



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:27 PM GMT

PDB ID : 3B3O
Title : Structure of neuronal nos heme domain in complex with a inhibitor (+-)-n1-{
cis-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-n2-(4'-chlor
obenzyl)ethane-1,2-diamine
Authors : Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on : 2007-10-22
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

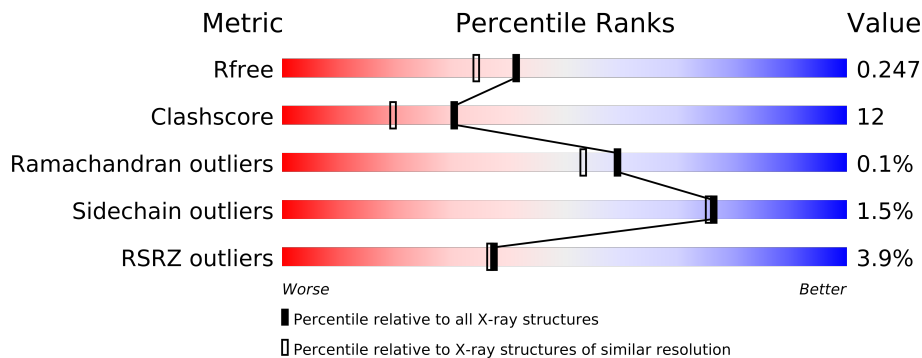
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.05 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	A	860	-	X
6	JI3	A	800	-	X
6	JI3	B	800	-	X

2 Entry composition i

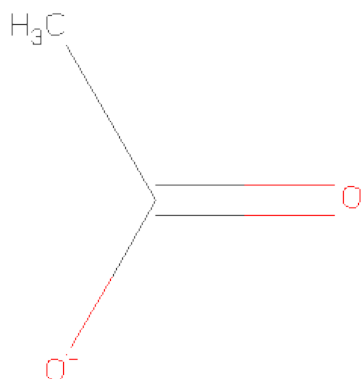
There are 7 unique types of molecules in this entry. The entry contains 7275 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3331	2132	571	607	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

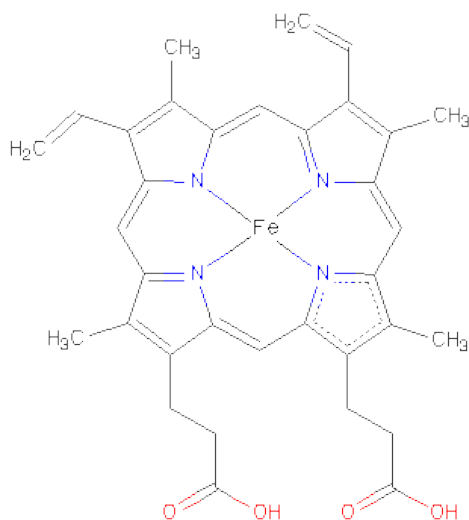


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

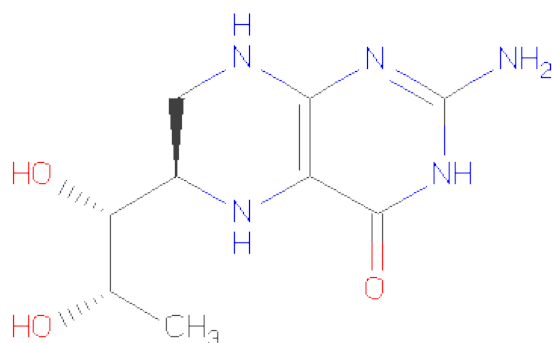
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



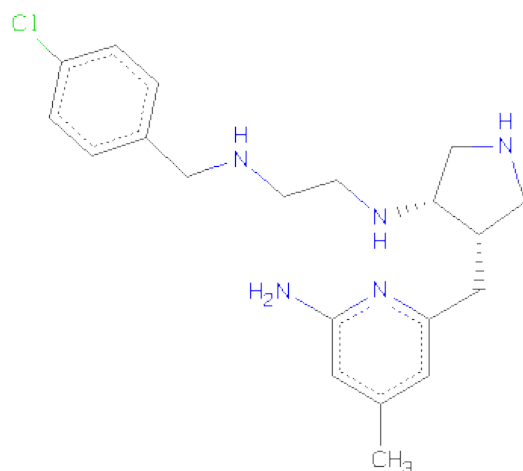
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 6 is N-{(3S,4S)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-(4-CHLOROBENZYL)ETHANE-1,2-DIAMINE (three-letter code: JI3) (formula: C₂₀H₂₈ClN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	0	0
			26	20	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	Cl	N	0	0
			26	20	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	246	Total	O	0	0
			246	246		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.21Å 111.53Å 164.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 2.05 49.77 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.77-2.05) 97.4 (49.77-2.04)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.253 0.209 , 0.247	Depositor DCC
R_{free} test set	3017 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 60532 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7275	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, ACT, H4B, JI3

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	0.44	0/3424	0.65	1/4645 (0.0%)
1	B	0.46	0/3438	0.65	2/4661 (0.0%)
All	All	0.45	0/6862	0.65	3/9306 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	MET	N-CA-C	-5.97	94.89	111.00
1	B	589	MET	N-CA-C	-5.15	97.09	111.00
1	B	326	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3331	0	3243	113	0
1	B	3345	0	3259	47	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	6	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	26	0	28	1	0
