Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:42 PM GMT

PDB ID	:	3RQJ
Title	:	Structure of the neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((1S,2R)-2-(3-Fluorophenyl)cyclopropylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on	:	2011-04-28
Resolution	:	1.84 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
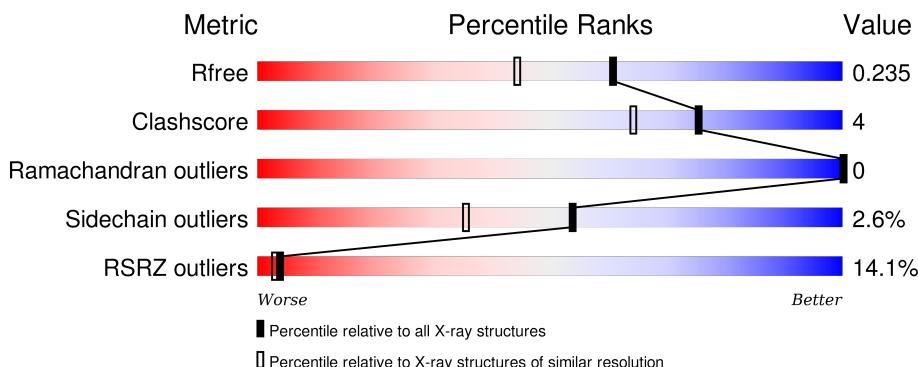
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
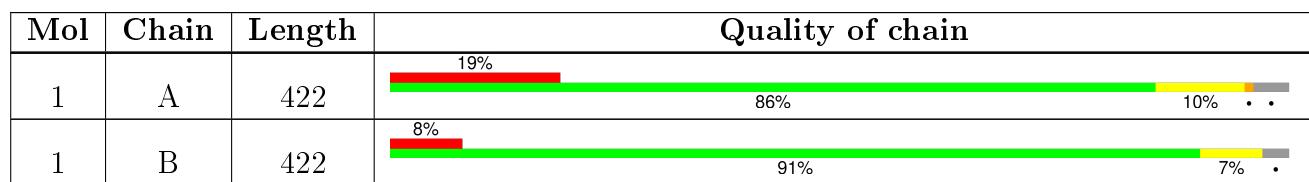
The reported resolution of this entry is 1.84 Å.

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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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
4	ACT	A	860	-	-	-	X

2 Entry composition (i)
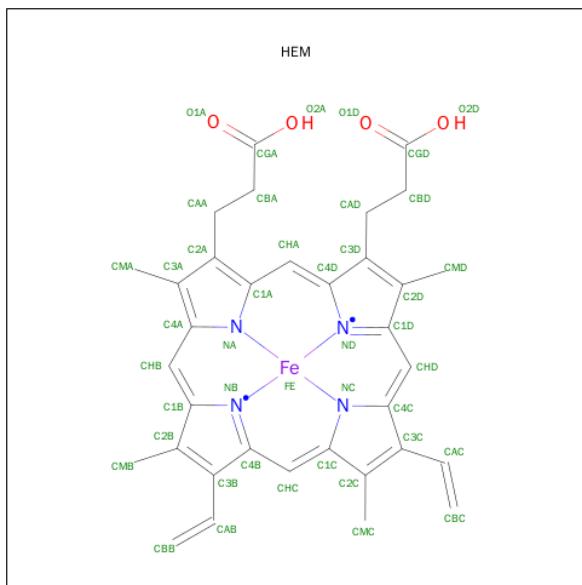
There are 7 unique types of molecules in this entry. The entry contains 7189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.
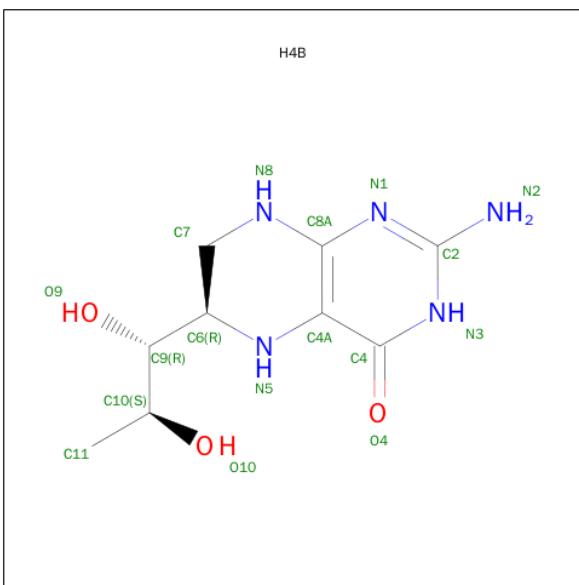
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total 3322	C 2127	N 566	O 608	S 21	0	2	0
1	B	411	Total 3354	C 2146	N 574	O 612	S 22	0	2	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
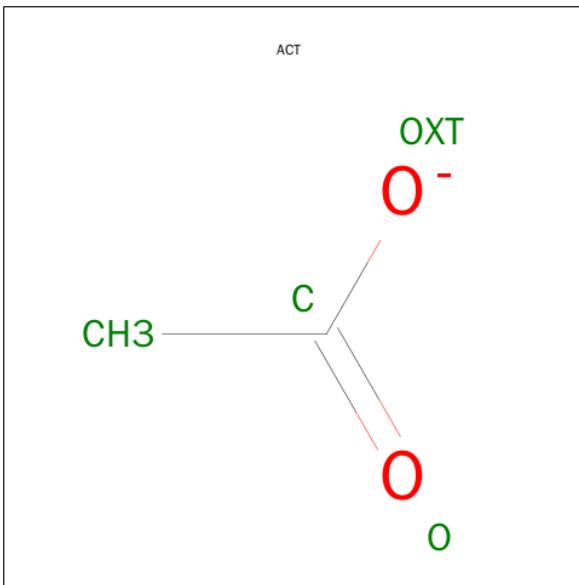
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).

