



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:01 AM UTC

PDB ID : 1M9R / pdb_00001m9r
Title : human endothelial nitric oxide synthase with 3-Bromo-7-Nitroindazole bound
Authors : Rosenfeld, R.J.; Garcin, E.D.; Panda, K.; Andersson, G.; Aberg, A.; Wallace, A.V.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2002-07-29
Resolution : 2.56 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

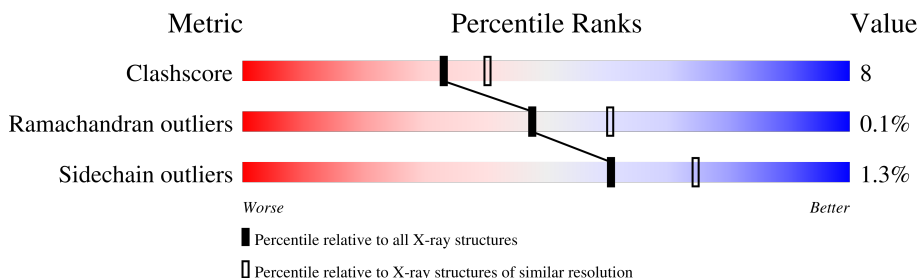
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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))
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

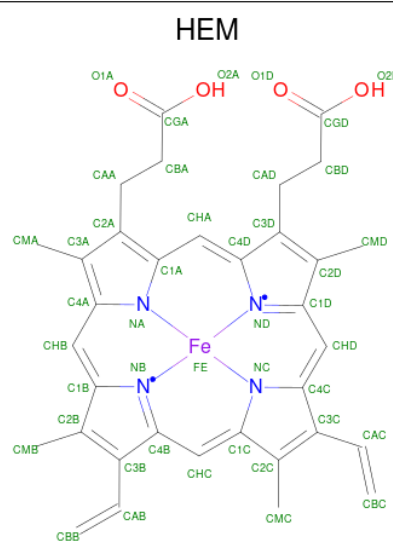
Mol	Chain	Length	Quality of chain
1	A	415	
1	B	415	

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 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- $$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$



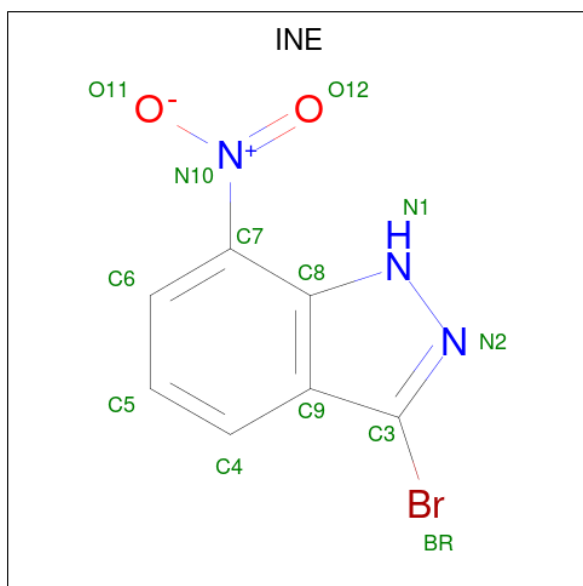
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 4 is 3-BROMO-7-NITROINDAZOLE (CCD ID: INE) (formula: $C_7H_4BrN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 13	Br 1	C 7	N 3	O 2	0	0
4	A	1	Total 13	Br 1	C 7	N 3	O 2	0	0
4	B	1	Total 13	Br 1	C 7	N 3	O 2	0	0
4	B	1	Total 13	Br 1	C 7	N 3	O 2	0	0

- Molecule 5 is water.

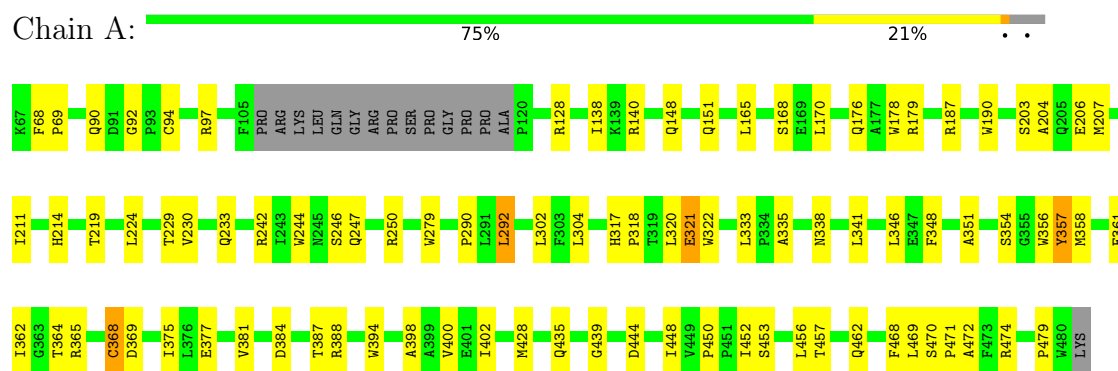
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 95 95	0	0
5	B	77	Total O 77 77	0	0