6	B	26	0	28	3	0
7	A	172	0	0	10	0
7	B	246	0	0	6	0
All	All	7275	0	6654	161	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.40	1.04
1:A:350:THR:HB	1:A:353:GLN:HG3	1.58	0.86
1:B:355:PHE:HZ	1:B:389:GLU:HG3	1.41	0.84
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.57	0.83
1:A:467:ASP:OD2	1:A:469:LYS:HB2	1.86	0.76
1:B:350:THR:HG22	1:B:352:ASP:H	1.52	0.72
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.04	0.72
1:B:355:PHE:CZ	1:B:389:GLU:HG3	2.26	0.70
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.58	0.69
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.74	0.69
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.09	0.68
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.07	0.68
1:A:620:LYS:HE3	1:A:622:SER:OG	1.94	0.67
1:A:488:PRO:C	1:A:490:GLY:H	1.98	0.66
1:A:350:THR:HG22	1:A:352:ASP:H	1.60	0.66
1:A:522:LEU:HB3	7:A:1019:HOH:O	1.97	0.65
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.23	0.64
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.79	0.64
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.34	0.62
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.63	0.62
1:A:489:ASP:C	1:A:491:SER:H	2.01	0.61
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.82	0.61
1:B:504:ILE:O	1:B:508:GLN:HG2	2.02	0.60
1:A:355:PHE:CZ	1:A:381:LEU:HD11	2.36	0.60
1:A:380:ARG:NH1	1:A:397:LYS:HG2	2.18	0.59
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:GLU:H	1:A:328:GLU:CD	2.08	0.57
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.86	0.57
1:A:569:ASN:H	1:A:569:ASN:HD22	1.53	0.57
1:B:393:THR:HG23	7:B:983:HOH:O	2.06	0.56
1:A:504:ILE:O	1:A:508:GLN:HG2	2.05	0.56
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.71	0.55
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.88	0.55
1:B:514:ARG:HD2	7:B:1069:HOH:O	2.07	0.55
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.88	0.55
1:B:391:THR:O	1:B:392:SER:HB2	2.07	0.55
1:B:513:PRO:HG2	1:B:518:ASP:OD2	2.08	0.54
1:B:350:THR:O	1:B:353:GLN:HG2	2.06	0.54
1:A:488:PRO:C	1:A:490:GLY:N	2.62	0.53
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.44	0.53
1:A:659:ILE:O	1:A:663:GLU:HG3	2.09	0.53
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.39	0.53
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.74	0.53
1:B:304:LYS:NZ	7:B:1085:HOH:O	2.42	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.91	0.52
1:A:545:PRO:HD2	1:A:644:ASP:OD2	2.08	0.52
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.73	0.52
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.25	0.52