H4B
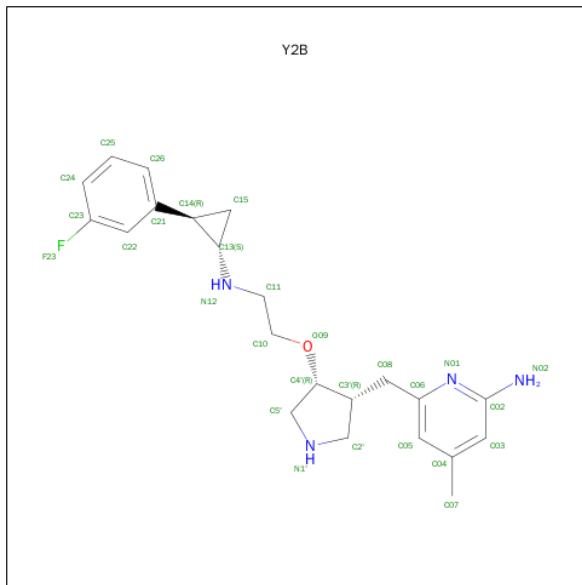
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

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

ACT

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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[(1S,2R)-2-(3-FLUOROPHENYL)CYCLOPROPYL] AMINO}ETHOXY)PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: Y2B) (formula: $C_{22}H_{29}FN_4O$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			28	22	1	4	1		
5	B	1	Total	C	F	N	O	0	0
			28	22	1	4	1		