3 Residue-property plots

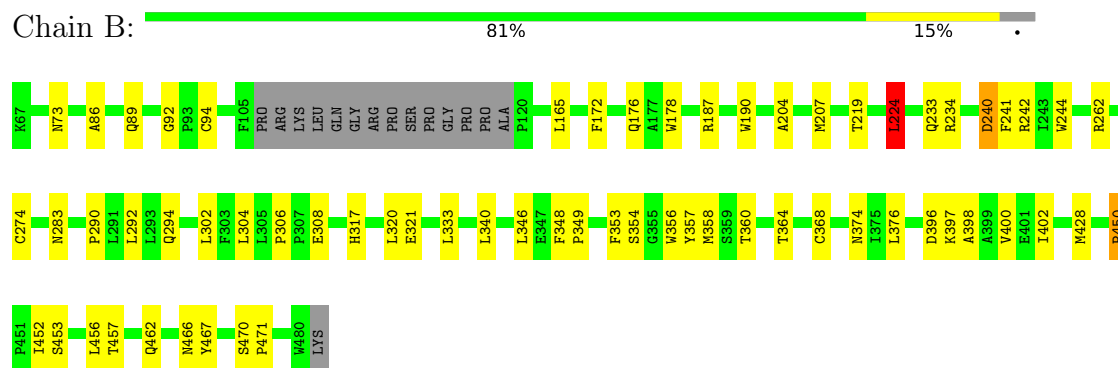
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: endothelial Nitric-oxide synthase



- Molecule 1: endothelial Nitric-oxide synthase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.62Å 90.28Å 155.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 2.56	Depositor
% Data completeness (in resolution range)	95.5 (29.65-2.56)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: INE, ZN, HEM