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.29	0.52
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.09	0.52
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.25	0.52
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.91	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.25	0.52
1:A:569:ASN:N	1:A:569:ASN:HD22	2.08	0.52
1:A:701:THR:HG23	7:A:1039:HOH:O	2.09	0.52
1:A:715:VAL:HG23	1:A:715:VAL:O	2.09	0.52
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.46	0.51
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.37	0.51
1:A:608:GLU:HB2	7:A:1060:HOH:O	2.09	0.51
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.92	0.51
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.26	0.51
1:A:547:ARG:NH1	1:A:643:SER:HB2	2.26	0.50
1:A:374:SER:O	1:A:378:MET:HG2	2.12	0.50
1:A:675:ASP:O	1:A:679:ILE:HG12	2.11	0.50
1:A:488:PRO:O	1:A:490:GLY:N	2.44	0.50
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.42	0.50
1:B:525:GLN:HE21	1:B:528:GLY:HA2	1.75	0.50
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.92	0.49
1:B:631:VAL:HB	7:B:961:HOH:O	2.12	0.49
1:A:554:PHE:HB3	7:A:1057:HOH:O	2.12	0.49
1:B:355:PHE:N	1:B:356:PRO:HD2	2.28	0.49
1:A:524:LEU:O	1:A:531:PRO:HA	2.13	0.49
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.43	0.49
1:A:508:GLN:OE1	1:A:716:TRP:CH2	2.66	0.49
1:B:364:GLN:NE2	7:B:1054:HOH:O	2.46	0.49
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.42	0.48
1:A:353:GLN:O	1:A:356:PRO:HG2	2.14	0.48
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.96	0.48
1:A:350:THR:HG22	1:A:351:LYS:N	2.29	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.48
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.95	0.47
1:A:351:LYS:HE2	1:A:392:SER:HA	1.96	0.47
1:A:567:VAL:HG23	6:A:800:JI3:H3	1.96	0.47
1:B:614:MET:CE	1:B:632:GLU:HG3	2.45	0.47
1:A:551:PHE:CD2	1:A:551:PHE:N	2.81	0.47
1:A:498:ASN:HA	7:A:1028:HOH:O	2.15	0.47
1:B:362:LEU:HD12	1:B:381:LEU:HD23	1.96	0.47
1:A:489:ASP:C	1:A:491:SER:N	2.69	0.47
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.44	0.46
4:B:750:HEM:O2A	6:B:800:JI3:H102	2.16	0.46
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.97	0.46
1:B:302:LYS:HA	1:B:312:LEU:O	2.15	0.46
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.04	0.46
1:B:328:GLU:H	1:B:328:GLU:CD	2.19	0.46
1:A:678:TRP:HA	5:A:760:H4B:N1	2.31	0.45
1:A:571:LEU:C	1:A:571:LEU:HD23	2.36	0.45
1:A:387:GLU:OE1	1:A:394:TYR:HA	2.16	0.45
1:A:489:ASP:O	1:A:489:ASP:OD2	2.34	0.45
1:A:314:ASP:HB2	1:A:666:TYR:HE2	1.82	0.45
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.52	0.45
