W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:42 PM GMT

PDB ID	:	4FVX
Title	:	Structure of rat nNOS heme domain in complex with N(omega)-ethoxy-L-arginine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2012-06-29
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) 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 2.00 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.
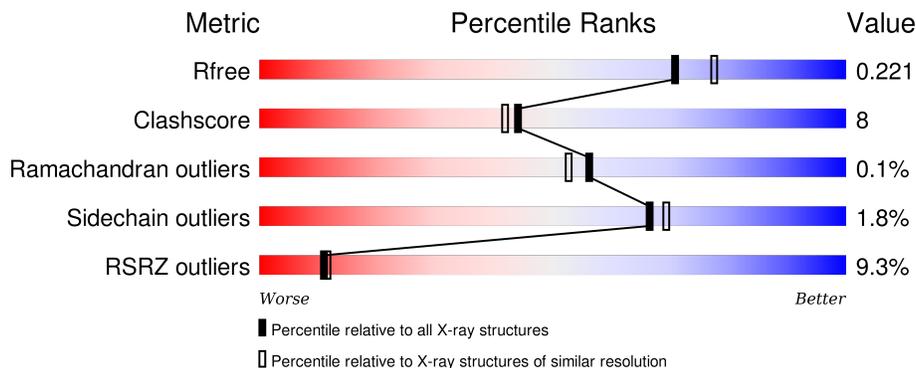
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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
5	TFA	B	804	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7211 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	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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

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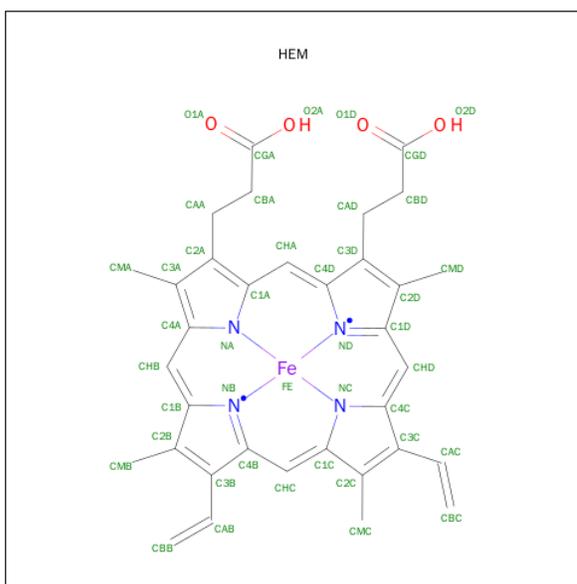
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
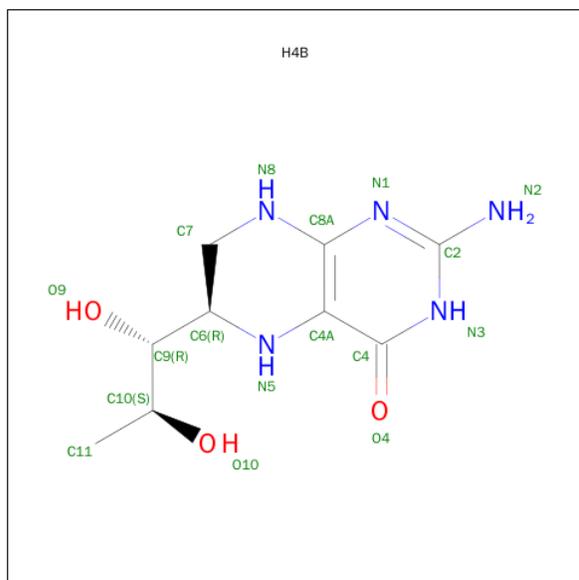
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is N 5 -(N-ETHOXYCARBAMIMIDOYL)-L-ORNITHINE (three-letter code: 2KJ) (formula: $C_8H_{18}N_4O_3$).
