



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:56 AM GMT

PDB ID : 3NLN
Title : Structure of neuronal nitric oxide synthase R349A mutant heme domain in complex with 6-{{(3'R,4'S)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
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Deposited on : 2010-06-21
Resolution : 2.00 Å(reported)

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

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

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

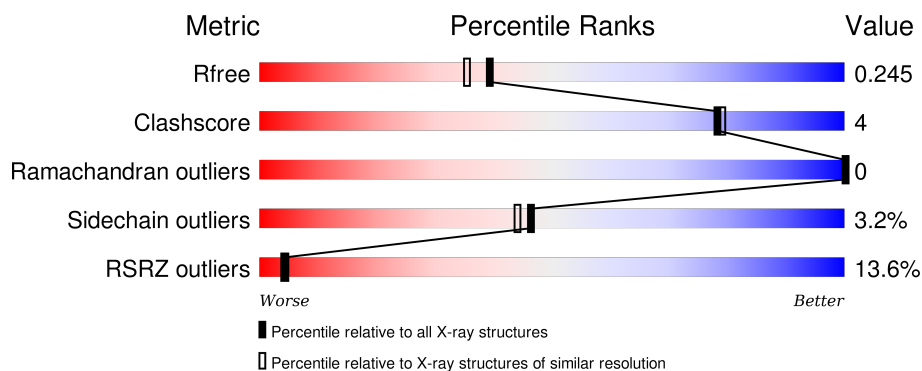
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 $\leq 5\%$. 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	
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	ACT	A	860	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7141 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
			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 MUTATION	UNP P29476
B	349	ALA	ARG	ENGINEERED MUTATION	UNP P29476

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



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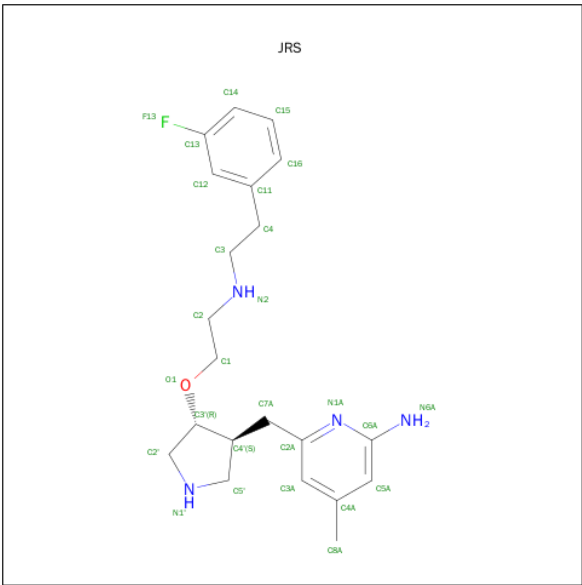
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



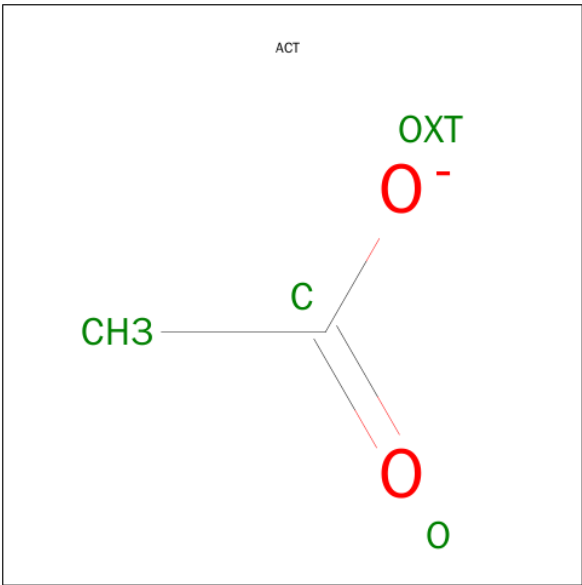
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[[[(3S,4R)-4-(2-[[2-(3-FLUOROPHENYL)ETHYL]AMINO}ETHOXY)PYRROLIDIN-3-YL]METHYL]-4-METHYLPYRIDIN-2-AMINE (three-letter code: JRS) (formula: $C_{21}H_{29}FN_4O$).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 123	O 123	0	0
7	B	183	Total 183	O 183	0	0