1:A:657:SER:HB2	7:A:1068:HOH:O	2.17	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.52	0.45
1:A:480:ILE:HA	7:A:974:HOH:O	2.16	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.98	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.45
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.47	0.45
1:A:614:MET:CE	1:A:632:GLU:HG3	2.46	0.44
1:A:361:PHE:O	1:A:364:GLN:HG2	2.17	0.44
1:A:494:GLY:O	1:A:496:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:608:GLU:O	1:A:611:ALA:HB3	2.18	0.44
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.44
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.48	0.44
1:A:610:VAL:O	1:A:614:MET:HG3	2.16	0.44
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.32	0.44
1:B:388:ILE:O	1:B:392:SER:N	2.43	0.44
1:A:507:GLN:HG2	1:A:507:GLN:O	2.16	0.44
1:B:557:LEU:HD23	1:B:609:GLU:OE1	2.18	0.43
1:A:569:ASN:H	1:A:569:ASN:ND2	2.15	0.43
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.33	0.43
1:B:409:TRP:CH2	4:B:750:HEM:HMC3	2.53	0.43
1:A:523:LEU:HG	1:A:533:LEU:HD21	2.00	0.43
1:A:354:LEU:HD11	1:A:394:TYR:HE2	1.84	0.43
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.32	0.43
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.53	0.43
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.00	0.42
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.54	0.42
1:B:355:PHE:HZ	1:B:389:GLU:CG	2.22	0.42
1:B:409:TRP:CZ3	4:B:750:HEM:HMC3	2.54	0.42
1:A:553:TRP:CZ3	1:A:613:LYS:HB3	2.54	0.42
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.48	0.42
1:B:567:VAL:HG23	6:B:800:JI3:H3	2.01	0.42
1:B:328:GLU:OE1	1:B:328:GLU:N	2.51	0.42
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.82	0.42
1:B:362:LEU:CD1	1:B:381:LEU:HD23	2.49	0.42
1:A:706:TYR:HD1	7:A:956:HOH:O	2.02	0.42
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.13	0.42
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.89	0.42
1:B:351:LYS:HE2	1:B:392:SER:HA	2.01	0.42
1:B:652:HIS:ND1	7:B:1103:HOH:O	2.37	0.42
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.19	0.42
1:A:436:HIS:ND1	7:A:1052:HOH:O	2.36	0.42
1:A:664:ASN:HA	1:A:667:ARG:NH1	2.34	0.42
1:B:608:GLU:O	1:B:612:LYS:HG3	2.20	0.42
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.02	0.42
1:A:393:THR:OG1	1:A:394:TYR:N	2.53	0.41
1:B:684:SER:HB3	1:B:687:ILE:HG12	2.01	0.41
1:A:355:PHE:HZ	1:A:381:LEU:HD11	1.79	0.41
4:B:750:HEM:C1C	6:B:800:JI3:H83	2.56	0.41
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
1:A:350:THR:N	1:A:353:GLN:OE1	2.50	0.41