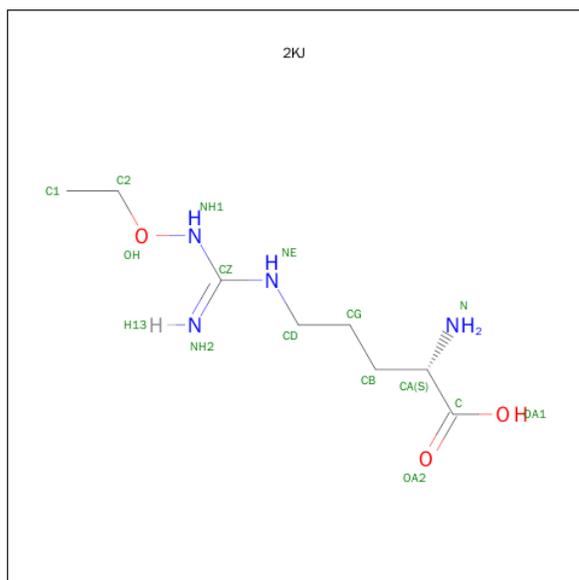
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 15	C 8	N 4	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 15	C 8	N 4	O 3	0	0

- Molecule 5 is TRIFLUOROACETIC ACID (three-letter code: TFA) (formula: $C_2HF_3O_2$).
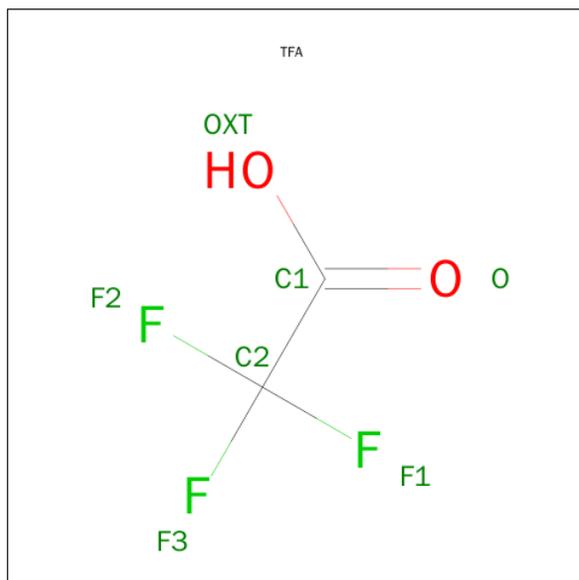
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 7	C 2	F 3	O 2	0	0
5	B	1	Total 7	C 2	F 3	O 2	0	0

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total 161	O 161	0	0
7	B	227	Total 227	O 227	0	0

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
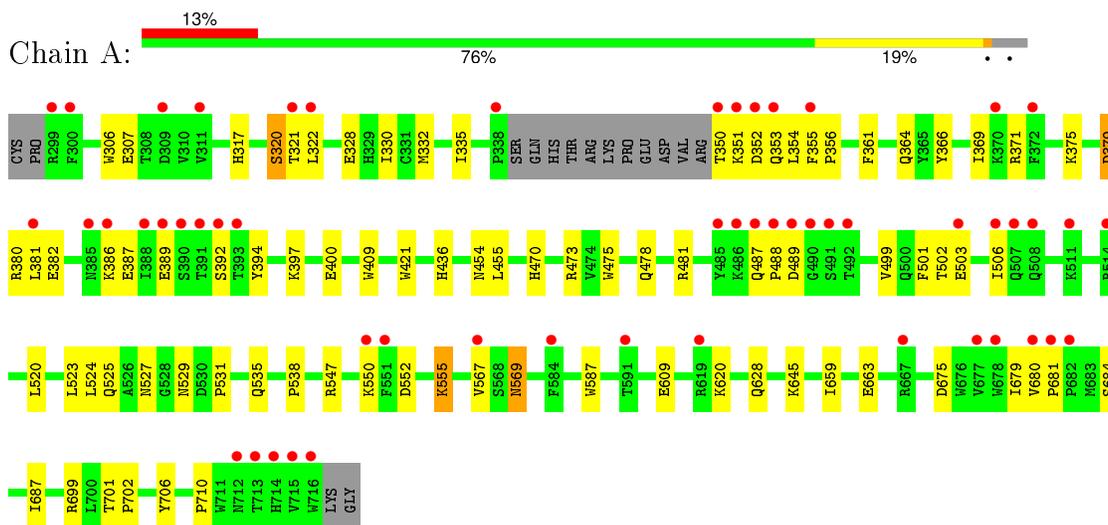
• Molecule 1: Nitric oxide synthase, brain
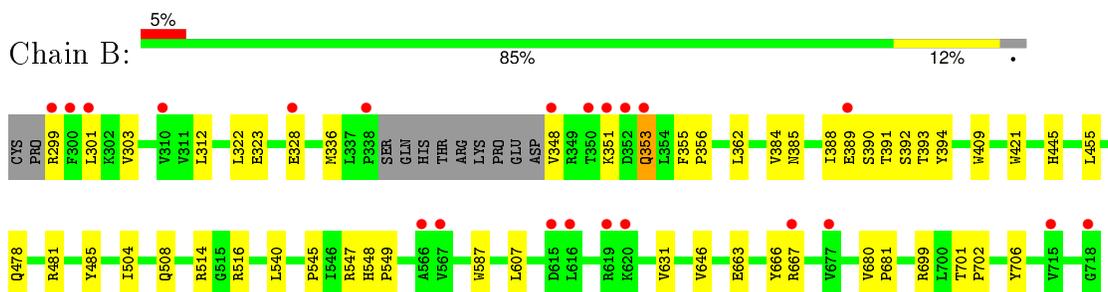
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.00Å 111.28Å 165.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 2.00 37.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.80-2.00) 99.5 (37.80-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.181 , 0.221 0.180 , 0.221	Depositor DCC
R_{free} test set	3215 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	1 of 65204 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7211	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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, TFA, H4B, 2KJ

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	0.60	0/3406	0.67	2/4621 (0.0%)
1	B	0.66	0/3438	0.67	0/4661
All	All	0.63	0/6844	0.67	2/9282 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	381	LEU	CA-CB-CG	5.32	127.54	115.30

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	3313	0	3221	68	0
1	B	3345	0	3259	43	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	15	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	16	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
6	A	1	0	0	0	0
7	A	161	0	0	2	0
7	B	227	0	0	9	0
All	All	7211	0	6602	107	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 (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:TYR:OH	2:B:801:HEM:O1D	1.92	0.86
1:B:303:VAL:HG12	7:B:1049:HOH:O	1.82	0.79
1:A:350:THR:HG22	1:A:352:ASP:H	1.49	0.76
1:A:335:ILE:HD11	7:B:1049:HOH:O	1.92	0.70
1:B:646:VAL:HG12	7:B:1033:HOH:O	1.93	0.67
1:A:350:THR:HB	1:A:353:GLN:HG3	1.76	0.67
