



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3JWV
Title : Structure of rat neuronal nitric oxide synthase R349A mutant heme domain
in complex with N1-{(3'S,4'R)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]
pyrrolidin-3'-yl}-N2-(3'-fluorophenethyl)ethane-1,2-diamine
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2009-09-18
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

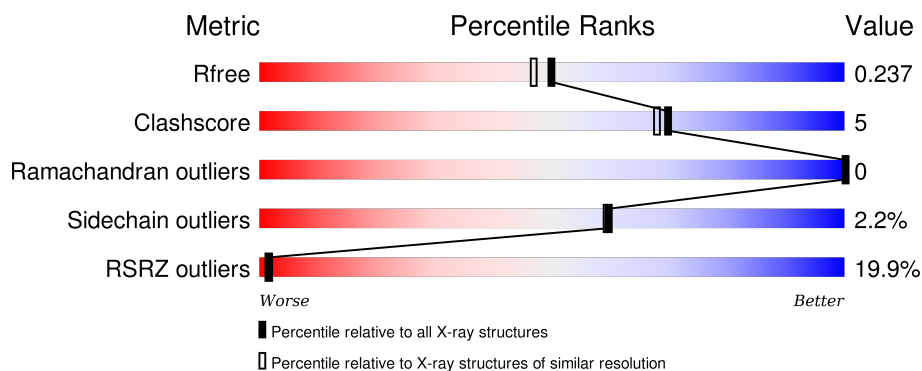
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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>28%</div> <div>87%</div> <div>9%</div> <div>...</div> </div>
1	B	422	<div> <div>11%</div> <div>89%</div> <div>9%</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
4	J14	A	800	-	-	-	X
4	J14	B	800	-	-	-	X
5	ACT	A	860	-	-	-	X

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.

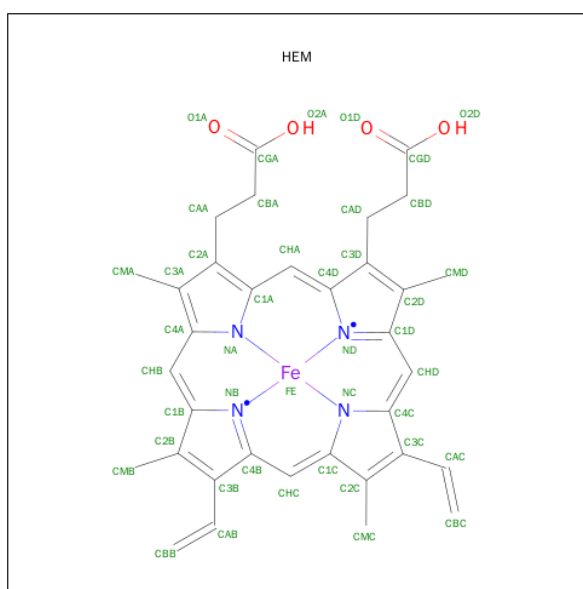
- Molecule 1 is a protein called Nitric oxide synthase, brain.

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
			3339	2137	571	610	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ALA	ARG	ENGINEERED	UNP P29476
B	349	ALA	ARG	ENGINEERED	UNP P29476

- 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		

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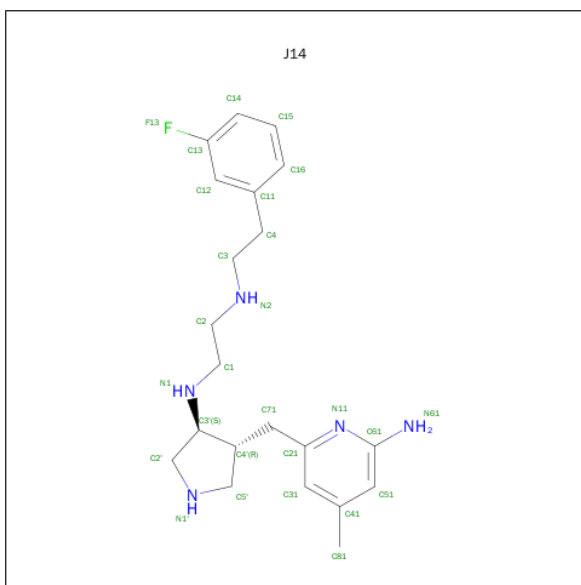
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