- 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		
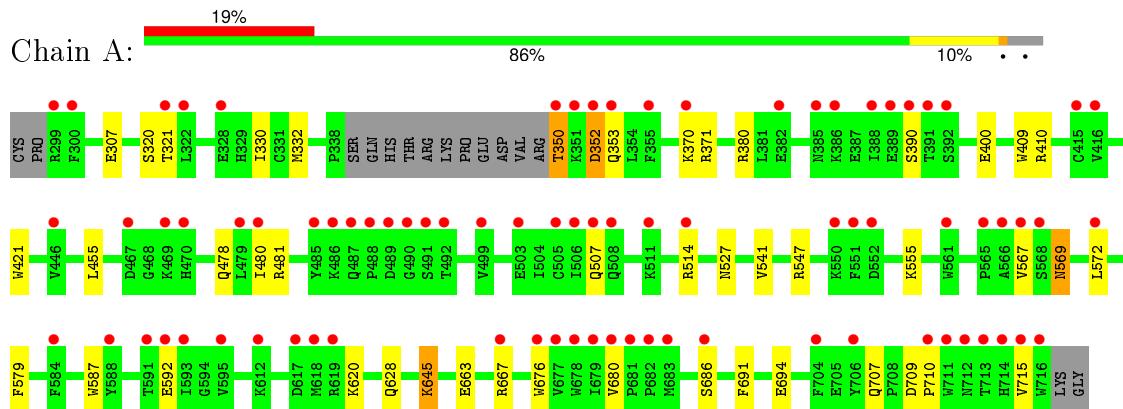
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	190	Total	O	0	0
			190	190		
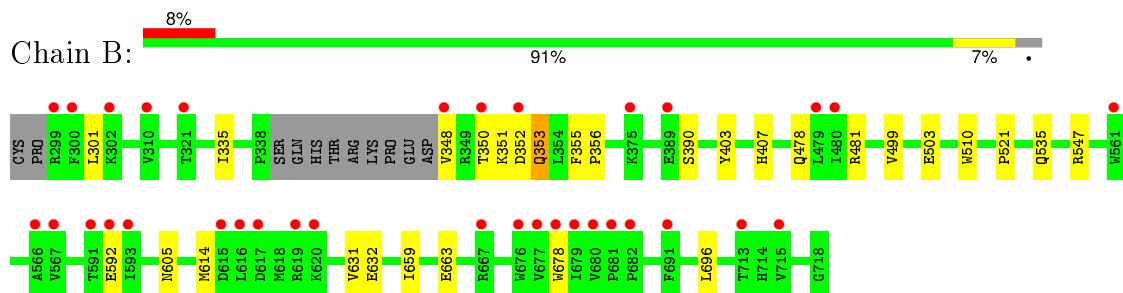
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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	51.84Å 110.74Å 164.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 1.84 37.84 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.11-1.84) 98.3 (37.84-1.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	2.46 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.221 0.208 , 0.235	Depositor DCC
R_{free} test set	4057 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	2 of 82102 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7189	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 4.33% 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: Y2B, ZN, H4B, HEM, 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	0.69	0/3421	0.69	1/4641 (0.0%)
1	B	0.77	0/3453	0.73	0/4681
All	All	0.73	0/6874	0.71	1/9322 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	410	ARG	NE-CZ-NH2	5.17	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3232	31	0
1	B	3354	0	3270	21	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	29	6	0
5	B	28	0	29	4	0
6	A	1	0	0	0	0
7	A	138	0	0	0	0
7	B	190	0	0	3	0
All	All	7189	0	6656	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (52) 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:A:592[A]:GLU:OE1	5:A:800:Y2B:H26	1.72	0.89
1:B:592[A]:GLU:OE1	5:B:800:Y2B:H26	1.81	0.79
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.70	0.73
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.71	0.72
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.55	0.72
1:A:307:GLU:HG3	7:B:1003:HOH:O	1.94	0.68
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.09	0.65
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.01	0.60
1:A:592[A]:GLU:OE1	5:A:800:Y2B:H14	2.03	0.58
1:B:350:THR:HG22	1:B:352:ASP:H	1.70	0.57
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.66	0.56
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.88	0.55
1:B:659:ILE:O	1:B:663:GLU:HG3	2.07	0.55
1:A:592[A]:GLU:CD	5:A:800:Y2B:H26	2.28	0.52
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.92	0.52
1:A:645:LYS:HB2	1:A:645:LYS:HZ1	1.75	0.52
1:A:332:MET:CE	1:B:301:LEU:HD22	2.40	0.51
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.41	0.51
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.95	0.49
1:B:499:VAL:O	1:B:503:GLU:HG3	2.13	0.49
1:A:569:ASN:H	1:A:569:ASN:HD22	1.58	0.48
1:B:614:MET:CE	1:B:632:GLU:HG3	2.44	0.48
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.96	0.48
2:A:750:HEM:HBA1	5:A:800:Y2B:H14	1.97	0.47
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.97	0.47
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.98	0.46
1:A:645:LYS:NZ	1:A:645:LYS:HB2	2.29	0.45
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:TRP:CH2	5:B:800:Y2B:H2'A	2.52	0.45
1:B:592[A]:GLU:CD	5:B:800:Y2B:H26	2.38	0.45
1:B:605:ASN:ND2	7:B:1019:HOH:O	2.39	0.44
1:B:535:GLN:HG3	7:B:1188:HOH:O	2.18	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.52	0.44
1:B:355:PHE:N	1:B:356:PRO:HD2	2.33	0.43
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.43
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	2.01	0.43
1:B:351:LYS:H	1:B:351:LYS:HG3	1.69	0.43
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.85	0.42
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.66	0.42
1:A:663:GLU:O	1:A:667:ARG:HG2	2.19	0.42
1:A:592[B]:GLU:OE2	5:A:800:Y2B:N12	2.49	0.42
1:A:569:ASN:O	1:A:707:GLN:HG2	2.20	0.42
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.42
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.01	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.55	0.42
1:A:350:THR:N	1:A:353:GLN:HE21	2.18	0.41
1:A:572:LEU:HB3	1:A:579:PHE:HB2	2.03	0.41
1:A:628:GLN:HG2	1:B:631:VAL:HG11	2.03	0.41
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.56	0.41
1:A:352:ASP:N	1:A:352:ASP:OD2	2.54	0.41
1:A:567:VAL:CG2	5:A:800:Y2B:H15A	2.50	0.41
1:B:592[A]:GLU:OE1	5:B:800:Y2B:H14	2.22	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	405/422 (96%)	393 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	409/422 (97%)	403 (98%)	6 (2%)	0	100	100
All	All	814/844 (96%)	796 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	365/377 (97%)	350 (96%)	15 (4%)	37	16
1	B	368/377 (98%)	364 (99%)	4 (1%)	80	72
All	All	733/754 (97%)	714 (97%)	19 (3%)	54	35

