	0	0	2	0
All	All	7025	0	6623	108	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 8.

All (108) 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:750:HEM:O2A	4:B:800:S8F:H17A	1.67	0.95
1:A:350:THR:HB	1:A:353:GLN:NE2	1.89	0.86
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.39	0.85
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.59	0.84
1:A:371:ARG:HG2	1:A:371:ARG:NH1	1.95	0.81
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.05	0.73
1:A:375:LYS:HD3	1:A:379:ASP:OD2	1.89	0.72
1:A:371:ARG:CG	1:A:371:ARG:HH11	2.01	0.72
1:A:350:THR:HG22	1:A:353:GLN:H	1.54	0.72
1:B:447:LYS:HD2	1:B:540:LEU:HD11	1.71	0.71
2:A:750:HEM:HMB3	5:A:860:ACT:H3	1.73	0.71
1:A:350:THR:N	1:A:353:GLN:NE2	2.42	0.68
1:A:571:LEU:HD21	1:A:578:GLU:HB3	1.76	0.66
1:A:675:ASP:O	1:A:679:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:O	1:B:392:SER:N	2.28	0.65
1:A:350:THR:HB	1:A:353:GLN:CD	2.20	0.62
1:A:350:THR:HG22	1:A:353:GLN:HG3	1.80	0.62
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.00	0.62
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.81	0.60
1:A:524:LEU:O	1:A:531:PRO:HA	2.01	0.60
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.33	0.59
2:A:750:HEM:O2A	4:A:800:S8F:H17A	2.02	0.59
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.65	0.59
1:A:350:THR:CG2	1:A:353:GLN:HG3	2.33	0.58
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.39	0.58
1:B:391:THR:O	1:B:392:SER:CB	2.52	0.57
1:A:350:THR:N	1:A:353:GLN:HE21	2.03	0.57
1:A:525:GLN:HG3	1:A:529:ASN:O	2.06	0.56
1:B:325:GLY:O	1:B:332:MET:HG3	2.06	0.56
1:B:353:GLN:O	1:B:356:PRO:HG2	2.06	0.55
1:A:460:THR:O	1:A:583:PRO:HD2	2.06	0.55
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.40	0.54
1:A:450:THR:HA	1:A:455:LEU:HD22	1.90	0.53
2:A:750:HEM:HMC1	2:A:750:HEM:HBC2	1.90	0.53
1:B:554:PHE:HB3	7:B:2063:HOH:O	2.08	0.53
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.89	0.53
1:A:352:ASP:O	1:A:356:PRO:HD2	2.09	0.52
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.40	0.52
1:A:686:SER:HA	1:A:691:PHE:CG	2.45	0.52
1:A:678:TRP:HH2	4:A:800:S8F:H21A	1.75	0.52
1:A:455:LEU:HD13	1:A:564:LEU:HD12	1.93	0.51
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.48	0.49
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.94	0.49
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.94	0.48
1:A:299:ARG:O	1:A:318:LEU:HD11	2.14	0.48
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.48	0.48
1:A:601:ASN:HB2	7:A:2071:HOH:O	2.14	0.47
1:B:459:ILE:HG13	1:B:583:PRO:O	2.13	0.47
1:A:536:ILE:O	1:A:538:PRO:HD3	2.15	0.47
1:A:535:GLN:HE21	1:A:536:ILE:H	1.61	0.47
1:A:595:VAL:O	1:A:599:CYS:HB2	2.15	0.47
