



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:30 AM UTC

PDB ID : 4JS9 / pdb_00004js9
Title : Structural Characterization of Inducible Nitric Oxide Synthase Substituted With Mesoheme
Authors : Hannibal, L.; Page, R.C.; Bolisetty, K.; Yu, Z.; Misra, S.; Stuehr, D.J.
Deposited on : 2013-03-22
Resolution : 2.78 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

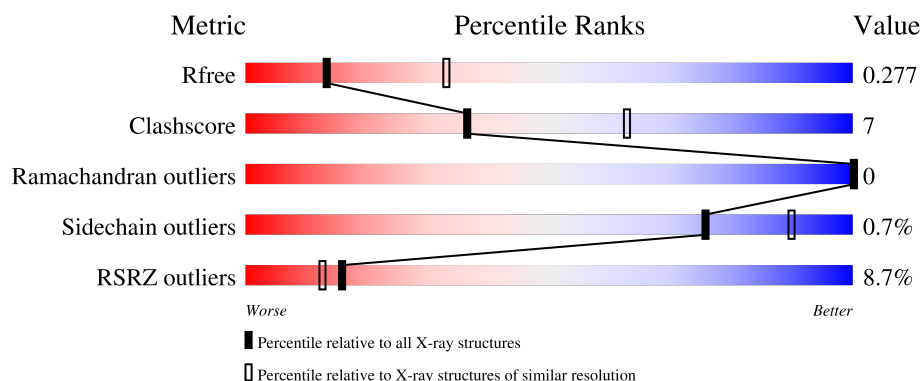
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 $\leq 5\%$. 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	431	9% 80% 14% 6%
1	B	431	7% 77% 16% 7%



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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

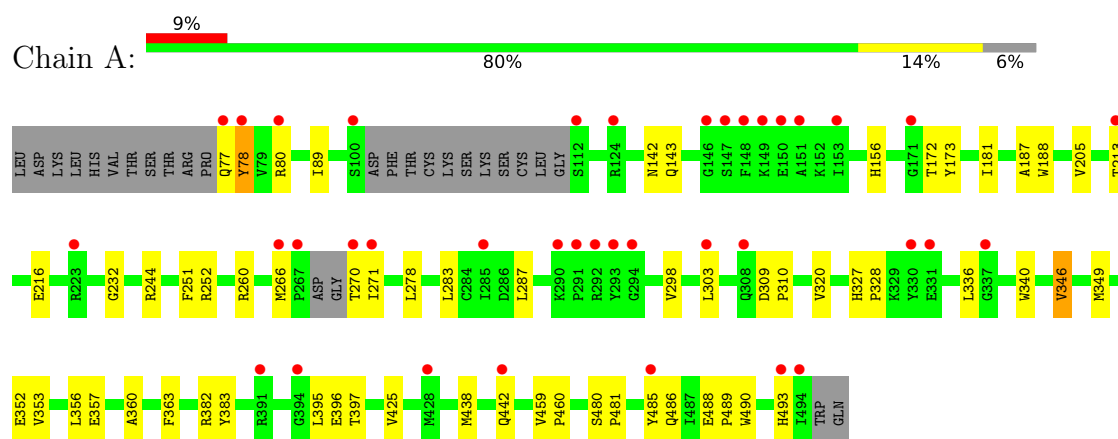
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	76	Total 76	O 76	0	0

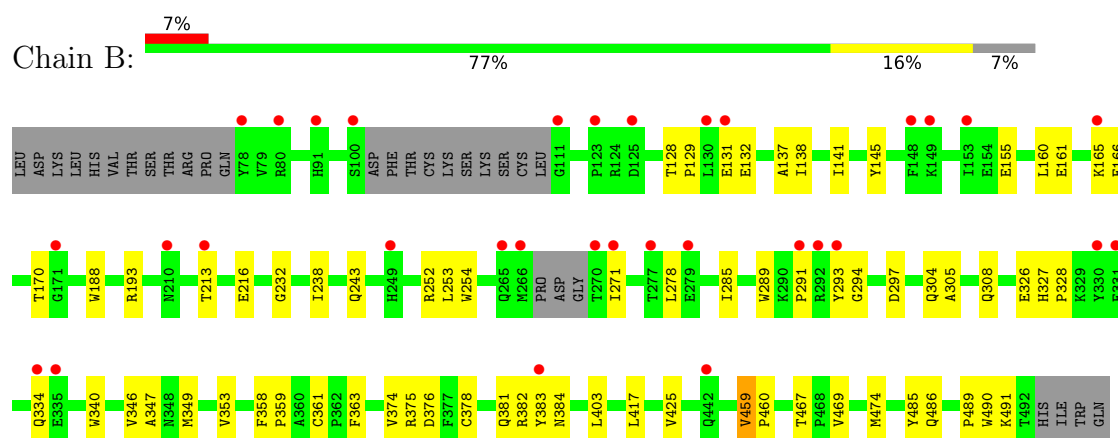
3 Residue-property plots

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 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, inducible