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 1.00). The x-axis lists amino acids. A bar chart at the top shows the percentage of each amino acid: 19% (red), 87% (green), 9% (yellow), and 2% (grey).
- | Amino Acid | Percentage |
|------------|------------|
| CYS | 19% |
| PRO | 19% |
| R299 | 19% |
| F300 | 19% |
| E307 | 19% |
| T308 | 19% |
| D309 | 19% |
| H317 | 19% |
| L318 | 19% |
| T321 | 19% |
| L322 | 19% |
| E328 | 19% |
| M332 | 19% |
| P338 | 19% |
| SER | 19% |
| GLN | 19% |
| HIS | 19% |
| THR | 19% |
| ARG | 19% |
| LYS | 19% |
| PRO | 19% |
| GLU | 19% |
| ASP | 19% |
| VAL | 19% |
| ALA | 19% |
| T350 | 19% |
| K351 | 19% |
| D352 | 19% |
| Q353 | 19% |
| L354 | 19% |
| F355 | 19% |
| P356 | 19% |
| R371 | 19% |
| F372 | 19% |
| G373 | 19% |
| R380 | 19% |
| E382 | 19% |
| N385 | 19% |
| K386 | 19% |
| E387 | 19% |
| I388 | 19% |
| E389 | 19% |
| S390 | 19% |
| T391 | 19% |
| S392 | 19% |
| T393 | 19% |
| Y394 | 19% |
| Y403 | 19% |
| H407 | 19% |
| A412 | 19% |
| C415 | 19% |
| V416 | 19% |
| F439 | 19% |
| C443 | 19% |
| N444 | 19% |
| H445 | 19% |
| N451 | 19% |
| N454 | 19% |
| L455 | 19% |
| I459 | 19% |
| Q464 | 19% |
| D467 | 19% |
| G468 | 19% |
| K469 | 19% |
| H470 | 19% |
| Q478 | 19% |
| L479 | 19% |
| I480 | 19% |
| R481 | 19% |
| K486 | 19% |
| Q487 | 19% |
| P488 | 19% |
| D489 | 19% |
| G490 | 19% |
| S491 | 19% |
| E503 | 19% |
| I506 | 19% |
| Q507 | 19% |
| Q508 | 19% |
| K511 | 19% |
| R514 | 19% |
| L523 | 19% |
| D530 | 19% |
| P531 | 19% |
| R547 | 19% |
| W553 | 19% |
| F554 | 19% |
| K555 | 19% |
| W561 | 19% |
| P565 | 19% |
| A566 | 19% |
| V567 | 19% |
| S568 | 19% |
| N569 | 19% |
| F579 | 19% |
| G582 | 19% |
| P583 | 19% |
| F584 | 19% |
| W587 | 19% |
| Y588 | 19% |
| T591 | 19% |
| E592 | 19% |
| I593 | 19% |
| G594 | 19% |
| V595 | 19% |
| A611 | 19% |
| K612 | 19% |
| D615 | 19% |
| L616 | 19% |
| D617 | 19% |
| M618 | 19% |
| R619 | 19% |
| K620 | 19% |
| L630 | 19% |
| V631 | 19% |
| Y639 | 19% |
| S643 | 19% |
| D644 | 19% |
| K645 | 19% |
| R667 | 19% |
| W676 | 19% |
| V677 | 19% |
| H678 | 19% |
| I679 | 19% |
| V680 | 19% |
| P681 | 19% |
| P682 | 19% |
| G685 | 19% |
| S686 | 19% |
| F691 | 19% |
| F704 | 19% |
| E705 | 19% |
| W706 | 19% |