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	0.55	0/3275	0.91	5/4464 (0.1%)
1	B	0.54	0/3275	0.91	8/4464 (0.2%)
All	All	0.54	0/6550	0.91	13/8928 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	PRO	CA-C-N	7.09	126.77	119.82
1	B	450	PRO	C-N-CA	7.09	126.77	119.82
1	A	333	LEU	N-CA-C	6.04	119.28	108.47
1	A	357	TYR	N-CA-C	5.86	119.15	110.48
1	B	224	LEU	N-CA-C	5.62	118.00	110.35
1	B	357	TYR	N-CA-C	5.60	118.40	110.50
1	A	368	CYS	N-CA-C	5.46	120.09	113.38
1	B	92	GLY	CA-C-N	5.42	125.89	120.04
1	B	92	GLY	C-N-CA	5.42	125.89	120.04
1	B	187	ARG	N-CA-C	5.42	119.37	112.87
1	A	92	GLY	CA-C-N	5.22	124.91	119.64
1	A	92	GLY	C-N-CA	5.22	124.91	119.64
1	B	333	LEU	N-CA-C	5.14	117.95	108.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3184	0	3081	56	0
1	B	3184	0	3081	45	0
2	A	1	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	26	0	8	2	0
4	B	26	0	8	4	0
5	A	95	0	0	3	0
5	B	77	0	0	3	0
All	All	6679	0	6238	99	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 (99) 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:365:ARG:HH22	4:B:902:INE:H41	1.41	0.85
1:A:365:ARG:NH2	4:B:902:INE:H41	1.92	0.84
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.66	0.78
1:B:244:TRP:HE1	1:B:294:GLN:NE2	1.80	0.78
1:B:73:ASN:HD22	1:B:462:GLN:NE2	1.89	0.69
1:B:207:MET:HE2	1:B:241:PHE:HD2	1.58	0.69
1:A:400:VAL:HG11	1:B:397:LYS:HG3	1.77	0.67
1:A:128:ARG:HD2	5:A:726:HOH:O	1.96	0.64
1:A:361:GLU:HG3	4:A:906:INE:O11	1.97	0.64
1:A:428:MET:HE1	1:A:462:GLN:HE21	1.62	0.64
1:B:466:ASN:HD22	1:B:467:TYR:N	1.96	0.64
1:B:292:LEU:HD13	1:B:302:LEU:HD23	1.80	0.62
1:A:292:LEU:HD13	1:A:302:LEU:HD23	1.81	0.61
1:A:341:LEU:HB3	1:A:348:PHE:HB2	1.83	0.60
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.42	0.59
1:B:73:ASN:HD22	1:B:462:GLN:HE21	1.48	0.59
1:B:244:TRP:HE1	1:B:294:GLN:HE21	1.47	0.57
1:A:219:THR:HA	1:A:224:LEU:HD22	1.85	0.57
1:B:207:MET:HE2	1:B:241:PHE:CD2	2.40	0.57
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.86	0.57
1:A:304:LEU:HD23	5:A:661:HOH:O	2.06	0.56
1:B:428:MET:HE1	1:B:462:GLN:HE21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ALA:HB2	1:A:354:SER:HB3	1.88	0.56
1:A:148:GLN:O	1:A:151:GLN:HG2	2.05	0.55
1:A:138:ILE:O	1:A:140:ARG:HG2	2.07	0.55
1:A:470:SER:HA	1:A:471:PRO:C	2.33	0.54
1:B:358:MET:HE3	1:B:360:THR:OG1	2.08	0.54
1:A:320:LEU:HD13	1:A:322:TRP:CZ2	2.43	0.53
1:B:204:ALA:HA	1:B:207:MET:HE3	1.91	0.53
1:A:94:CYS:HB3	1:B:94:CYS:HB3	1.90	0.53
1:A:90:GLN:HB3	1:A:468:PHE:CD2	2.44	0.52
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.44	0.52
3:B:901:HEM:HMC2	3:B:901:HEM:HBC2	1.91	0.52
1:B:244:TRP:HB2	1:B:292:LEU:HB3	1.91	0.51
1:B:262:ARG:HD3	1:B:283:ASN:O	2.10	0.51
1:A:290:PRO:HB3	1:A:304:LEU:HD23	1.93	0.50
1:A:204:ALA:HA	1:A:207:MET:HE3	1.93	0.50
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.46	0.50
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.27	0.50
1:B:234:ARG:HG3	1:B:240:ASP:OD1	2.12	0.49