- Molecule 1: Nitric oxide synthase, inducible



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	215.04Å 215.04Å 115.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.78 49.09 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.09-2.78) 99.0 (49.09-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.250 , 0.290 (Not available) , 0.277	Depositor DCC
R_{free} test set	1974 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6836	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, MH0, SO4

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	0.62	1/3373 (0.0%)	0.91	3/4591 (0.1%)
1	B	0.60	0/3362	0.92	2/4569 (0.0%)
All	All	0.61	1/6735 (0.0%)	0.92	5/9160 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	VAL	CA-CB	5.17	1.60	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLN	N-CA-C	-5.54	105.14	111.07
1	A	78	TYR	N-CA-C	5.19	116.08	107.73
1	A	336	LEU	N-CA-C	-5.12	106.29	112.54
1	B	459	VAL	CA-C-N	5.09	123.38	119.66
1	B	459	VAL	C-N-CA	5.09	123.38	119.66

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	3278	0	3150	43	0
1	B	3269	0	3170	47	0
2	A	43	0	34	7	0
2	B	43	0	34	7	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	5	0	0	0	0
5	A	88	0	0	1	0
5	B	76	0	0	0	0
All	All	6836	0	6418	94	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 7.

All (94) 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:188:TRP:HB2	2:B:900:MH0:H28	1.52	0.91
2:B:900:MH0:H27	2:B:900:MH0:H21	1.56	0.86
1:A:188:TRP:HB2	2:A:501:MH0:H28	1.69	0.73
1:B:188:TRP:CB	2:B:900:MH0:H28	2.18	0.72
1:A:188:TRP:CG	2:A:501:MH0:H28	2.26	0.70
1:B:326:GLU:HG2	1:B:334:GLN:HG2	1.71	0.70
1:B:376:ASP:OD1	1:B:382:ARG:NH1	2.26	0.69
1:B:188:TRP:CG	2:B:900:MH0:H28	2.28	0.69
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.75	0.67
1:B:469:VAL:HG13	1:B:474:MET:HE1	1.78	0.65
1:B:285:ILE:HG12	1:B:291:PRO:HG3	1.80	0.63
1:A:252:ARG:HH21	1:A:489:PRO:HG3	1.64	0.62
1:B:188:TRP:HB2	2:B:900:MH0:CBC	2.29	0.62
1:A:188:TRP:CB	2:A:501:MH0:H28	2.30	0.62
1:B:166:GLU:O	1:B:170:THR:HG22	1.99	0.62
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.63	0.61
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.82	0.61
1:A:77:GLN:HG3	1:A:78:TYR:H	1.66	0.60
1:B:381:GLN:HG2	1:B:382:ARG:HG3	1.83	0.60
1:A:382:ARG:O	1:A:383:TYR:HB2	2.03	0.58
1:A:142:ASN:OD1	1:A:156:HIS:NE2	2.30	0.58
1:B:131:GLU:HA	1:B:131:GLU:OE1	2.04	0.57
1:B:460:PRO:HG2	1:B:467:THR:HG21	1.85	0.56
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.88	0.56
1:A:80:ARG:HE	1:A:89:ILE:HG21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CE1	1:A:356:LEU:HD11	2.41	0.55
1:A:187:ALA:HB2	1:A:481:PRO:HB2	1.89	0.54
1:B:382:ARG:O	1:B:384:ASN:N	2.40	0.53
1:A:363:PHE:CD1	2:A:501:MH0:H25	2.43	0.53
1:B:129:PRO:HB2	1:B:132:GLU:HG3	1.91	0.53
1:A:77:GLN:O	1:A:78:TYR:HB3	2.08	0.53
1:A:260:ARG:HH21	1:A:382:ARG:NH2	2.07	0.53
1:A:438:MET:O	1:A:442:GLN:HG2	2.08	0.52
2:A:501:MH0:CMC	2:A:501:MH0:H27	2.39	0.52
1:B:490:TRP:CD1	1:B:491:LYS:HD3	2.45	0.52
1:B:213:THR:CG2	1:B:216:GLU:HG3	2.40	0.52
1:B:193:ARG:NH1	1:B:485:TYR:OH	2.44	0.50
1:B:349:MET:C	1:B:486:GLN:HE21	2.19	0.50
1:B:291:PRO:HB2	1:B:293:TYR:CE2	2.46	0.50
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.26	0.50
1:B:161:GLU:HG2	1:B:165:LYS:HZ2	1.77	0.49
1:A:77:GLN:CG	1:A:78:TYR:H	2.25	0.49
1:A:352:GLU:OE1	1:A:480:SER:OG	2.24	0.49
1:A:80:ARG:NE	1:A:89:ILE:HG21	2.27	0.48