1:A:355:PHE:N	1:A:356:PRO:HD2	2.10	0.66
1:A:350:THR:HB	1:A:353:GLN:CG	2.27	0.65
1:A:436:HIS:ND1	7:A:980:HOH:O	2.30	0.65
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.80	0.64
1:A:350:THR:HB	1:A:353:GLN:CD	2.22	0.60
1:A:307:GLU:HG3	7:B:939:HOH:O	2.01	0.60
1:A:355:PHE:N	1:A:356:PRO:CD	2.65	0.59
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.17	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.03	0.58
1:A:675:ASP:O	1:A:679:ILE:HG12	2.03	0.58
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.84	0.58
1:A:569:ASN:HD22	1:A:569:ASN:H	1.50	0.58
1:B:504:ILE:HD11	7:B:1052:HOH:O	2.03	0.58
1:A:353:GLN:O	1:A:356:PRO:HG2	2.04	0.57
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.19	0.57
1:B:328:GLU:OE1	1:B:328:GLU:N	2.37	0.57
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.87	0.57
1:A:306:TRP:CD2	1:B:336:MET:HE2	2.40	0.56
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.86	0.56
1:B:355:PHE:N	1:B:356:PRO:HD2	2.19	0.56
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:HIS:O	1:A:320:SER:HB3	2.06	0.55
1:B:646:VAL:CG1	7:B:1033:HOH:O	2.53	0.55
1:A:361:PHE:O	1:A:364:GLN:HG2	2.06	0.54
1:A:609:GLU:HG3	7:A:974:HOH:O	2.07	0.54
1:A:350:THR:HG22	1:A:352:ASP:N	2.20	0.54
1:A:354:LEU:C	1:A:356:PRO:HD2	2.28	0.54
1:A:306:TRP:CG	1:B:336:MET:HE1	2.43	0.54
1:A:567:VAL:HG23	4:A:803:2KJ:H19	1.90	0.53
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.71	0.53
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.23	0.53
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.23	0.53
1:A:306:TRP:CE2	1:B:336:MET:HE2	2.44	0.52
1:A:535:GLN:HE21	1:A:538:PRO:HD3	1.75	0.52
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.46	0.51
1:A:332:MET:HE2	1:B:301:LEU:HD13	1.92	0.51
1:B:391:THR:O	1:B:392:SER:HB2	2.11	0.51
1:B:323:GLU:O	1:B:699:ARG:HD3	2.11	0.50
1:A:525:GLN:HG3	1:A:529:ASN:O	2.11	0.50
2:A:801:HEM:HMC1	2:A:801:HEM:HBC2	1.93	0.50
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.93	0.50
1:B:701:THR:HA	1:B:702:PRO:C	2.32	0.49
2:B:801:HEM:HBC2	2:B:801:HEM:CMC	2.42	0.49
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.43	0.49
1:B:445:HIS:CD2	1:B:445:HIS:C	2.87	0.48
1:B:516:ARG:HD2	7:B:1111:HOH:O	2.11	0.48