1:B:306:PRO:HB3	1:B:308:GLU:OE2	2.13	0.49
1:A:377:GLU:O	1:A:381:VAL:HG23	2.12	0.49
1:B:317:HIS:HB3	1:B:320:LEU:HB2	1.95	0.49
1:A:398:ALA:O	1:A:402:ILE:HG13	2.12	0.49
1:A:335:ALA:CB	1:A:354:SER:HB3	2.42	0.48
1:A:165:LEU:HG	1:A:346:LEU:HD12	1.96	0.48
1:A:279:TRP:HB2	1:A:302:LEU:HD13	1.95	0.48
1:B:219:THR:HA	1:B:224:LEU:HD22	1.96	0.48
1:A:247:GLN:HB2	1:A:250:ARG:CG	2.44	0.48
1:B:354:SER:HA	4:B:907:INE:BR	2.68	0.47
1:B:240:ASP:HB3	5:B:519:HOH:O	2.13	0.47
1:A:229:THR:O	1:A:351:ALA:HA	2.14	0.47
1:B:470:SER:HA	1:B:471:PRO:C	2.40	0.47
1:A:211:ILE:O	1:A:214:HIS:HB3	2.14	0.46
1:A:354:SER:HA	4:A:906:INE:BR	2.70	0.46
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.97	0.46
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.50	0.46
1:A:203:SER:OG	1:A:206:GLU:HG3	2.16	0.46
1:B:292:LEU:HD13	1:B:302:LEU:CD2	2.45	0.46
1:B:450:PRO:HG3	1:B:457:THR:HG21	1.98	0.46
1:A:469:LEU:O	1:A:472:ALA:HB2	2.16	0.45
3:A:901:HEM:HMC2	3:A:901:HEM:HBC2	1.98	0.45
1:B:396:ASP:O	1:B:400:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TRP:HB2	1:A:292:LEU:HB3	1.99	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.52	0.45
1:A:246:SER:HA	1:A:338:ASN:HB3	1.99	0.44
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.44
1:B:165:LEU:HG	1:B:346:LEU:HD12	2.00	0.44
1:B:374:ASN:ND2	5:B:707:HOH:O	2.51	0.44
1:A:304:LEU:CD2	5:A:661:HOH:O	2.64	0.44
1:A:97:ARG:HE	1:B:86:ALA:HA	1.83	0.43
1:B:376:LEU:HB2	5:B:606:HOH:O	2.18	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.18	0.43
1:A:356:TRP:H	3:A:901:HEM:HAB	1.82	0.43
1:A:170:LEU:HD11	1:A:230:VAL:HG21	2.01	0.43
1:B:364:THR:HG21	1:B:452:ILE:HG23	2.00	0.43
1:A:435:GLN:O	1:A:439:GLY:HA2	2.18	0.43
1:B:398:ALA:O	1:B:402:ILE:HG13	2.19	0.43
1:B:466:ASN:HD22	1:B:466:ASN:C	2.24	0.43
1:B:242:ARG:HD3	1:B:349:PRO:HB3	2.01	0.43
1:A:450:PRO:HG3	1:A:457:THR:HG21	2.00	0.42
1:A:388:ARG:HB2	1:A:388:ARG:NH1	2.33	0.42
1:A:321:GLU:CD	1:A:321:GLU:H	2.27	0.42
1:A:400:VAL:CG1	1:B:397:LYS:HG3	2.49	0.42
1:B:178:TRP:CZ3	1:B:190:TRP:HA	2.55	0.42
1:B:340:LEU:C	1:B:340:LEU:HD23	2.45	0.42
1:B:356:TRP:H	3:B:901:HEM:HAB	1.85	0.42
1:B:353:PHE:HD1	4:B:907:INE:BR	2.58	0.41
1:B:172:PHE:O	1:B:176:GLN:HG2	2.20	0.41
1:A:365:ARG:NH1	1:A:369:ASP:OD2	2.53	0.41
1:A:375:ILE:HD11	1:A:402:ILE:HD13	2.02	0.41
1:B:274:CYS:SG	1:B:290:PRO:HG2	2.61	0.41
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.89	0.40
1:A:444:ASP:O	1:A:448:ILE:HG12	2.21	0.40
1:B:290:PRO:HB3	1:B:304:LEU:HD23	2.03	0.40
1:A:387:THR:HA	1:A:394:TRP:CD1	2.56	0.40
1:A:187:ARG:O	1:A:190:TRP:HD1	2.03	0.40
1:A:176:GLN:HE22	1:A:179:ARG:HH11	1.70	0.40
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.56	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	396/415 (95%)	380 (96%)	16 (4%)	0	100	100
1	B	396/415 (95%)	376 (95%)	19 (5%)	1 (0%)	36	44
All	All	792/830 (95%)	756 (96%)	35 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	GLN