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	321	THR
1	A	350	THR
1	A	352	ASP
1	A	370	LYS
1	A	390	SER
1	A	507	GLN
1	A	514	ARG
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	348	VAL
1	B	353	GLN
1	B	390	SER

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Mol	Chain	Res	Type
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	601	ASN
1	B	605	ASN
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	750	1	30,50,50	2.28	8 (26%)	24,82,82	2.79	11 (45%)
3	H4B	A	760	-	13,18,18	0.73	0	11,26,26	2.43	5 (45%)
5	Y2B	A	800	-	26,31,31	0.91	0	30,43,43	2.47	9 (30%)
4	ACT	A	860	-	1,3,3	1.25	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.15	9 (30%)	24,82,82	2.99	13 (54%)
3	H4B	B	760	-	13,18,18	1.24	1 (7%)	11,26,26	2.53	5 (45%)
5	Y2B	B	800	-	26,31,31	0.83	0	30,43,43	2.42	8 (26%)
4	ACT	B	860	-	1,3,3	1.70	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	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	Y2B	A	800	-	-	0/13/30/30	0/3/4/4
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	Y2B	B	800	-	-	0/13/30/30	0/3/4/4
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-6.59	1.46	1.51
2	A	750	HEM	C3D-C4D	-5.40	1.44	1.51
2	B	750	HEM	C3D-C4D	-5.37	1.44	1.51
2	B	750	HEM	C3B-C4B	-5.10	1.47	1.51
2	B	750	HEM	C2C-C1C	-4.27	1.44	1.52
2	A	750	HEM	C2C-C1C	-3.98	1.45	1.52
2	A	750	HEM	C2D-C1D	-2.13	1.44	1.51
2	B	750	HEM	C2B-C1B	-2.12	1.44	1.51
2	B	750	HEM	C2D-C1D	-2.11	1.44	1.51
2	B	750	HEM	CAD-C3D	2.24	1.58	1.54
2	B	750	HEM	CAA-C2A	2.25	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CMA-C3A	2.35	1.56	1.51
3	B	760	H4B	C7-N8	2.46	1.49	1.46
2	A	750	HEM	CMA-C3A	2.60	1.57	1.51
2	A	750	HEM	FE-ND	2.64	2.11	1.97
2	A	750	HEM	C1C-NC	2.66	1.39	1.36
2	A	750	HEM	FE-NC	3.73	2.10	1.95
2	B	750	HEM	FE-NC	4.27	2.12	1.95