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.44	0.47
1:A:380:ARG:NH1	1:A:397:LYS:HG2	2.29	0.47
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.96	0.46
1:A:659:ILE:O	1:A:663:GLU:HG3	2.15	0.46
1:A:524:LEU:O	1:A:531:PRO:HA	2.15	0.46
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.31	0.46
1:A:328:GLU:H	1:A:328:GLU:CD	2.18	0.46
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.83	0.46
1:A:502:THR:O	1:A:506:ILE:HG13	2.15	0.45
1:A:382:GLU:O	1:A:386:LYS:HG3	2.17	0.45
1:B:389:GLU:HG3	1:B:390:SER:N	2.30	0.45
1:A:353:GLN:C	1:A:356:PRO:HD2	2.38	0.45
1:A:306:TRP:CD2	1:B:336:MET:CE	2.99	0.45
1:B:348:VAL:HG13	1:B:348:VAL:O	2.18	0.44
1:A:684:SER:HB3	1:A:687:ILE:HG12	2.00	0.44
2:B:801:HEM:HBC2	2:B:801:HEM:HMC1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:O	1:B:392:SER:N	2.45	0.44
1:A:569:ASN:ND2	1:A:569:ASN:H	2.15	0.43
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.00	0.43
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.83	0.43
1:A:375:LYS:NZ	1:A:379:ASP:OD1	2.49	0.43
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.00	0.43
1:B:504:ILE:O	1:B:508:GLN:HG2	2.18	0.43
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.00	0.43
1:A:569:ASN:N	1:A:569:ASN:HD22	2.09	0.43
1:A:330:ILE:O	1:A:330:ILE:HG23	2.17	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.55	0.43
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.34	0.43
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.49	0.43
1:B:699:ARG:NE	7:B:1026:HOH:O	2.52	0.43
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.43
1:B:351:LYS:HE3	1:B:392:SER:OG	2.18	0.42
1:A:306:TRP:CD1	1:B:336:MET:HE1	2.54	0.42
1:A:353:GLN:O	1:A:356:PRO:HD2	2.20	0.42
1:A:321:THR:HG23	1:A:322:LEU:N	2.35	0.42
1:A:706:TYR:OH	2:A:801:HEM:O1D	2.13	0.41
1:A:321:THR:HG23	1:A:322:LEU:HG	2.02	0.41
1:B:393:THR:OG1	1:B:394:TYR:N	2.52	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.41
1:A:351:LYS:HE3	1:A:392:SER:HB3	2.01	0.41
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.50	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.41	0.41
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.01	0.41
1:B:322:LEU:HB2	1:B:699:ARG:HB2	2.03	0.41
1:A:306:TRP:CG	1:B:336:MET:CE	3.04	0.41