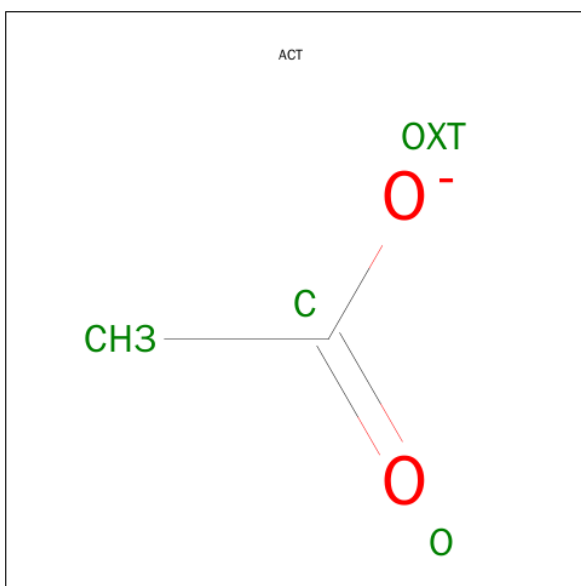
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-{(3S,4R)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-[2-(3-FLUOROPHENYL)ETHYL]ETHANE-1,2-DIAMINE (three-letter code: J14) (formula: $C_{21}H_{30}FN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 27	C 21	F 1	N 5	0	0
4	B	1	Total 27	C 21	F 1	N 5	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	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 1	Zn 1	0	0

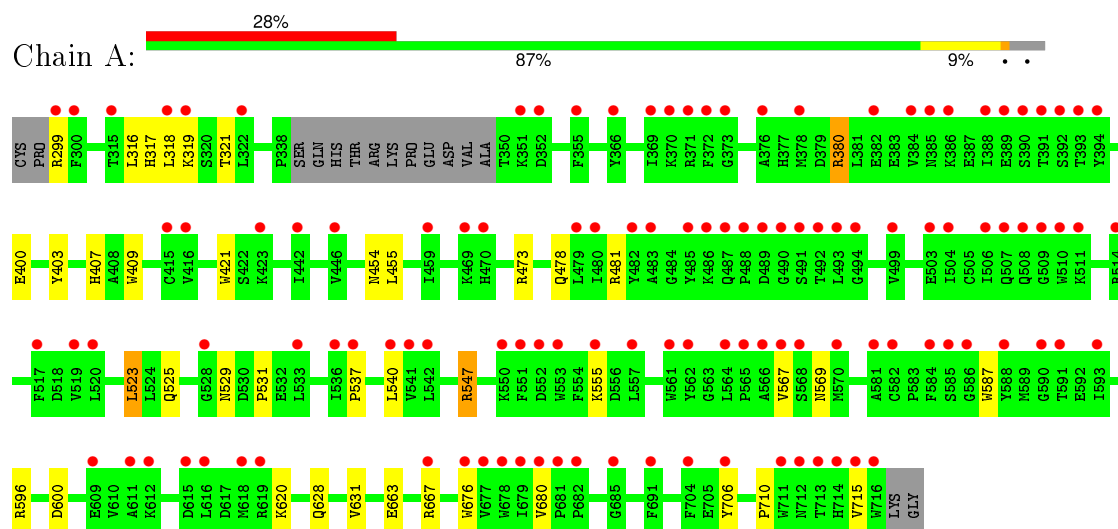
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total 137	O 137	0	0
7	B	202	Total 202	O 202	0	0