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-7.26	99.51	112.53
5	B	800	Y2B	C15-C14-C21	-7.01	109.73	122.30
5	A	800	Y2B	C15-C14-C21	-6.91	109.91	122.30
5	B	800	Y2B	C15-C13-N12	-5.96	101.90	118.20
5	A	800	Y2B	C15-C13-N12	-5.55	103.02	118.20
2	A	750	HEM	CBA-CAA-C2A	-4.80	103.92	112.53
2	A	750	HEM	CBD-CAD-C3D	-4.32	100.99	113.55
2	B	750	HEM	CAA-C2A-C1A	-4.17	122.48	127.01
2	A	750	HEM	CAA-C2A-C1A	-3.83	122.85	127.01
2	B	750	HEM	CBD-CAD-C3D	-3.75	102.63	113.55
5	A	800	Y2B	C26-C25-C24	-3.74	114.90	120.24
3	B	760	H4B	N3-C2-N1	-3.23	120.24	125.53
3	A	760	H4B	N3-C2-N1	-3.18	120.31	125.53
5	A	800	Y2B	C05-C06-N01	-2.79	119.82	122.96
2	B	750	HEM	C3B-C4B-NB	-2.57	106.72	111.63
5	B	800	Y2B	C04-C05-C06	-2.52	118.70	120.28
5	A	800	Y2B	C21-C14-C13	-2.49	116.22	121.50
5	B	800	Y2B	C24-C23-C22	-2.20	120.51	123.35
2	A	750	HEM	C3C-CAC-CBC	-2.15	121.15	124.46
2	B	750	HEM	C3C-CAC-CBC	-2.13	121.18	124.46
5	A	800	Y2B	C24-C23-C22	-2.13	120.60	123.35
5	B	800	Y2B	C05-C06-N01	-2.12	120.57	122.96
5	A	800	Y2B	C26-C21-C22	2.07	121.28	118.79
5	A	800	Y2B	C25-C24-C23	2.11	123.11	118.12
2	A	750	HEM	C2D-C3D-C4D	2.17	105.19	101.50
2	B	750	HEM	C3B-C4B-CHC	2.23	126.30	123.16
3	B	760	H4B	C2-N1-C8A	2.26	119.62	114.54
5	B	800	Y2B	N02-C02-N01	2.38	120.84	116.50
2	B	750	HEM	C4B-CHC-C1C	2.44	129.91	125.82
2	B	750	HEM	CMD-C2D-C3D	2.49	125.36	114.35
3	B	760	H4B	N2-C2-N1	2.62	121.54	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	800	Y2B	C11-N12-C13	2.92	118.30	113.89
2	B	750	HEM	C2C-C1C-CHC	2.93	128.13	123.68
3	A	760	H4B	C4A-C8A-N8	2.94	121.89	118.43
2	A	750	HEM	CMD-C2D-C3D	3.05	127.86	114.35
3	A	760	H4B	C4-N3-C2	3.12	120.27	115.94
3	A	760	H4B	C2-N1-C8A	3.22	121.79	114.54
2	B	750	HEM	CMC-C2C-C3C	3.28	124.73	116.53
2	A	750	HEM	C3B-C4B-CHC	3.35	127.87	123.16
2	A	750	HEM	CMB-C2B-C3B	3.97	126.44	116.53
3	B	760	H4B	C4-N3-C2	4.06	121.57	115.94
3	A	760	H4B	C4-C4A-C8A	4.30	118.45	114.56
2	A	750	HEM	CAD-C3D-C4D	4.33	127.73	112.47
2	B	750	HEM	CMB-C2B-C3B	4.67	128.19	116.53
2	B	750	HEM	CAD-C3D-C4D	4.70	129.04	112.47
2	A	750	HEM	CAD-C3D-C2D	4.79	127.00	113.22
2	B	750	HEM	CAD-C3D-C2D	4.83	127.09	113.22
2	A	750	HEM	CMC-C2C-C3C	5.31	129.79	116.53
3	B	760	H4B	C4-C4A-C8A	5.33	119.39	114.56
5	B	800	Y2B	C02-N01-C06	5.70	122.28	118.23
5	A	800	Y2B	C02-N01-C06	6.30	122.71	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	2	0
5	A	800	Y2B	6	0
2	B	750	HEM	3	0
5	B	800	Y2B	4	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%)	1.02	81 (19%)	1	1	28, 53, 92, 121	0
1	B	411/422 (97%)	0.51	34 (8%)	14	13	28, 41, 66, 80	0