1:B:516:ARG:CD	7:B:1111:HOH:O	2.66	0.41
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.51	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.85	0.41
1:B:455:LEU:HD23	1:B:587:TRP:HB3	2.03	0.41
1:B:663:GLU:O	1:B:667:ARG:HD2	2.22	0.40
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.56	0.40
1:A:499:VAL:O	1:A:503:GLU:HG3	2.22	0.40
1:A:387:GLU:OE1	1:A:394:TYR:HA	2.22	0.40
1:B:607:LEU:HA	1:B:607:LEU:HD23	1.97	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	403/422 (96%)	390 (97%)	12 (3%)	1 (0%)	52	48
1	B	407/422 (96%)	399 (98%)	8 (2%)	0	100	100
All	All	810/844 (96%)	789 (97%)	20 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

5.3.2 Protein sidechains (i)

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%)	354 (98%)	9 (2%)	55	55
1	B	366/377 (97%)	362 (99%)	4 (1%)	80	83
All	All	729/754 (97%)	716 (98%)	13 (2%)	66	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	389	GLU
1	A	454	ASN
1	A	547	ARG
1	A	552	ASP

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Mol	Chain	Res	Type
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	B	353	GLN
1	B	540	LEU
1	B	545	PRO
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	535	GLN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	801	1	30,50,50	2.35	10 (33%)	24,82,82	2.88	13 (54%)
3	H4B	A	802	-	13,18,18	0.77	0	11,26,26	2.55	6 (54%)
4	2KJ	A	803	-	7,14,14	0.99	1 (14%)	4,16,16	0.62	0
5	TFA	A	804	-	3,6,6	0.10	0	3,9,9	1.15	0
2	HEM	B	801	1	30,50,50	1.89	7 (23%)	24,82,82	2.78	13 (54%)
3	H4B	B	802	-	13,18,18	1.17	2 (15%)	11,26,26	2.24	6 (54%)
4	2KJ	B	803	-	7,14,14	0.67	0	4,16,16	1.15	1 (25%)
5	TFA	B	804	-	3,6,6	0.12	0	3,9,9	1.41	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	801	1	-	0/10/54/54	0/0/8/8
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	2KJ	A	803	-	-	0/6/15/15	0/0/0/0
5	TFA	A	804	-	-	0/0/6/6	0/0/0/0
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2KJ	B	803	-	-	0/6/15/15	0/0/0/0
5	TFA	B	804	-	-	0/0/6/6	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C4B	-6.67	1.45	1.51
2	A	801	HEM	C3D-C4D	-6.29	1.43	1.51
2	B	801	HEM	C3D-C4D	-4.18	1.46	1.51
2	B	801	HEM	C2C-C1C	-3.99	1.45	1.52
2	B	801	HEM	C3B-C4B	-3.79	1.48	1.51
2	A	801	HEM	C2C-C1C	-3.45	1.46	1.52