4:B:750:HEM:HMC1	4:B:750:HEM:HBC2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.90	0.41
1:A:484:GLY:O	1:A:499:VAL:HA	2.21	0.41
1:B:335:ILE:HB	1:B:338:PRO:HG3	2.02	0.40
1:A:475:TRP:CZ3	1:A:711:TRP:HB3	2.56	0.40
1:A:351:LYS:HE2	1:A:392:SER:CA	2.52	0.40
1:A:553:TRP:O	1:A:556:ASP:HB2	2.21	0.40
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	2.03	0.40
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.86	0.40
1:A:524:LEU:CD2	7:A:1019:HOH:O	2.68	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	405/422 (96%)	376 (93%)	28 (7%)	1 (0%)	56	47
1	B	407/422 (96%)	397 (98%)	10 (2%)	0	100	100
All	All	812/844 (96%)	773 (95%)	38 (5%)	1 (0%)	59	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/377 (97%)	358 (98%)	7 (2%)	69	66
1	B	366/377 (97%)	362 (99%)	4 (1%)	84	83
All	All	731/754 (97%)	720 (98%)	11 (2%)	76	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	GLU
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	B	328	GLU
1	B	445	HIS
1	B	454	ASN
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN

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Mol	Chain	Res	Type
1	B	697	ASN
1	B	712	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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$
4	HEM	A	750	1	49,50,50	2.29	18 (36%)	46,82,82	1.43	7 (15%)
5	H4B	A	760	-	18,18,18	1.63	3 (16%)	24,26,26	2.44	7 (29%)
6	JI3	A	800	-	28,28,28	2.31	15 (53%)	37,37,37	1.76	6 (16%)
2	ACT	A	860	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
4	HEM	B	750	1	49,50,50	2.07	14 (28%)	46,82,82	1.81	11 (23%)
5	H4B	B	760	-	18,18,18	1.78	5 (27%)	24,26,26	2.50	7 (29%)
6	JI3	B	800	-	28,28,28	2.34	12 (42%)	37,37,37	1.99	5 (13%)
2	ACT	B	860	-	1,3,3	3.98	1 (100%)	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
4	HEM	A	750	1	-	0/14/114/114	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/0/2/2
6	JI3	A	800	-	-	0/12/22/22	0/3/3/3
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/14/114/114	0/0/8/8
5	H4B	B	760	-	-	0/8/17/17	0/0/2/2
6	JI3	B	800	-	-	0/12/22/22	0/3/3/3
2	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	HEM	C2B-C1B	6.90	1.46	1.44
4	B	750	HEM	C2D-C1D	5.75	1.46	1.44
4	A	750	HEM	C3D-C4D	-5.42	1.43	1.44
4	B	750	HEM	C3C-C2C	-5.15	1.34	1.43
4	B	750	HEM	C3B-C2B	-4.62	1.35	1.43
5	B	760	H4B	C6-N5	4.33	1.55	1.46
5	A	760	H4B	C6-N5	4.27	1.55	1.46
6	B	800	JI3	C7-C4'	4.18	1.60	1.53
4	B	750	HEM	C3D-C2D	-4.17	1.36	1.43
6	B	800	JI3	C2'-C3'	4.16	1.59	1.53
6	B	800	JI3	C5-C4	4.14	1.46	1.38
6	B	800	JI3	C3-C4	4.10	1.46	1.38
4	A	750	HEM	C3D-C2D	-4.07	1.36	1.43
4	A	750	HEM	CHA-C4D	4.06	1.41	1.35