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.95Å 112.19Å 164.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 2.00 38.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.20-2.00) 98.8 (38.67-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.225 0.208 , 0.245	Depositor DCC
R_{free} test set	3236 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.3	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 65124 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7141	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 3.72% 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, JRS, 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	0.67	0/3406	0.65	0/4621
1	B	0.71	0/3432	0.70	2/4654 (0.0%)
All	All	0.69	0/6838	0.67	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	B	418	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	430	ARG	NE-CZ-NH1	5.53	123.06	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	20	0
1	B	3339	0	3251	21	0
2	A	43	0	30	7	0
2	B	43	0	30	7	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	29	4	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	123	0	0	2	0
7	B	183	0	0	1	0
All	All	7141	0	6626	48	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 (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:HEM:O2D	4:A:800:JRS:H2	1.69	0.91
1:A:706:TYR:OH	2:A:750:HEM:O1D	1.89	0.90
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.93	0.86
2:B:750:HEM:O2D	4:B:800:JRS:H2	1.90	0.71
1:A:328:GLU:OE2	7:A:1049:HOH:O	2.09	0.70
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.77	0.67
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.79	0.65
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.78	0.65
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.79	0.64
2:B:750:HEM:HBA1	4:B:800:JRS:H7AA	1.80	0.61
1:B:706:TYR:CZ	4:B:800:JRS:H16	2.36	0.60
1:B:391:THR:O	1:B:392:SER:HB2	2.04	0.57
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.86	0.57
1:A:508:GLN:HA	1:A:508:GLN:HE21	1.70	0.55
2:A:750:HEM:HBA1	4:A:800:JRS:H7AA	1.89	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.37	0.55
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.90	0.53
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.91	0.53
1:A:299:ARG:O	1:A:317:HIS:CE1	2.62	0.52
1:A:350:THR:HG22	1:A:351:LYS:H	1.73	0.52
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.41	0.51
1:B:701:THR:HA	1:B:702:PRO:C	2.32	0.49
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.49	0.48
1:A:307:GLU:HG3	7:B:1045:HOH:O	2.14	0.48
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.61	0.47
2:A:750:HEM:HMC1	2:A:750:HEM:HBC2	1.97	0.47
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.50	0.46
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.99	0.45
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.99	0.44
1:B:337:LEU:HG	4:B:800:JRS:H15	2.00	0.44
1:A:451:ASN:HB3	1:A:454:ASN:O	2.18	0.44
1:B:595:VAL:O	1:B:599:CYS:HB2	2.18	0.44
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.53	0.43
1:B:325:GLY:O	1:B:332:MET:HG3	2.19	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.43
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.43
2:A:750:HEM:O2A	7:A:1083:HOH:O	2.21	0.42
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.42
1:A:299:ARG:HG3	1:A:318:LEU:HD11	2.01	0.42
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.56	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.14	0.41
1:B:386:LYS:O	1:B:389:GLU:HG2	2.21	0.41
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.36	0.40
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.40
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	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%)	395 (98%)	8 (2%)	0	100	100
1	B	407/422 (96%)	397 (98%)	10 (2%)	0	100	100
All	All	810/844 (96%)	792 (98%)	18 (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%)	350 (96%)	13 (4%)	42	39
1	B	365/376 (97%)	355 (97%)	10 (3%)	52	52
All	All	728/752 (97%)	705 (97%)	23 (3%)	46	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	390	SER
1	A	508	GLN
1	A	523	LEU
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	313	THR
1	B	321	THR
1	B	332	MET
1	B	353	GLN
1	B	360	GLU
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	620	LYS
1	B	653	SER

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	440	ASN
1	A	454	ASN
1	A	508	GLN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	385	ASN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	527	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	750	1	30,50,50	2.36	10 (33%)	24,82,82	2.51	12 (50%)
3	H4B	A	760	-	13,18,18	1.24	2 (15%)	11,26,26	2.89	6 (54%)
4	JRS	A	800	-	26,29,29	0.71	0	27,38,38	1.55	3 (11%)
5	ACT	A	860	-	1,3,3	1.30	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.05	8 (26%)	24,82,82	2.53	12 (50%)
3	H4B	B	760	-	13,18,18	0.93	0	11,26,26	2.76	4 (36%)
4	JRS	B	800	-	26,29,29	0.74	0	27,38,38	1.36	2 (7%)
5	ACT	B	860	-	1,3,3	1.33	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
4	JRS	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	JRS	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-7.39	1.42	1.51
2	B	750	HEM	C3D-C4D	-6.31	1.43	1.51
2	A	750	HEM	C3B-C4B	-6.25	1.46	1.51
2	B	750	HEM	C3B-C4B	-3.92	1.48	1.51
2	A	750	HEM	C2C-C1C	-3.46	1.46	1.52
2	B	750	HEM	C2C-C1C	-3.43	1.46	1.52
2	A	750	HEM	C2B-C1B	-2.31	1.44	1.51
2	A	750	HEM	C2D-C1D	-2.27	1.44	1.51
2	B	750	HEM	C2B-C1B	-2.12	1.44	1.51
2	B	750	HEM	C3C-CAC	2.04	1.55	1.51
2	A	750	HEM	CMA-C3A	2.17	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NC	2.20	2.04	1.95
2	B	750	HEM	FE-ND	2.30	2.09	1.97
3	A	760	H4B	C2-N2	2.51	1.39	1.34
2	A	750	HEM	FE-NB	2.53	2.10	1.97
2	A	750	HEM	FE-ND	2.58	2.11	1.97
3	A	760	H4B	C4-N3	2.58	1.37	1.33
2	A	750	HEM	C1C-NC	2.60	1.39	1.36
2	B	750	HEM	C1C-NC	2.87	1.39	1.36
2	B	750	HEM	FE-NC	3.17	2.08	1.95