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.47
1:A:321:THR:HG21	1:A:701:THR:HG22	1.97	0.47
1:A:425:GLN:HG2	1:A:448:TYR:CE2	2.50	0.47
1:A:555:LYS:HG3	1:A:556:ASP:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:SER:OG	1:B:682:PRO:HB2	2.15	0.46
1:B:363:ASP:HB3	1:B:372:PHE:HE2	1.80	0.46
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.46
1:B:355:PHE:CE2	1:B:385:ASN:HB2	2.50	0.46
1:A:330:ILE:HG23	1:A:330:ILE:O	2.15	0.46
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.65	0.46
1:B:525:GLN:HB2	1:B:531:PRO:HB3	1.98	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.15	0.46
1:A:569:ASN:H	1:A:569:ASN:ND2	2.14	0.46
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.31	0.46
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.81	0.46
1:A:314:ASP:HB2	1:A:666:TYR:HE2	1.81	0.45
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.46	0.45
1:A:388:ILE:O	1:A:392:SER:HA	2.17	0.44
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.82	0.44
1:B:476:ASN:O	1:B:568:SER:OG	2.30	0.44
1:B:370:LYS:O	1:B:371:ARG:HD3	2.17	0.44
1:A:413:SER:CB	1:A:697:ASN:HD21	2.30	0.44
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.52	0.44
1:A:645:LYS:HA	1:A:645:LYS:HD3	1.45	0.44
1:A:536:ILE:O	1:A:537:PRO:C	2.55	0.44
1:B:353:GLN:HG2	1:B:353:GLN:H	1.38	0.44
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.97	0.44
1:B:462:PHE:HB2	1:B:581:ALA:HB3	2.00	0.43
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.43
1:B:547:ARG:HD3	1:B:547:ARG:H	1.83	0.43
1:A:565:PRO:HB2	4:A:800:S8F:H04	1.99	0.43
1:A:487:GLN:CB	1:A:489:ASP:OD1	2.66	0.43
1:A:350:THR:CB	1:A:353:GLN:NE2	2.74	0.42
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.54	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.42
1:B:681:PRO:HG2	1:B:688:THR:HG21	2.02	0.42
1:A:550:LYS:HD3	1:A:550:LYS:HA	1.89	0.42
2:B:750:HEM:HMB3	5:B:860:ACT:H2	2.02	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.02	0.41
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.85	0.41
1:A:300:PHE:N	1:A:300:PHE:CD1	2.89	0.41
1:A:487:GLN:HB2	1:A:489:ASP:OD1	2.20	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.41
1:B:684:SER:HB3	1:B:687:ILE:HD11	2.01	0.41
1:A:352:ASP:O	1:A:356:PRO:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:HG2	1:B:328:GLU:HB3	2.03	0.41
1:B:684:SER:O	1:B:685:GLY:C	2.59	0.41
1:B:512:ALA:HA	1:B:513:PRO:HD2	1.92	0.41
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.69	0.41
1:A:418:ARG:C	1:A:420:GLN:N	2.73	0.41
1:A:413:SER:CB	1:A:697:ASN:ND2	2.84	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.41
1:B:428:ASP:OD1	1:B:430:ARG:HB2	2.21	0.41