4	A	750	HEM	C4A-C3A	4.03	1.45	1.40
4	A	750	HEM	C3B-C2B	-4.02	1.36	1.43
2	B	860	ACT	CH3-C	3.98	1.54	1.48
6	A	800	JI3	C3-C4	3.85	1.46	1.38
4	B	750	HEM	C2B-C1B	3.80	1.45	1.44
6	A	800	JI3	C2'-C3'	3.70	1.58	1.53
6	A	800	JI3	C5-C4	3.67	1.45	1.38
5	B	760	H4B	C4-N3	3.62	1.43	1.37
4	B	750	HEM	C3B-C4B	3.50	1.48	1.44
5	A	760	H4B	C4-N3	3.44	1.43	1.37
4	A	750	HEM	C2D-C1D	-3.42	1.43	1.44
6	A	800	JI3	C5-C6	3.41	1.46	1.40
6	A	800	JI3	C3-C2	3.36	1.45	1.38
4	A	750	HEM	CHD-C4C	3.35	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	JI3	C5-C6	3.31	1.46	1.40
6	B	800	JI3	C3-C2	3.31	1.45	1.38
6	A	800	JI3	C7-C4'	3.27	1.58	1.53
4	A	750	HEM	FE-NA	3.27	2.06	1.92
4	B	750	HEM	CHB-C1B	3.23	1.40	1.35
6	A	800	JI3	C22-C23	3.14	1.44	1.38
6	B	800	JI3	C24-C23	3.11	1.44	1.38
4	B	750	HEM	CHA-C4D	3.11	1.40	1.35
4	B	750	HEM	CMD-C2D	3.10	1.57	1.47
4	B	750	HEM	CHD-C4C	3.00	1.41	1.36
6	B	800	JI3	C2-N1	2.90	1.40	1.34
4	A	750	HEM	C3B-C4B	2.88	1.47	1.44
6	A	800	JI3	C24-C23	2.87	1.43	1.38
6	B	800	JI3	C22-C23	2.81	1.43	1.38
4	A	750	HEM	C3C-C2C	-2.80	1.38	1.43
5	A	760	H4B	C4A-N5	2.76	1.47	1.38
5	B	760	H4B	C4A-N5	2.63	1.47	1.38
6	A	800	JI3	C6-N1	2.60	1.40	1.35
4	A	750	HEM	CMB-C2B	2.58	1.55	1.47
4	A	750	HEM	CMD-C2D	2.49	1.55	1.47
6	B	800	JI3	C6-N1	2.49	1.40	1.35
4	B	750	HEM	CMB-C2B	2.49	1.55	1.47
4	A	750	HEM	C1A-NA	2.48	1.41	1.36
6	A	800	JI3	C2-N1	2.44	1.39	1.34
4	B	750	HEM	CMC-C2C	2.42	1.54	1.47
6	A	800	JI3	C22-C21	2.41	1.43	1.38
4	B	750	HEM	C4A-C3A	2.37	1.43	1.40
4	A	750	HEM	CHC-C1C	2.37	1.40	1.36
2	A	860	ACT	CH3-C	2.30	1.52	1.48
6	A	800	JI3	C25-C24	2.30	1.43	1.38
4	A	750	HEM	CMC-C2C	2.27	1.54	1.47
6	B	800	JI3	C22-C21	2.26	1.43	1.38
6	B	800	JI3	C25-C24	2.26	1.43	1.38
6	A	800	JI3	C4'-C3'	2.20	1.56	1.53
4	A	750	HEM	FE-NB	2.18	2.05	1.97
5	B	760	H4B	C8A-N1	2.14	1.38	1.34
4	B	750	HEM	FE-NA	2.13	2.01	1.92
4	A	750	HEM	C1D-ND	2.06	1.42	1.37
6	A	800	JI3	C23-CL	2.06	1.79	1.74
5	B	760	H4B	C7-C6	2.05	1.54	1.52
6	A	800	JI3	C21-C26	2.04	1.43	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	760	H4B	C4-C4A-C8A	8.84	122.75	114.56
6	B	800	JI3	C6-N1-C2	8.59	124.26	118.23
5	A	760	H4B	C4-C4A-C8A	8.31	122.26	114.56
6	A	800	JI3	C6-N1-C2	7.65	123.61	118.23
4	B	750	HEM	C3B-C4B-NB	-4.97	110.44	114.00
4	B	750	HEM	C3A-C4A-NA	4.50	112.81	109.41
6	B	800	JI3	C4-C3-C2	-4.47	117.31	120.29
4	B	750	HEM	CBA-CAA-C2A	-4.16	105.36	112.69
4	A	750	HEM	CBA-CAA-C2A	-3.94	105.74	112.69
4	B	750	HEM	C4A-C3A-C2A	-3.87	104.31	107.00
5	A	760	H4B	C2-N1-C8A	3.68	122.84	117.61
4	A	750	HEM	CBD-CAD-C3D	-3.58	106.57	114.37
5	A	760	H4B	C4A-N5-C6	-3.50	111.62	121.16