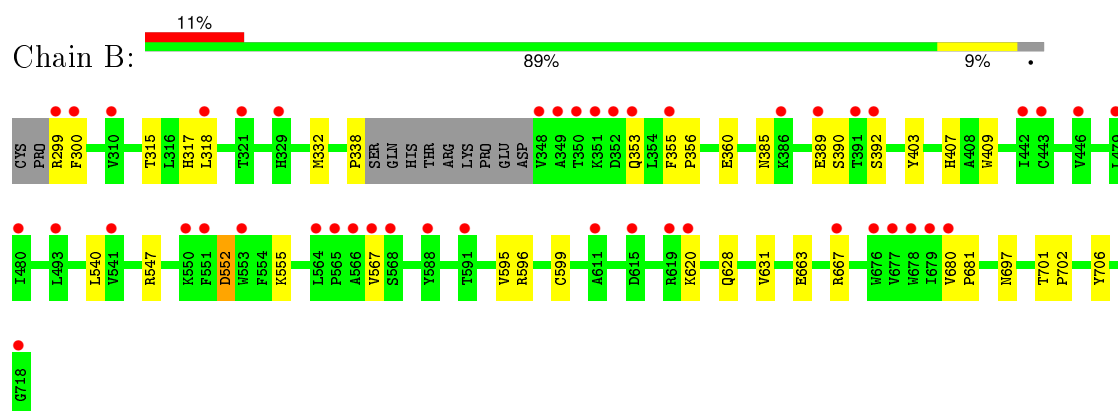
3 Residue-property plots

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.91Å 111.90Å 164.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 1.98 40.86 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.86-1.98) 97.7 (40.86-1.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.181 , 0.213 0.210 , 0.237	Depositor DCC
R_{free} test set	3299 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 66154 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, J14, H4B, 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	0.60	0/3406	0.63	1/4621 (0.0%)
1	B	0.65	0/3432	0.64	1/4654 (0.0%)
All	All	0.62	0/6838	0.64	2/9275 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	596	ARG	NE-CZ-NH1	-5.19	117.70	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	3313	0	3221	25	0
1	B	3339	0	3251	28	0
2	A	43	0	30	4	0
2	B	43	0	30	9	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	30	7	0
5	A	4	0	3	0	0
6	A	1	0	0	0	0
7	A	137	0	0	0	0
7	B	202	0	0	2	0
All	All	7170	0	6625	61	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 5.

All (61) 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:567:VAL:CG2	4:B:800:J14:H5'A	1.84	1.07
1:A:567:VAL:HG22	4:A:800:J14:H5'A	1.41	0.98
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.84	0.94
1:B:567:VAL:HG21	4:B:800:J14:H5'A	1.49	0.93
1:A:706:TYR:OH	2:A:750:HEM:O1D	1.92	0.88
1:A:567:VAL:CG2	4:A:800:J14:H5'A	2.09	0.82
1:B:567:VAL:HG22	4:B:800:J14:H5'A	1.59	0.82
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.68	0.75
1:B:567:VAL:HG21	4:B:800:J14:C5'	2.18	0.72
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.71	0.72
1:A:567:VAL:CG2	4:A:800:J14:C5'	2.68	0.71
1:B:299:ARG:HG2	1:B:317:HIS:NE2	2.12	0.65
1:B:299:ARG:HB2	1:B:299:ARG:NH1	2.12	0.65
1:B:706:TYR:HH	2:B:750:HEM:CGD	2.06	0.65
1:B:567:VAL:CG2	4:B:800:J14:C5'	2.71	0.61
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.83	0.61
2:A:750:HEM:HBA1	4:A:800:J14:H71A	1.82	0.60
1:A:567:VAL:HG21	4:A:800:J14:H5'	1.85	0.59
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.83	0.59
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.33	0.59
1:A:663:GLU:O	1:A:667:ARG:HG2	2.04	0.57
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.85	0.57
1:B:332:MET:CE	1:B:338:PRO:HB3	2.34	0.57
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
4:B:800:J14:H1A	7:B:1103:HOH:O	2.05	0.55
1:B:552:ASP:OD1	1:B:555:LYS:NZ	2.39	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.36	0.55
1:B:299:ARG:HB2	1:B:299:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.23	0.53
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.91	0.53
1:A:299:ARG:O	1:A:317:HIS:CE1	2.62	0.52
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.92	0.51
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.93	0.51
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.54	0.51
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.43	0.50
1:B:332:MET:HE3	1:B:338:PRO:HB3	1.92	0.50
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.11	0.50
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.28	0.49
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.95	0.48
1:A:525:GLN:HG3	1:A:529:ASN:O	2.14	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.47
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.04	0.46
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.52	0.46
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45
4:B:800:J14:H2A	7:B:1176:HOH:O	2.16	0.45
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.51	0.45
1:A:567:VAL:HG21	4:A:800:J14:C5'	2.41	0.44
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.83	0.44
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.42	0.43
1:A:567:VAL:CG2	4:A:800:J14:H5'	2.41	0.43
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.54	0.42
1:B:356:PRO:O	1:B:360:GLU:HG3	2.20	0.42
1:B:389:GLU:HG2	1:B:390:SER:N	2.34	0.42
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.01	0.42
1:A:631:VAL:HG11	1:B:628:GLN:HG2	2.02	0.41
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.41
2:B:750:HEM:CBC	2:B:750:HEM:HMC1	2.51	0.41
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.56	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.94	0.41
2:A:750:HEM:O2A	4:A:800:J14:H2'A	2.22	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	403/422 (96%)	393 (98%)	10 (2%)	0	100	100
1	B	407/422 (96%)	402 (99%)	5 (1%)	0	100	100
All	All	810/844 (96%)	795 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	363/376 (96%)	354 (98%)	9 (2%)	55	53
1	B	365/376 (97%)	358 (98%)	7 (2%)	65	65
All	All	728/752 (97%)	712 (98%)	16 (2%)	60	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	380	ARG
1	A	454	ASN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS