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	337/352 (96%)	331 (98%)	6 (2%)	51	67
1	B	337/352 (96%)	334 (99%)	3 (1%)	70	80
All	All	674/704 (96%)	665 (99%)	9 (1%)	61	74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	SER
1	A	292	LEU
1	A	321	GLU
1	A	358	MET
1	A	384	ASP

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Mol	Chain	Res	Type
1	A	474	ARG
1	B	224	LEU
1	B	240	ASP
1	B	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	176	GLN
1	A	205	GLN
1	A	233	GLN
1	A	277	HIS
1	A	294	GLN
1	A	403	ASN
1	A	462	GLN
1	A	466	ASN
1	B	133	GLN
1	B	148	GLN
1	B	151	GLN
1	B	233	GLN
1	B	277	HIS
1	B	294	GLN
1	B	462	GLN
1	B	466	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	INE	B	907	-	14,14,14	2.56	3 (21%)	11,20,20	2.56	4 (36%)
4	INE	B	902	-	14,14,14	2.85	4 (28%)	11,20,20	3.00	4 (36%)
3	HEM	A	901	1	50,50,50	1.69	9 (18%)	67,82,82	1.10	2 (2%)
4	INE	A	903	-	14,14,14	2.83	5 (35%)	11,20,20	2.84	4 (36%)
4	INE	A	906	-	14,14,14	2.66	4 (28%)	11,20,20	2.21	4 (36%)
3	HEM	B	901	1	50,50,50	1.64	8 (16%)	67,82,82	1.00	3 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	INE	B	907	-	-	0/2/4/4	0/2/2/2
4	INE	B	902	-	-	0/2/4/4	0/2/2/2
3	HEM	A	901	1	-	7/14/54/54	-
4	INE	A	903	-	-	0/2/4/4	0/2/2/2
4	INE	A	906	-	-	0/2/4/4	0/2/2/2
3	HEM	B	901	1	-	7/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	INE	BR-C3	-8.89	1.75	1.87
4	A	903	INE	BR-C3	-8.75	1.75	1.87
4	B	907	INE	BR-C3	-8.17	1.76	1.87
4	A	906	INE	BR-C3	-8.12	1.76	1.87
3	A	901	HEM	FE-NB	4.38	2.08	1.94
3	B	901	HEM	FE-NC	4.27	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	HEM	FE-NA	4.25	2.09	1.95
3	A	901	HEM	C4D-ND	-4.03	1.33	1.40
3	A	901	HEM	FE-ND	3.92	2.07	1.94
3	B	901	HEM	FE-NB	3.76	2.06	1.94
3	B	901	HEM	CAC-C3C	-3.54	1.37	1.47
4	B	902	INE	C8-N1	3.53	1.38	1.36
3	B	901	HEM	FE-ND	3.35	2.05	1.94
3	A	901	HEM	FE-NC	3.31	2.06	1.95
3	A	901	HEM	CAB-C3B	-3.25	1.38	1.47
4	A	906	INE	C8-C7	-3.07	1.36	1.42
3	A	901	HEM	FE-NA	3.01	2.05	1.95
4	A	906	INE	C5-C4	2.84	1.43	1.38
3	B	901	HEM	CAB-C3B	-2.82	1.39	1.47
4	A	903	INE	C8-N1	2.73	1.38	1.36
4	B	907	INE	C5-C4	2.63	1.43	1.38
4	B	902	INE	C4-C9	-2.60	1.36	1.39
3	A	901	HEM	C1D-C2D	-2.59	1.39	1.44
3	A	901	HEM	C1A-NA	-2.52	1.34	1.39
4	A	903	INE	C8-C7	-2.47	1.37	1.42
4	B	907	INE	C8-C7	-2.44	1.37	1.42
3	B	901	HEM	CMB-C2B	2.38	1.55	1.50
3	A	901	HEM	CAC-C3C	-2.38	1.41	1.47
4	A	906	INE	C3-N2	2.32	1.37	1.32
4	A	903	INE	C4-C9	-2.17	1.36	1.39
4	A	903	INE	C7-N10	-2.11	1.41	1.45
3	B	901	HEM	C4D-ND	-2.10	1.36	1.40
4	B	902	INE	C8-C7	-2.02	1.38	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	INE	C9-C8-N1	-6.86	103.63	106.95
4	A	903	INE	C9-C8-N1	-6.24	103.93	106.95
4	B	907	INE	C9-C8-N1	-5.22	104.43	106.95
4	A	906	INE	BR-C3-N2	5.18	127.20	119.74
4	B	907	INE	BR-C3-N2	5.09	127.07	119.74
4	B	902	INE	BR-C3-N2	4.91	126.81	119.74
4	A	903	INE	BR-C3-N2	4.57	126.32	119.74
4	A	903	INE	C3-N2-N1	4.16	111.17	106.27
4	B	902	INE	C3-N2-N1	4.10	111.10	106.27
3	A	901	HEM	CBD-CAD-C3D	-3.85	101.88	112.53
4	A	906	INE	C9-C8-N1	-3.23	105.39	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	INE	C3-N2-N1	3.06	109.87	106.27
4	A	903	INE	O12-N10-C7	-2.87	114.12	119.03
4	B	902	INE	O12-N10-C7	-2.83	114.18	119.03
3	B	901	HEM	CAD-C3D-C4D	2.66	129.33	124.70
4	A	906	INE	C3-N2-N1	2.45	109.16	106.27
3	A	901	HEM	CAA-C2A-C1A	2.32	129.47	124.94
3	B	901	HEM	CMB-C2B-C1B	2.28	128.60	125.03
3	B	901	HEM	CHD-C1D-C2D	-2.27	121.44	125.03
4	A	906	INE	O12-N10-C7	-2.26	115.16	119.03
4	B	907	INE	O12-N10-C7	-2.03	115.55	119.03