2:B:750:HEM:CHA	4:B:800:S8F:H02	2.51	0.41
1:B:605:ASN:ND2	7:B:2075:HOH:O	2.47	0.40
1:A:587:TRP:NE1	5:A:860:ACT:H1	2.37	0.40
2:B:750:HEM:CBC	2:B:750:HEM:CMC	2.99	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	404/422 (96%)	382 (95%)	19 (5%)	3 (1%)	26	14
1	B	409/422 (97%)	389 (95%)	19 (5%)	1 (0%)	52	43
All	All	813/844 (96%)	771 (95%)	38 (5%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLY
1	A	489	ASP
1	A	575	GLY
1	B	352	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	363/377 (96%)	333 (92%)	30 (8%)	14	6
1	B	368/377 (98%)	348 (95%)	20 (5%)	27	17
All	All	731/754 (97%)	681 (93%)	50 (7%)	19	11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	321	THR
1	A	322	LEU
1	A	337	LEU
1	A	350	THR
1	A	360	GLU
1	A	370	LYS
1	A	371	ARG
1	A	375	LYS
1	A	380	ARG
1	A	381	LEU
1	A	423	LYS
1	A	476	ASN
1	A	486	LYS
1	A	489	ASP
1	A	507	GLN
1	A	511	LYS
1	A	523	LEU
1	A	533	LEU
1	A	547	ARG
1	A	552	ASP
1	A	569	ASN
1	A	608	GLU
1	A	620	LYS
1	A	645	LYS
1	A	653	SER
1	A	660	LYS

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Mol	Chain	Res	Type
1	A	701	THR
1	A	713	THR
1	A	715	VAL
1	B	309	ASP
1	B	330	ILE
1	B	332	MET
1	B	337	LEU
1	B	353	GLN
1	B	382	GLU
1	B	392	SER
1	B	423	LYS
1	B	445	HIS
1	B	454	ASN
1	B	481	ARG
1	B	486	LYS
1	B	507	GLN
1	B	540	LEU
1	B	547	ARG
1	B	612	LYS
1	B	621	THR
1	B	627	ASP
1	B	643	SER
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	364	GLN
1	A	454	ASN
1	A	527	ASN
1	A	535	GLN
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	454	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	750	1,4	30,50,50	2.41	9 (30%)	24,82,82	2.79	12 (50%)
3	H4B	A	760	-	13,18,18	1.14	1 (7%)	11,26,26	3.12	7 (63%)
4	S8F	A	800	2	23,25,25	1.94	4 (17%)	30,32,32	2.80	13 (43%)
5	ACT	A	860	-	1,3,3	1.31	0	0,3,3	0.00	-
2	HEM	B	750	1,4	30,50,50	2.31	8 (26%)	24,82,82	3.27	12 (50%)
3	H4B	B	760	-	13,18,18	1.47	3 (23%)	11,26,26	3.06	4 (36%)
4	S8F	B	800	2	23,25,25	1.61	3 (13%)	30,32,32	2.70	14 (46%)
5	ACT	B	860	-	1,3,3	0.07	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	1,4	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	S8F	A	800	2	-	0/8/12/12	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1,4	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	S8F	B	800	2	-	0/8/12/12	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C2D-C3D	-7.55	1.31	1.54
2	B	750	HEM	C2D-C3D	-7.41	1.32	1.54
2	B	750	HEM	C2C-C1C	-6.29	1.40	1.52
2	A	750	HEM	C2C-C1C	-5.25	1.42	1.52
4	A	800	S8F	C04-N03	-4.83	1.32	1.39
2	A	750	HEM	C3D-C4D	-4.65	1.45	1.51
4	B	800	S8F	C04-N03	-4.48	1.32	1.39
2	B	750	HEM	C3D-C4D	-3.89	1.46	1.51
2	A	750	HEM	C3B-C4B	-3.10	1.49	1.51