4	A	803	2KJ	OH-NH1	-2.28	1.42	1.45
2	A	801	HEM	C2D-C1D	-2.06	1.45	1.51
2	B	801	HEM	C1C-NC	2.08	1.38	1.36
2	B	801	HEM	C3C-CAC	2.10	1.55	1.51
2	A	801	HEM	FE-NB	2.10	2.08	1.97
2	A	801	HEM	C3B-CAB	2.22	1.55	1.51
2	A	801	HEM	C3C-CAC	2.25	1.55	1.51
3	B	802	H4B	C7-N8	2.30	1.49	1.46
3	B	802	H4B	C4-N3	2.35	1.37	1.33
2	A	801	HEM	FE-NC	2.36	2.05	1.95
2	B	801	HEM	FE-ND	2.50	2.10	1.97
2	B	801	HEM	FE-NC	2.77	2.06	1.95
2	A	801	HEM	FE-ND	3.30	2.15	1.97
2	A	801	HEM	C1C-NC	3.50	1.40	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-6.35	101.15	112.53
2	A	801	HEM	CBA-CAA-C2A	-6.27	101.29	112.53
2	A	801	HEM	CBD-CAD-C3D	-4.11	101.59	113.55
2	B	801	HEM	CAA-C2A-C1A	-3.72	122.97	127.01
2	A	801	HEM	C3C-CAC-CBC	-3.61	118.92	124.46
2	B	801	HEM	CBD-CAD-C3D	-3.20	104.23	113.55
3	A	802	H4B	N3-C2-N1	-3.04	120.55	125.53
3	B	802	H4B	N3-C2-N1	-2.85	120.87	125.53
2	A	801	HEM	CMA-C3A-C4A	-2.57	124.11	128.36
2	B	801	HEM	C3B-C4B-NB	-2.28	107.26	111.63
2	A	801	HEM	CAA-C2A-C1A	-2.24	124.57	127.01
2	B	801	HEM	CMA-C3A-C4A	-2.13	124.85	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	H4B	N2-C2-N3	2.05	120.60	117.20
2	B	801	HEM	C2C-C1C-CHC	2.09	126.86	123.68
2	B	801	HEM	C2D-C3D-C4D	2.10	105.06	101.50
4	B	803	2KJ	OH-C2-C1	2.14	110.94	107.45
3	B	802	H4B	C4-N3-C2	2.58	119.51	115.94
3	B	802	H4B	C4A-C8A-N8	2.66	121.56	118.43
2	A	801	HEM	CMD-C2D-C3D	2.77	126.60	114.35
2	B	801	HEM	CMD-C2D-C3D	2.85	126.96	114.35
3	A	802	H4B	N2-C2-N3	2.86	121.93	117.20
3	B	802	H4B	C2-N1-C8A	2.89	121.04	114.54
2	A	801	HEM	C3B-C4B-CHC	2.91	127.25	123.16
2	A	801	HEM	C3B-CAB-CBB	2.91	128.92	124.46
2	A	801	HEM	CMB-C2B-C3B	2.93	123.84	116.53
3	A	802	H4B	C4-N3-C2	2.99	120.08	115.94
2	A	801	HEM	C2D-C3D-C4D	3.09	106.74	101.50
2	B	801	HEM	C3B-C4B-CHC	3.16	127.61	123.16
3	A	802	H4B	C4A-C8A-N8	3.30	122.32	118.43
3	A	802	H4B	C2-N1-C8A	3.37	122.12	114.54
2	A	801	HEM	CAD-C3D-C4D	3.82	125.93	112.47
2	B	801	HEM	CMC-C2C-C3C	4.06	126.68	116.53
2	B	801	HEM	CMB-C2B-C3B	4.11	126.80	116.53
3	B	802	H4B	C4-C4A-C8A	4.19	118.36	114.56
2	B	801	HEM	CAD-C3D-C4D	4.30	127.62	112.47
3	A	802	H4B	C4-C4A-C8A	4.53	118.66	114.56
2	A	801	HEM	CAD-C3D-C2D	4.89	127.28	113.22
2	B	801	HEM	CAD-C3D-C2D	4.91	127.32	113.22