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	HEM	C2B-C3B-CAB-CBB
3	B	901	HEM	C4B-C3B-CAB-CBB
3	B	901	HEM	C3D-CAD-CBD-CGD
3	A	901	HEM	C2A-CAA-CBA-CGA
3	A	901	HEM	C2B-C3B-CAB-CBB
3	A	901	HEM	C4B-C3B-CAB-CBB
3	B	901	HEM	CAD-CBD-CGD-O1D
3	A	901	HEM	CAD-CBD-CGD-O1D
3	B	901	HEM	CAD-CBD-CGD-O2D
3	A	901	HEM	CAD-CBD-CGD-O2D
3	B	901	HEM	CAA-CBA-CGA-O1A
3	B	901	HEM	CAA-CBA-CGA-O2A
3	A	901	HEM	CAA-CBA-CGA-O2A
3	A	901	HEM	CAA-CBA-CGA-O1A

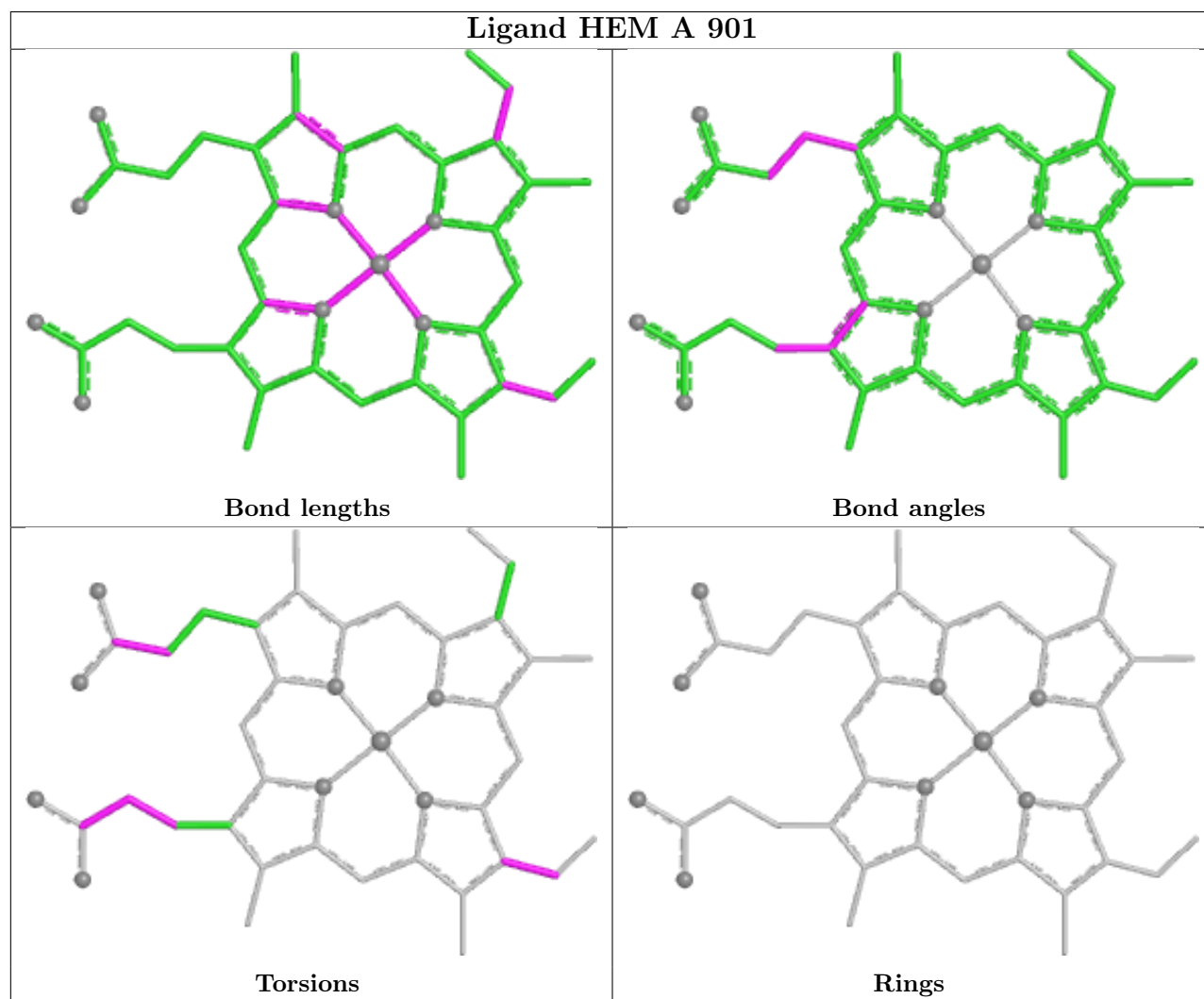
There are no ring outliers.