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Mol	Chain	Res	Type
1	A	715	VAL
1	B	353	GLN
1	B	392	SER
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP
1	B	620	LYS
1	B	697	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	A	714	HIS
1	B	364	GLN
1	B	385	ASN
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 ⓘ

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	2.33	10 (33%)	24,82,82	2.84	12 (50%)
3	H4B	A	760	-	13,18,18	1.00	0	11,26,26	2.84	6 (54%)
4	J14	A	800	-	26,29,29	0.70	0	30,38,38	1.83	6 (20%)
5	ACT	A	860	-	1,3,3	1.38	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.07	9 (30%)	24,82,82	2.59	11 (45%)
3	H4B	B	760	-	13,18,18	0.92	0	11,26,26	2.68	6 (54%)
4	J14	B	800	-	26,29,29	0.75	0	30,38,38	2.31	7 (23%)

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
4	J14	A	800	-	-	0/13/23/23	0/3/3/3
5	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
4	J14	B	800	-	-	0/13/23/23	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-6.55	1.43	1.51
2	B	750	HEM	C3D-C4D	-6.16	1.43	1.51
2	A	750	HEM	C3B-C4B	-6.06	1.46	1.51
2	B	750	HEM	C3B-C4B	-4.52	1.47	1.51
2	A	750	HEM	C2C-C1C	-3.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C2C-C1C	-3.70	1.45	1.52
2	A	750	HEM	C2B-C1B	-2.44	1.43	1.51
2	B	750	HEM	C2B-C1B	-2.13	1.44	1.51
2	A	750	HEM	C2D-C1D	-2.08	1.45	1.51
2	B	750	HEM	C3C-CAC	2.01	1.55	1.51
2	B	750	HEM	CAA-C2A	2.05	1.55	1.52
2	A	750	HEM	CMA-C3A	2.17	1.56	1.51
2	B	750	HEM	CMA-C3A	2.20	1.56	1.51
2	A	750	HEM	FE-NC	2.55	2.05	1.95
2	A	750	HEM	C1C-NC	2.56	1.39	1.36
2	B	750	HEM	FE-NC	2.65	2.06	1.95
2	B	750	HEM	FE-ND	2.65	2.11	1.97
2	A	750	HEM	FE-NB	2.68	2.11	1.97
2	A	750	HEM	FE-ND	3.25	2.14	1.97