All	All	818/844 (96%)	0.76	115 (14%)	4	3	28, 47, 86, 121	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.8
1	A	488	PRO	8.4
1	A	716	TRP	8.2
1	A	713	THR	6.0
1	A	351	LYS	6.0
1	A	355	PHE	6.0
1	B	619	ARG	5.6
1	A	352	ASP	5.6
1	A	486	LYS	5.4
1	A	388	ILE	4.8
1	A	506	ILE	4.6
1	A	300	PHE	4.4
1	B	348	VAL	4.4
1	A	715	VAL	4.3
1	B	350	THR	4.2
1	A	514	ARG	4.1
1	A	491	SER	3.8
1	A	714	HIS	3.8
1	A	567	VAL	3.8
1	A	487	GLN	3.8
1	A	507	GLN	3.8
1	A	678	TRP	3.7
1	A	385	ASN	3.6
1	B	667	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	616	LEU	3.6
1	A	389	GLU	3.5
1	A	386	LYS	3.5
1	A	392	SER	3.4
1	A	551	PHE	3.4
1	A	479	LEU	3.4
1	A	490	GLY	3.4
1	A	592[A]	GLU	3.4
1	A	390	SER	3.3
1	A	552	ASP	3.3
1	A	593	ILE	3.3
1	A	503	GLU	3.2
1	B	677	VAL	3.2
1	B	567	VAL	3.2
1	A	469	LYS	3.2
1	A	299	ARG	3.2
1	B	620	LYS	3.2
1	A	619	ARG	3.1
1	B	680	VAL	3.1
1	A	391	THR	3.1
1	A	511	LYS	3.1
1	A	480	ILE	3.1
1	B	691	PHE	3.0
1	A	680	VAL	3.0
1	B	479	LEU	3.0
1	A	584	PHE	2.9
1	A	489	ASP	2.9
1	A	591	THR	2.9
1	B	310	VAL	2.9
1	B	561	TRP	2.9
1	B	566	ALA	2.9
1	A	682	PRO	2.8
1	A	321	THR	2.8
1	A	382	GLU	2.8
1	A	676	TRP	2.8
1	A	350	THR	2.8
1	A	561	TRP	2.8
1	B	592[A]	GLU	2.8
1	B	302	LYS	2.8
1	B	591	THR	2.8
1	A	416	VAL	2.8
1	A	677	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	715	VAL	2.7
1	A	492	THR	2.7
1	B	713	THR	2.7
1	A	415	CYS	2.7
1	B	480	ILE	2.7
1	A	588	TYR	2.7
1	B	617	ASP	2.6
1	A	712	ASN	2.6
1	A	505	CYS	2.6
1	B	682	PRO	2.6
1	A	508	GLN	2.6
1	A	595	VAL	2.6
1	A	499	VAL	2.5
1	A	681	PRO	2.5
1	A	566	ALA	2.5
1	B	352	ASP	2.5
1	B	299	ARG	2.5
1	B	615	ASP	2.5
1	A	565	PRO	2.5
1	A	667	ARG	2.4
1	A	467	ASP	2.4
1	B	321	THR	2.4
1	B	389	GLU	2.4
1	A	470	HIS	2.3
1	A	683	MET	2.3
1	B	679	ILE	2.3
1	B	681	PRO	2.3
1	A	322	LEU	2.3
1	A	550	LYS	2.3
1	A	686	SER	2.3
1	A	679	ILE	2.3
1	A	370	LYS	2.3
1	A	446	VAL	2.3
1	A	572	LEU	2.2
1	B	375	LYS	2.2
1	B	678	TRP	2.2
1	A	328	GLU	2.2
1	B	676	TRP	2.2
1	A	485	TYR	2.2
1	A	704	PHE	2.1
1	B	593	ILE	2.1
1	A	568	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	617	ASP	2.1
1	A	618	MET	2.1
1	A	710	PRO	2.1
1	A	711	TRP	2.1
1	A	353	GLN	2.0
1	A	706	TYR	2.0
1	A	612	LYS	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
4	ACT	A	860	4/4	0.93	0.22	5.24	51,53,53,55	0
3	H4B	A	760	17/17	0.95	0.20	0.72	32,35,39,40	0
3	H4B	B	760	17/17	0.96	0.18	0.66	32,34,38,39	0
4	ACT	B	860	4/4	0.97	0.10	0.26	47,47,49,49	0
2	HEM	A	750	43/43	0.97	0.21	0.16	26,34,41,44	0
2	HEM	B	750	43/43	0.98	0.17	0.14	24,31,41,46	0
5	Y2B	B	800	28/28	0.83	0.17	-0.16	31,38,42,47	0
5	Y2B	A	800	28/28	0.81	0.20	-0.26	33,42,44,44	0
6	ZN	A	900	1/1	0.99	0.07	-1.09	38,38,38,38	0

6.5　Other polymers ⓘ

There are no such residues in this entry.