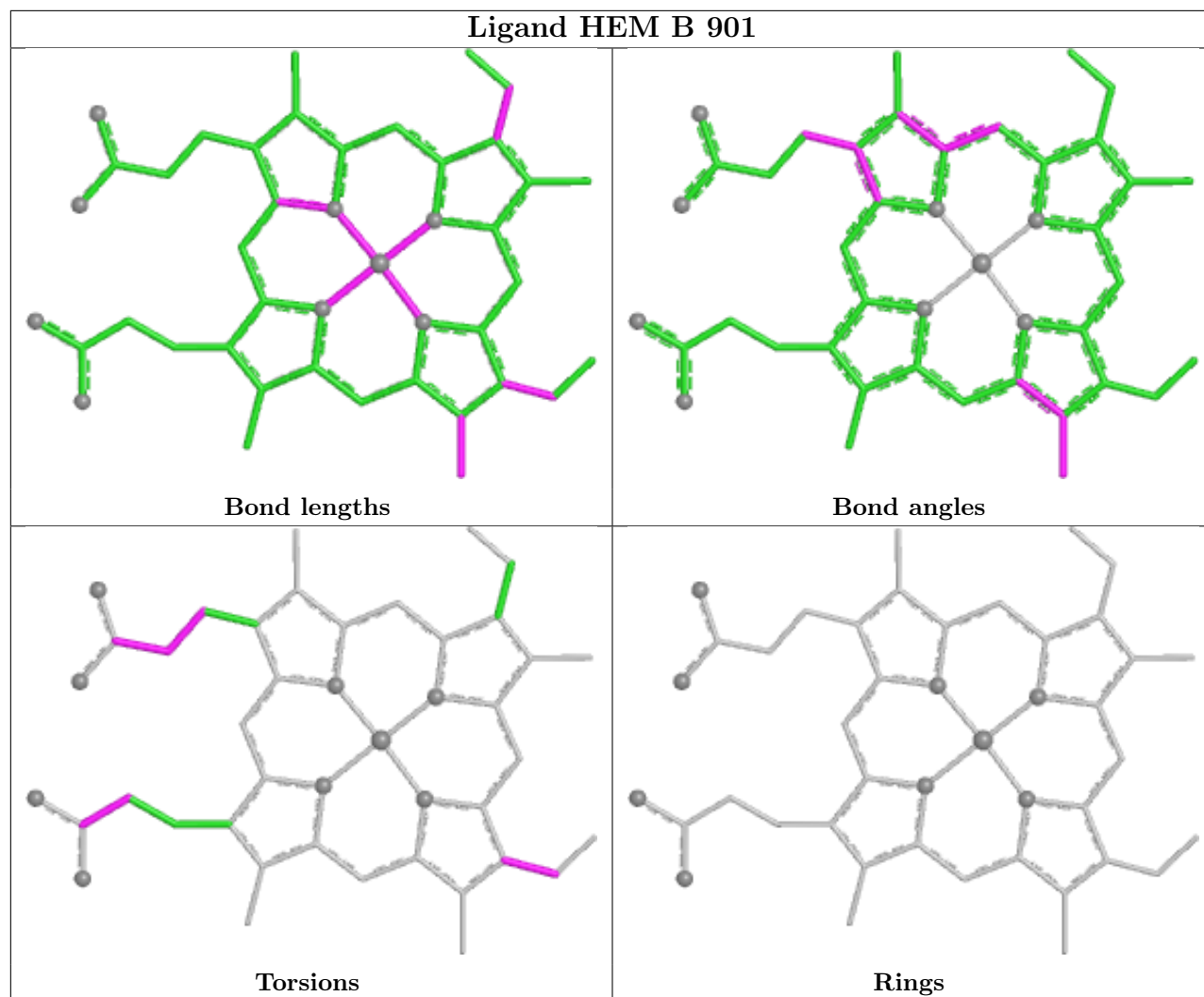
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	907	INE	2	0
4	B	902	INE	2	0
3	A	901	HEM	2	0
4	A	906	INE	2	0
3	B	901	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.