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-5.78	102.17	112.53
4	B	800	J14	C31-C21-N11	-5.45	116.81	122.96
4	A	800	J14	C31-C21-N11	-4.27	118.14	122.96
2	B	750	HEM	C3C-CAC-CBC	-4.05	118.25	124.46
2	A	750	HEM	CBD-CAD-C3D	-3.75	102.64	113.55
3	A	760	H4B	N3-C2-N1	-3.69	119.48	125.53
2	B	750	HEM	CAA-C2A-C1A	-3.61	123.09	127.01
3	B	760	H4B	N3-C2-N1	-3.61	119.62	125.53
4	B	800	J14	C2'-C3'-N1	-3.37	104.84	111.90
2	B	750	HEM	CBD-CAD-C3D	-3.05	104.67	113.55
2	A	750	HEM	CAA-C2A-C1A	-2.88	123.89	127.01
2	B	750	HEM	C3B-CAB-CBB	-2.75	120.24	124.46
4	B	800	J14	C14-C13-C12	-2.24	120.46	123.35
2	A	750	HEM	C3C-CAC-CBC	-2.18	121.11	124.46
4	A	800	J14	C14-C13-C12	-2.06	120.69	123.35
2	A	750	HEM	C3B-C4B-NB	-2.03	107.75	111.63
4	B	800	J14	C3-N2-C2	2.15	120.95	113.35
3	B	760	H4B	N2-C2-N3	2.16	120.77	117.20
3	B	760	H4B	C4A-C8A-N8	2.30	121.14	118.43
4	A	800	J14	C3-N2-C2	2.41	121.88	113.35
3	A	760	H4B	N2-C2-N3	2.62	121.54	117.20
3	A	760	H4B	C4A-C8A-N8	2.65	121.55	118.43
3	A	760	H4B	C2-N1-C8A	2.72	120.65	114.54
3	B	760	H4B	C2-N1-C8A	2.76	120.73	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C3B-C4B-CHC	3.06	127.47	123.16
2	B	750	HEM	CMD-C2D-C3D	3.07	127.94	114.35
2	B	750	HEM	C2D-C3D-C4D	3.10	106.76	101.50
4	A	800	J14	C2-C1-N1	3.21	115.28	110.67
2	A	750	HEM	C2D-C3D-C4D	3.25	107.02	101.50
2	A	750	HEM	CMD-C2D-C3D	3.27	128.83	114.35
4	B	800	J14	C2-C1-N1	3.33	115.44	110.67
2	A	750	HEM	CAD-C3D-C4D	3.95	126.41	112.47
4	B	800	J14	C1-N1-C3'	3.97	119.88	113.89
2	A	750	HEM	C3B-C4B-CHC	4.06	128.87	123.16
3	B	760	H4B	C4-N3-C2	4.11	121.64	115.94
2	B	750	HEM	CMC-C2C-C3C	4.18	126.98	116.53
2	B	750	HEM	CAD-C3D-C4D	4.29	127.61	112.47
2	B	750	HEM	CAD-C3D-C2D	4.31	125.60	113.22
2	B	750	HEM	CMB-C2B-C3B	4.33	127.34	116.53
2	A	750	HEM	CMB-C2B-C3B	4.37	127.45	116.53
4	A	800	J14	C1-N1-C3'	4.38	120.49	113.89
3	A	760	H4B	C4-N3-C2	4.56	122.27	115.94
2	A	750	HEM	CAD-C3D-C2D	4.64	126.57	113.22
2	A	750	HEM	CMC-C2C-C3C	4.86	128.66	116.53
4	A	800	J14	C61-N11-C21	5.31	122.00	118.23
3	B	760	H4B	C4-C4A-C8A	5.32	119.37	114.56
3	A	760	H4B	C4-C4A-C8A	5.55	119.59	114.56
4	B	800	J14	C61-N11-C21	7.66	123.67	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	4	0
4	A	800	J14	8	0
2	B	750	HEM	9	0
4	B	800	J14	7	0