2	A	801	HEM	CMC-C2C-C3C	5.26	129.67	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	3	0
4	A	803	2KJ	1	0
2	B	801	HEM	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	407/422 (96%)	0.57	54 (13%)	4	5	26, 50, 91, 116	0
1	B	411/422 (97%)	0.09	22 (5%)	29	31	25, 39, 66, 85	0
All	All	818/844 (96%)	0.33	76 (9%)	11	11	25, 44, 85, 116	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.4
1	A	716	TRP	6.8
1	A	352	ASP	5.8
1	A	488	PRO	5.7
1	A	355	PHE	5.3
1	B	348	VAL	5.2
1	B	350	THR	5.1
1	B	718	GLY	5.0
1	B	619	ARG	4.5
1	A	300	PHE	4.5
1	A	388	ILE	4.4
1	A	351	LYS	4.3
1	A	299	ARG	4.0
1	B	352	ASP	3.9
1	A	715	VAL	3.7
1	A	507	GLN	3.7
1	A	491	SER	3.7
1	A	350	THR	3.6
1	A	322	LEU	3.5
1	A	514	ARG	3.5
1	A	567	VAL	3.4
1	A	503	GLU	3.4
1	A	392	SER	3.4
1	B	616	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	3.3
1	A	390	SER	3.1
1	A	486	LYS	3.0
1	B	351	LYS	3.0
1	A	713	THR	3.0
1	A	393	THR	3.0
1	A	712	ASN	3.0
1	A	489	ASP	2.9
1	B	338	PRO	2.9
1	A	311	VAL	2.8
1	A	678	TRP	2.8
1	A	682	PRO	2.8
1	A	619	ARG	2.8
1	A	511	LYS	2.8
1	A	391	THR	2.6
1	A	667	ARG	2.6
1	A	714	HIS	2.6
1	B	299	ARG	2.5
1	A	584	PHE	2.5
1	A	506	ILE	2.4
1	A	370	LYS	2.4
1	A	385	ASN	2.4
1	B	389	GLU	2.4
1	B	567	VAL	2.4
1	A	381	LEU	2.4
1	B	353	GLN	2.4
1	A	321	THR	2.4
1	A	680	VAL	2.4
1	A	386	LYS	2.3
1	A	551	PHE	2.3
1	B	566	ALA	2.3
1	A	508	GLN	2.3
1	A	338	PRO	2.3
1	A	677	VAL	2.3
1	B	615	ASP	2.3
1	A	485	TYR	2.3
1	B	620	LYS	2.3
1	A	487	GLN	2.2
1	B	677	VAL	2.2
1	A	681	PRO	2.2
1	A	353	GLN	2.2
1	A	492	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	2.1
1	B	301	LEU	2.1
1	A	591	THR	2.1
1	B	328	GLU	2.1
1	B	667	ARG	2.1
1	B	310	VAL	2.1
1	A	490	GLY	2.1
1	B	715	VAL	2.0
1	A	372	PHE	2.0
1	A	309	ASP	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
5	TFA	B	804	7/7	0.92	0.20	5.58	49,51,54,55	7
4	2KJ	A	803	15/15	0.95	0.26	1.54	32,35,44,46	0
5	TFA	A	804	7/7	0.97	0.17	1.34	60,60,61,61	7
2	HEM	A	801	43/43	0.98	0.19	0.61	26,31,39,46	0
4	2KJ	B	803	15/15	0.95	0.18	0.48	30,34,44,47	0
2	HEM	B	801	43/43	0.98	0.15	0.47	23,28,36,44	0
3	H4B	A	802	17/17	0.96	0.17	0.43	26,30,35,36	0
3	H4B	B	802	17/17	0.97	0.14	0.08	24,28,32,34	0
6	ZN	A	805	1/1	0.99	0.07	-0.94	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.