4	B	750	HEM	C4A-CHB-C1B	-3.48	122.90	127.47
5	B	760	H4B	C4A-N5-C6	-3.42	111.84	121.16
6	A	800	JI3	C4-C3-C2	-3.40	118.03	120.29
5	B	760	H4B	C2-N1-C8A	3.20	122.16	117.61
5	A	760	H4B	C4-N3-C2	3.15	125.02	119.51
4	A	750	HEM	C3B-C4B-NB	-3.14	111.75	114.00
5	B	760	H4B	C4-N3-C2	3.11	124.95	119.51
6	B	800	JI3	C9-N8-C3'	3.09	118.36	113.21
4	A	750	HEM	CHC-C4B-NB	-2.92	122.15	124.58
6	A	800	JI3	C9-N8-C3'	2.69	117.69	113.21
5	A	760	H4B	N3-C2-N1	-2.65	118.07	121.78
5	A	760	H4B	C4A-C8A-N8	2.65	122.86	119.23
6	A	800	JI3	C3-C2-N1	-2.62	120.08	122.99
5	B	760	H4B	N3-C2-N1	-2.59	118.16	121.78
6	B	800	JI3	C3-C4-C5	2.54	121.51	118.10
5	B	760	H4B	C4A-C8A-N8	2.54	122.72	119.23
6	B	800	JI3	C3-C2-N1	-2.50	120.20	122.99
4	A	750	HEM	C1A-CHA-C4D	-2.50	124.19	127.47
4	B	750	HEM	C1A-CHA-C4D	-2.47	124.22	127.47
4	B	750	HEM	C4C-NC-C1C	-2.44	103.00	105.53
4	B	750	HEM	C4A-NA-C1A	-2.32	103.71	106.76
4	B	750	HEM	CBD-CAD-C3D	-2.28	109.39	114.37
6	A	800	JI3	C3-C4-C5	2.27	121.14	118.10
4	A	750	HEM	C2D-C1D-ND	-2.17	110.37	112.93
4	B	750	HEM	C1A-C2A-C3A	2.16	109.15	106.92
4	A	750	HEM	C4A-C3A-C2A	2.15	108.49	107.00
6	A	800	JI3	C5'-C4'-C3'	-2.14	99.47	103.31
4	B	750	HEM	CMA-C3A-C2A	2.12	128.94	124.94
5	B	760	H4B	N8-C8A-N1	2.07	118.86	115.82
5	A	760	H4B	N8-C8A-N1	2.01	118.77	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.52	27 (6%) 18 16	22, 46, 76, 94	0
1	B	411/422 (97%)	0.09	5 (1%) 75 77	22, 36, 63, 79	0
All	All	820/844 (97%)	0.31	32 (3%) 37 37	22, 40, 73, 94	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	6.0
1	A	355	PHE	5.2
1	B	348	VAL	4.2
1	A	716	TRP	4.2
1	A	370	LYS	3.7
1	A	351	LYS	3.5
1	A	373	GLY	3.4
1	A	381	LEU	3.4
1	B	300	PHE	3.0
1	B	321	THR	2.9
1	A	551	PHE	2.7
1	A	393	THR	2.7
1	A	553	TRP	2.7
1	A	388	ILE	2.7
1	A	391	THR	2.6
1	B	355	PHE	2.5
1	A	493	LEU	2.5
1	A	349	ARG	2.4
1	A	715	VAL	2.4
1	A	470	HIS	2.4
1	B	389	GLU	2.4
1	A	378	MET	2.2
1	A	321	THR	2.2
1	A	352	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	2.2
1	A	322	LEU	2.1
1	A	601	ASN	2.1
1	A	382	GLU	2.1
1	A	375	LYS	2.1
1	A	517	PHE	2.0
1	A	354	LEU	2.0
1	A	554	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ACT	A	860	4/4	0.27	19.51	52,52,53,54	0
6	J13	B	800	26/26	0.19	2.82	23,32,68,75	0
6	J13	A	800	26/26	0.18	2.16	23,33,65,71	0
5	H4B	B	760	17/17	0.14	1.25	22,26,30,30	0
2	ACT	B	860	4/4	0.14	1.19	37,39,40,41	0
3	ZN	A	900	1/1	0.11	0.61	30,30,30,30	0
4	HEM	A	750	43/43	0.11	0.27	20,26,33,41	0
4	HEM	B	750	43/43	0.12	-0.22	21,24,34,40	0
5	H4B	A	760	17/17	0.12	-0.30	28,31,32,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.