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	407/422 (96%)	1.42	118 (28%) ⓘ ⓘ	29, 57, 107, 139	0
1	B	411/422 (97%)	0.76	45 (10%) ⓘ ⓘ	29, 44, 68, 91	0
All	All	818/844 (96%)	1.09	163 (19%) ⓘ ⓘ	29, 49, 99, 139	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	9.1
1	B	300	PHE	7.4
1	A	488	PRO	7.2
1	B	350	THR	6.8
1	A	715	VAL	6.8
1	A	355	PHE	6.4
1	A	388	ILE	6.1
1	B	348	VAL	5.8
1	A	506	ILE	5.4
1	A	619	ARG	5.3
1	A	486	LYS	5.1
1	A	507	GLN	4.9
1	B	321	THR	4.9
1	A	390	SER	4.8
1	B	611	ALA	4.5
1	B	619	ARG	4.5
1	A	713	THR	4.3
1	A	351	LYS	4.3
1	A	389	GLU	4.3
1	A	490	GLY	4.3
1	A	479	LEU	4.2
1	A	352	ASP	4.1
1	B	352	ASP	4.1
1	A	508	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	714	HIS	4.0
1	A	469	LYS	4.0
1	A	493	LEU	3.9
1	B	677	VAL	3.9
1	A	470	HIS	3.9
1	B	351	LYS	3.8
1	A	553	TRP	3.8
1	A	491	SER	3.8
1	A	487	GLN	3.8
1	A	300	PHE	3.8
1	A	567	VAL	3.8
1	A	494	GLY	3.8
1	A	551	PHE	3.7
1	A	480	ILE	3.7
1	B	479	LEU	3.7
1	A	677	VAL	3.6
1	A	392	SER	3.6
1	A	509	GLY	3.5
1	B	567	VAL	3.5
1	A	678	TRP	3.5
1	A	492	THR	3.5
1	A	373	GLY	3.5
1	B	349	ALA	3.4
1	A	711	TRP	3.4
1	B	318	LEU	3.4
1	A	503	GLU	3.4
1	A	541	VAL	3.4
1	B	299	ARG	3.3
1	B	355	PHE	3.3
1	A	499	VAL	3.3
1	A	382	GLU	3.3
1	A	584	PHE	3.2
1	A	712	ASN	3.2
1	B	718	GLY	3.2
1	B	620	LYS	3.2
1	A	386	LYS	3.2
1	A	415	CYS	3.2
1	B	676	TRP	3.1
1	B	480	ILE	3.1
1	A	570	MET	3.1
1	A	679	ILE	3.0
1	A	511	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	3.0
1	A	528	GLY	3.0
1	A	485	TYR	3.0
1	B	310	VAL	3.0
1	A	566	ALA	3.0
1	A	582	CYS	3.0
1	A	442	ILE	3.0
1	A	593	ILE	3.0
1	B	553	TRP	2.9
1	A	416	VAL	2.9
1	B	564	LEU	2.9
1	A	369	ILE	2.9
1	B	442	ILE	2.9
1	A	612	LYS	2.9
1	B	566	ALA	2.9
1	A	510	TRP	2.9
1	A	676	TRP	2.9
1	B	680	VAL	2.8
1	A	391	THR	2.8
1	A	588	TYR	2.8
1	A	537	PRO	2.8
1	A	385	ASN	2.7
1	B	591	THR	2.7
1	A	591	THR	2.7
1	A	371	ARG	2.7
1	A	489	ASP	2.7
1	A	483	ALA	2.6
1	A	366	TYR	2.6
1	B	386	LYS	2.6
1	A	322	LEU	2.6
1	A	514	ARG	2.6
1	A	609	GLU	2.5
1	B	389	GLU	2.5
1	A	706	TYR	2.5
1	A	616	LEU	2.5
1	A	319	LYS	2.5
1	A	565	PRO	2.5
1	A	568	SER	2.5
1	A	517	PHE	2.5
1	A	564	LEU	2.5
1	A	682	PRO	2.5
1	A	446	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	590	GLY	2.4
1	A	533	LEU	2.4
1	B	568	SER	2.4
1	A	372	PHE	2.4
1	B	667	ARG	2.4
1	A	299	ARG	2.4
1	A	459	ILE	2.4
1	A	394	TYR	2.4
1	A	393	THR	2.4
1	B	679	ILE	2.3
1	B	615	ASP	2.3
1	B	493	LEU	2.3
1	A	519	VAL	2.3
1	A	555	LYS	2.3
1	B	588	TYR	2.3
1	A	691	PHE	2.3
1	A	540	LEU	2.3
1	B	565	PRO	2.3
1	B	391	THR	2.3
1	A	557	LEU	2.3
1	B	678	TRP	2.3
1	A	561	TRP	2.2
1	A	681	PRO	2.2
1	A	611	ALA	2.2
1	B	353	GLN	2.2
1	A	384	VAL	2.2
1	B	541	VAL	2.2
1	B	443	CYS	2.2
1	A	376	ALA	2.2
1	A	482	TYR	2.2
1	B	446	VAL	2.2
1	A	704	PHE	2.2
1	B	551	PHE	2.2
1	A	615	ASP	2.2
1	A	562	TYR	2.2
1	A	618	MET	2.2
1	B	329	HIS	2.1
1	A	667	ARG	2.1
1	A	370	LYS	2.1
1	A	550	LYS	2.1
1	A	542	LEU	2.1
1	A	586	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	520	LEU	2.1
1	A	685	GLY	2.1
1	A	585	SER	2.1
1	B	392	SER	2.1
1	A	423	LYS	2.1
1	A	581	ALA	2.1
1	A	378	MET	2.1
1	A	552	ASP	2.1
1	A	315	THR	2.1
1	B	550	LYS	2.0
1	A	504	ILE	2.0
1	A	318	LEU	2.0
1	A	536	ILE	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(\AA^2)	Q<0.9
4	J14	A	800	27/27	0.85	0.38	3.73	44,75,108,110	0
4	J14	B	800	27/27	0.84	0.30	3.56	51,73,84,85	0
5	ACT	A	860	4/4	0.94	0.18	2.26	63,65,65,65	0
2	HEM	A	750	43/43	0.97	0.21	0.42	32,36,54,56	0
3	H4B	B	760	17/17	0.95	0.19	0.35	36,38,41,41	0
2	HEM	B	750	43/43	0.97	0.16	0.21	31,35,51,55	0
3	H4B	A	760	17/17	0.96	0.18	0.11	37,41,45,46	0
6	ZN	A	900	1/1	0.99	0.12	-0.40	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.