2	B	750	HEM	C2B-C1B	-3.06	1.41	1.51
2	A	750	HEM	C2B-C1B	-2.78	1.42	1.51
2	B	750	HEM	C3B-CAB	-2.18	1.47	1.51
2	A	750	HEM	C3C-CAC	-2.18	1.47	1.51
3	B	760	H4B	C4A-N5	-2.16	1.33	1.38
2	B	750	HEM	C3B-C4B	-2.11	1.50	1.51
2	A	750	HEM	CHC-C1C	2.06	1.41	1.36
2	A	750	HEM	FE-NB	2.07	2.08	1.97
3	B	760	H4B	C7-N8	2.11	1.48	1.46
2	B	750	HEM	CHC-C1C	2.14	1.41	1.36
4	A	800	S8F	C4'-C3'	2.21	1.41	1.37
3	A	760	H4B	C2-N2	2.41	1.39	1.34
4	A	800	S8F	C12-N13	2.70	1.36	1.32
4	B	800	S8F	C4'-C3'	2.90	1.42	1.37
3	B	760	H4B	C2-N1	2.95	1.40	1.35
2	B	750	HEM	FE-NC	3.36	2.09	1.95
4	B	800	S8F	C12-N11	3.88	1.35	1.31
2	A	750	HEM	FE-NC	4.17	2.12	1.95
4	A	800	S8F	C12-N11	6.49	1.38	1.31

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-9.49	95.52	112.53
2	A	750	HEM	CBA-CAA-C2A	-6.57	100.75	112.53
4	A	800	S8F	N11-C12-N13	-6.56	118.21	126.44
4	B	800	S8F	N11-C12-N13	-5.78	119.19	126.44
4	A	800	S8F	C14-C17-N18	-5.33	102.50	113.26
3	A	760	H4B	N3-C2-N1	-4.39	118.34	125.53
2	B	750	HEM	C3C-CAC-CBC	-4.37	117.75	124.46
4	B	800	S8F	C15-C16-N11	-3.97	119.37	123.90
4	A	800	S8F	C15-C16-N11	-3.81	119.55	123.90
2	B	750	HEM	C1D-CHD-C4C	-3.63	119.75	125.82
2	A	750	HEM	C3B-CAB-CBB	-3.47	119.14	124.46
4	B	800	S8F	C05-C04-N03	-3.28	100.72	106.50
4	B	800	S8F	C02-N03-C12	-3.18	119.78	126.02
4	A	800	S8F	C05-C04-N03	-3.18	100.89	106.50
4	B	800	S8F	C4'-C3'-C2'	-3.09	119.36	123.35
4	A	800	S8F	C02-N03-C12	-2.82	120.49	126.02
4	A	800	S8F	C04-N03-C12	-2.79	122.55	125.61
2	A	750	HEM	C3C-CAC-CBC	-2.70	120.32	124.46
2	B	750	HEM	C3B-C4B-NB	-2.60	106.66	111.63
4	B	800	S8F	C21-C1'-C2'	-2.60	116.21	120.56
2	B	750	HEM	CAA-CBA-CGA	-2.59	107.99	112.75
4	A	800	S8F	C4'-C3'-C2'	-2.56	120.04	123.35
4	B	800	S8F	C04-N03-C12	-2.52	122.85	125.61
4	B	800	S8F	C19-C20-C21	-2.47	105.49	113.22
2	A	750	HEM	CBD-CAD-C3D	-2.44	106.44	113.55
4	B	800	S8F	C14-C17-N18	-2.43	108.36	113.26
4	B	800	S8F	C17-N18-C19	-2.37	104.74	113.48
4	A	800	S8F	C21-C1'-C2'	-2.33	116.65	120.56
4	A	800	S8F	C15-C14-N13	-2.28	119.62	122.41
2	A	750	HEM	C3B-C4B-NB	-2.27	107.29	111.63
2	B	750	HEM	CBD-CAD-C3D	-2.08	107.51	113.55
3	A	760	H4B	N2-C2-N1	2.03	120.56	117.20
2	A	750	HEM	C2C-C1C-CHC	2.07	126.83	123.68
2	A	750	HEM	CMD-C2D-C3D	2.10	123.65	114.35
4	A	800	S8F	F7'-C3'-C4'	2.11	122.05	118.52
3	A	760	H4B	N2-C2-N3	2.35	121.09	117.20
3	B	760	H4B	C2-N1-C8A	2.54	120.25	114.54
4	B	800	S8F	C6'-C1'-C2'	2.66	122.48	118.55
3	B	760	H4B	C4-N3-C2	2.91	119.98	115.94
2	B	750	HEM	C2D-C3D-C4D	2.94	106.48	101.50
2	B	750	HEM	CMD-C2D-C3D	3.03	127.74	114.35
2	A	750	HEM	C2D-C3D-C4D	3.16	106.85	101.50
3	A	760	H4B	C4A-C8A-N8	3.29	122.30	118.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CMB-C2B-C3B	3.40	125.02	116.53