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	N3-C2-N1	-4.24	118.59	125.53
2	B	750	HEM	C3C-CAC-CBC	-3.88	118.51	124.46
2	B	750	HEM	CBD-CAD-C3D	-3.86	102.33	113.55
4	A	800	JRS	C3A-C2A-N1A	-3.73	118.75	122.96
2	A	750	HEM	CBD-CAD-C3D	-3.69	102.81	113.55
4	B	800	JRS	C3A-C2A-N1A	-3.43	119.08	122.96
2	B	750	HEM	CAA-C2A-C1A	-3.39	123.32	127.01
2	A	750	HEM	CMA-C3A-C4A	-3.09	123.25	128.36
2	A	750	HEM	C3C-CAC-CBC	-3.07	119.75	124.46
4	A	800	JRS	C3-C4-C11	-2.93	106.75	112.83
3	B	760	H4B	N3-C2-N1	-2.66	121.18	125.53
2	B	750	HEM	C3B-C4B-NB	-2.16	107.50	111.63
2	A	750	HEM	C3B-C4B-NB	-2.13	107.55	111.63
2	A	750	HEM	CAA-C2A-C1A	-2.10	124.72	127.01
2	B	750	HEM	CAD-CBD-CGD	-2.06	104.63	113.02
2	B	750	HEM	C3B-C4B-CHC	2.53	126.72	123.16
3	A	760	H4B	C4A-C8A-N8	2.54	121.42	118.43
2	B	750	HEM	CMD-C2D-C3D	2.65	126.05	114.35
2	A	750	HEM	C2D-C3D-C4D	2.72	106.10	101.50
3	B	760	H4B	C4A-C8A-N8	2.87	121.81	118.43
3	A	760	H4B	C2-N1-C8A	2.89	121.03	114.54
2	A	750	HEM	CMD-C2D-C3D	3.10	128.06	114.35
2	B	750	HEM	C2D-C3D-C4D	3.24	106.99	101.50
2	A	750	HEM	C3B-C4B-CHC	3.34	127.87	123.16
3	A	760	H4B	N2-C2-N3	3.58	123.14	117.20
4	B	800	JRS	C6A-N1A-C2A	3.87	120.98	118.23
2	B	750	HEM	CAD-C3D-C2D	3.88	124.36	113.22
2	A	750	HEM	CMB-C2B-C3B	3.91	126.28	116.53
2	A	750	HEM	CAD-C3D-C4D	4.01	126.60	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CMB-C2B-C3B	4.07	126.69	116.53
2	B	750	HEM	CMC-C2C-C3C	4.18	126.95	116.53
2	A	750	HEM	CMC-C2C-C3C	4.29	127.24	116.53
3	A	760	H4B	C4-C4A-C8A	4.43	118.57	114.56
2	B	750	HEM	CAD-C3D-C4D	4.56	128.55	112.47
4	A	800	JRS	C6A-N1A-C2A	4.74	121.60	118.23
3	B	760	H4B	C4-N3-C2	4.77	122.56	115.94
2	A	750	HEM	CAD-C3D-C2D	4.89	127.28	113.22
3	A	760	H4B	C4-N3-C2	5.05	122.95	115.94
3	B	760	H4B	C4-C4A-C8A	6.17	120.14	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	7	0
4	A	800	JRS	2	0
2	B	750	HEM	7	0
4	B	800	JRS	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 ⓘ

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%)	1.00	80 (19%) 1 2	30, 56, 103, 131	0
1	B	411/422 (97%)	0.47	31 (7%) 17 18	30, 45, 71, 95	0
All	All	818/844 (96%)	0.73	111 (13%) 4 4	30, 50, 95, 131	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	6.9
1	B	350	THR	6.7
1	A	506	ILE	6.4
1	A	715	VAL	6.1
1	A	716	TRP	6.0
1	A	352	ASP	6.0
1	A	488	PRO	5.9
1	B	348	VAL	5.2
1	A	390	SER	5.1
1	A	355	PHE	4.8
1	A	388	ILE	4.8
1	A	487	GLN	4.8
1	A	350	THR	4.7
1	A	389	GLU	4.6
1	A	486	LYS	4.4
1	B	619	ARG	4.4
1	A	351	LYS	4.4
1	A	619	ARG	4.3
1	B	299	ARG	4.3
1	A	393	THR	4.2
1	B	667	ARG	4.2
1	A	470	HIS	4.1
1	A	507	GLN	4.0
1	A	567	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	3.9
1	A	713	THR	3.8
1	A	489	ASP	3.7
1	A	322	LEU	3.7
1	B	351	LYS	3.6
1	B	591	THR	3.6
1	B	321	THR	3.5
1	B	620	LYS	3.5
1	A	615	ASP	3.4
1	A	591	THR	3.4
1	A	300	PHE	3.4
1	A	391	THR	3.4
1	B	389	GLU	3.4
1	A	612	LYS	3.3
1	B	680	VAL	3.2
1	B	567	VAL	3.1
1	B	677	VAL	3.1
1	A	490	GLY	3.1
1	A	682	PRO	3.1
1	A	685	GLY	3.1
1	A	503	GLU	3.1
1	A	354	LEU	3.0
1	A	415	CYS	3.0
1	A	491	SER	3.0
1	A	714	HIS	3.0
1	A	678	TRP	2.9
1	A	679	ILE	2.9
1	B	310	VAL	2.9
1	A	299	ARG	2.9
1	A	677	VAL	2.9
1	A	479	LEU	2.9
1	A	712	ASN	2.8
1	A	582	CYS	2.8
1	A	416	VAL	2.8
1	A	459	ILE	2.7
1	B	301	LEU	2.7
1	A	584	PHE	2.7
1	B	352	ASP	2.6
1	B	678	TRP	2.6
1	B	679	ILE	2.6
1	A	511	LYS	2.6
1	A	514	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	676	TRP	2.6
1	A	711	TRP	2.6
1	A	392	SER	2.5
1	A	394	TYR	2.5
1	A	385	ASN	2.5
1	A	553	TRP	2.5
1	B	329	HIS	2.5
1	A	566	ALA	2.5
1	A	338	PRO	2.5
1	A	593	ILE	2.5
1	A	667	ARG	2.5
1	A	356	PRO	2.5
1	A	680	VAL	2.4
1	B	611	ALA	2.4
1	A	469	LYS	2.4
1	B	676	TRP	2.4
1	A	565	PRO	2.3
1	B	479	LEU	2.3
1	A	382	GLU	2.3
1	B	302	LYS	2.3
1	A	595	VAL	2.3
1	A	386	LYS	2.3
1	A	639	TYR	2.3
1	B	684	SER	2.3
1	B	615	ASP	2.3
1	B	691	PHE	2.3
1	B	565	PRO	2.2
1	A	480	ILE	2.2
1	A	568	SER	2.2
1	A	588	TYR	2.2
1	A	373	GLY	2.2
1	B	718	GLY	2.2
1	A	467	ASP	2.1
1	A	328	GLU	2.1
1	A	530	ASP	2.1
1	A	561	TRP	2.1
1	A	704	PHE	2.1
1	A	643	SER	2.1
1	A	630	LEU	2.1
1	A	412	ALA	2.1
1	B	713	THR	2.1
1	A	617	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	682	PRO	2.1
1	A	318	LEU	2.0
1	A	611	ALA	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	ACT	A	860	4/4	0.95	0.19	2.87	65,66,67,68	0
4	JRS	A	800	27/27	0.87	0.27	1.28	35,49,75,79	0
4	JRS	B	800	27/27	0.90	0.22	1.02	37,48,61,70	0
3	H4B	A	760	17/17	0.96	0.21	0.75	36,38,43,45	0
2	HEM	A	750	43/43	0.97	0.22	0.71	29,35,52,61	0
3	H4B	B	760	17/17	0.97	0.20	0.59	34,36,38,41	0
2	HEM	B	750	43/43	0.97	0.17	0.44	31,35,51,56	0
5	ACT	B	860	4/4	0.98	0.14	0.25	63,63,64,65	0
6	ZN	A	900	1/1	0.99	0.08	-1.07	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.