3	A	760	H4B	C2-N1-C8A	3.47	122.35	114.54
2	A	750	HEM	CAD-C3D-C4D	3.56	125.02	112.47
3	B	760	H4B	C4A-C8A-N8	3.76	122.86	118.43
2	B	750	HEM	CAD-C3D-C4D	4.22	127.36	112.47
2	B	750	HEM	CMC-C2C-C3C	4.36	127.42	116.53
4	A	800	S8F	C04-N03-C02	4.38	116.69	108.53
2	B	750	HEM	CAD-C3D-C2D	4.50	126.16	113.22
4	B	800	S8F	C04-N03-C02	4.68	117.24	108.53
4	B	800	S8F	C12-N13-C14	4.73	121.44	115.26
2	B	750	HEM	CMB-C2B-C3B	5.07	129.17	116.53
3	A	760	H4B	C4-N3-C2	5.08	122.99	115.94
2	A	750	HEM	CAD-C3D-C2D	5.19	128.13	113.22
3	A	760	H4B	C4-C4A-C8A	5.25	119.31	114.56
4	A	800	S8F	N11-C12-N03	5.37	123.90	115.16
2	A	750	HEM	CMC-C2C-C3C	5.39	129.98	116.53
4	A	800	S8F	C12-N13-C14	5.67	122.67	115.26
4	B	800	S8F	N11-C12-N03	6.13	125.14	115.16
3	B	760	H4B	C4-C4A-C8A	8.14	121.93	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
4	A	800	S8F	3	0
5	A	860	ACT	2	0
2	B	750	HEM	6	0
4	B	800	S8F	2	0
5	B	860	ACT	1	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%)	0.41	39 (9%) 10 11	30, 50, 79, 106	0
1	B	411/422 (97%)	0.02	13 (3%) 51 56	29, 43, 69, 88	0
All	All	819/844 (97%)	0.22	52 (6%) 23 25	29, 46, 77, 106	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	6.6
1	A	715	VAL	6.3
1	A	299	ARG	5.4
1	A	713	THR	5.1
1	B	300	PHE	4.9
1	A	488	PRO	4.8
1	B	619	ARG	4.7
1	B	718	GLY	4.1
1	B	348	VAL	4.1
1	B	616	LEU	4.0
1	A	489	ASP	4.0
1	A	352	ASP	3.9
1	A	351	LYS	3.9
1	A	486	LYS	3.6
1	A	507	GLN	3.6
1	A	487	GLN	3.4
1	A	355	PHE	3.3
1	A	619	ARG	3.1
1	A	388	ILE	3.1
1	A	321	THR	3.0
1	B	310	VAL	2.9
1	A	390	SER	2.9
1	A	490	GLY	2.8
1	A	677	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	503	GLU	2.6
1	A	392	SER	2.6
1	B	620	LYS	2.6
1	A	300	PHE	2.5
1	A	714	HIS	2.5
1	A	678	TRP	2.5
1	A	508	GLN	2.5
1	A	415	CYS	2.5
1	B	615	ASP	2.5
1	A	391	THR	2.5
1	B	667	ARG	2.5
1	B	677	VAL	2.4
1	A	667	ARG	2.4
1	A	643	SER	2.3
1	A	480	ILE	2.3
1	A	511	LYS	2.3
1	A	506	ILE	2.3
1	A	389	GLU	2.3
1	A	712	ASN	2.3
1	A	593	ILE	2.2
1	A	386	LYS	2.2
1	B	301	LEU	2.2
1	B	591	THR	2.2
1	A	302	LYS	2.2
1	A	469	LYS	2.1
1	B	678	TRP	2.0
1	A	685	GLY	2.0
1	A	567	VAL	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
2	HEM	A	750	43/43	0.97	0.20	1.03	34,38,50,54	0
5	ACT	B	860	4/4	0.97	0.11	0.77	52,53,55,59	0
4	S8F	B	800	23/23	0.94	0.18	0.69	40,51,68,70	0
4	S8F	A	800	23/23	0.95	0.20	0.57	38,51,77,80	0
2	HEM	B	750	43/43	0.98	0.15	0.38	34,37,47,54	0
3	H4B	A	760	17/17	0.94	0.17	0.36	37,41,44,44	0
6	ZN	A	900	1/1	0.98	0.11	0.31	45,45,45,45	0
3	H4B	B	760	17/17	0.94	0.16	0.31	34,37,46,46	0
5	ACT	A	860	4/4	0.95	0.11	0.01	70,71,74,78	0

6.5 Other polymers

There are no such residues in this entry.