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.29	0.48
1:A:213:THR:CG2	1:A:216:GLU:HG3	2.44	0.48
1:A:349:MET:HE3	1:A:485:TYR:CD1	2.50	0.47
1:B:326:GLU:HG2	1:B:334:GLN:CG	2.42	0.47
2:A:501:MH0:H27	2:A:501:MH0:H23	1.97	0.47
1:A:303:LEU:O	1:A:310:PRO:HA	2.15	0.47
1:A:356:LEU:HD12	1:A:356:LEU:N	2.30	0.47
1:B:137:ALA:O	1:B:141:ILE:HG12	2.14	0.46
1:A:251:PHE:O	1:A:360:ALA:HB2	2.16	0.46
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.75	0.46
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.51	0.45
1:B:294:GLY:N	1:B:297:ASP:OD2	2.48	0.45
1:B:305:ALA:O	1:B:308:GLN:HG2	2.17	0.45
1:B:161:GLU:HG2	1:B:165:LYS:NZ	2.30	0.45
1:A:232:GLY:O	1:A:425:VAL:HA	2.17	0.45
2:B:900:MH0:H19	2:B:900:MH0:CMB	2.47	0.45
1:B:254:TRP:NE1	1:B:304:GLN:OE1	2.33	0.44
1:B:238:ILE:HD11	1:B:361:CYS:HB2	1.99	0.44
1:A:252:ARG:NH2	1:A:489:PRO:HG3	2.30	0.44
1:A:213:THR:HG23	1:A:216:GLU:HG3	1.99	0.44
1:B:381:GLN:C	1:B:382:ARG:CG	2.90	0.43
1:A:244:ARG:HA	5:A:655:HOH:O	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:OG1	1:A:173:TYR:N	2.51	0.43
1:A:309:ASP:OD1	1:A:493:HIS:NE2	2.39	0.43
1:A:340:TRP:HZ3	1:A:383:TYR:CE1	2.36	0.43
1:A:266:MET:HB2	1:A:270:THR:OG1	2.19	0.43
1:A:244:ARG:HD2	1:A:357:GLU:OE1	2.18	0.43
1:A:188:TRP:HB2	2:A:501:MH0:CBC	2.45	0.43
1:B:128:THR:HA	1:B:129:PRO:HD2	1.94	0.42
1:A:252:ARG:NH1	1:A:486:GLN:OE1	2.52	0.42
1:B:232:GLY:O	1:B:425:VAL:HA	2.18	0.42
1:B:252:ARG:HD3	1:B:359:PRO:HB2	2.01	0.42
1:A:188:TRP:C	1:A:188:TRP:CD1	2.97	0.42
1:B:403:LEU:N	1:B:403:LEU:HD23	2.34	0.42
1:B:459:VAL:HA	1:B:460:PRO:HD3	1.91	0.42
1:B:363:PHE:CD1	2:B:900:MH0:H25	2.55	0.42
1:B:375:ARG:HH12	3:B:901:H4B:C4	2.33	0.42
1:B:417:LEU:HA	1:B:417:LEU:HD23	1.85	0.42
1:A:459:VAL:HA	1:A:460:PRO:HD3	1.94	0.41
1:A:181:ILE:HA	1:A:205:VAL:HG21	2.02	0.41
1:B:138:ILE:HG23	1:B:160:LEU:HD22	2.03	0.41
1:A:283:LEU:O	1:A:287:LEU:HG	2.21	0.41
1:A:395:LEU:O	1:A:397:THR:HG23	2.20	0.41
1:B:289:TRP:O	1:B:291:PRO:HD3	2.20	0.41
1:B:340:TRP:HZ3	1:B:383:TYR:CE1	2.39	0.41
1:B:213:THR:HG23	1:B:216:GLU:H	1.86	0.41
1:B:253:LEU:HD22	1:B:347:ALA:HB1	2.03	0.41
1:A:488:GLU:HB3	1:A:490:TRP:CE2	2.57	0.40
1:B:145:TYR:OH	1:B:155:GLU:HG2	2.22	0.40
1:B:374:VAL:O	1:B:378:CYS:HB2	2.21	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	399/431 (93%)	378 (95%)	21 (5%)	0	100	100
1	B	396/431 (92%)	373 (94%)	23 (6%)	0	100	100
All	All	795/862 (92%)	751 (94%)	44 (6%)	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	347/379 (92%)	344 (99%)	3 (1%)	70	87
1	B	349/379 (92%)	347 (99%)	2 (1%)	78	91
All	All	696/758 (92%)	691 (99%)	5 (1%)	76	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	VAL
1	A	353	VAL
1	A	396	GLU
1	B	346	VAL
1	B	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
1	A	364	ASN
1	B	215	GLN
1	B	219	GLN
1	B	423	GLN

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 ⓘ

5 ligands are modelled in this entry.

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	MH0	A	501	1	50,50,50	1.61	7 (14%)	68,82,82	1.46	14 (20%)
3	H4B	B	901	-	17,18,18	1.12	1 (5%)	14,26,26	2.08	5 (35%)
4	SO4	A	503	-	4,4,4	0.18	0	6,6,6	0.27	0
2	MH0	B	900	1	50,50,50	1.63	7 (14%)	68,82,82	1.56	11 (16%)
3	H4B	A	502	-	17,18,18	1.08	2 (11%)	14,26,26	2.18	6 (42%)

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	MH0	A	501	1	-	4/14/54/54	-
2	MH0	B	900	1	-	5/14/54/54	-
3	H4B	B	901	-	-	0/8/17/17	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MH0	C3D-C2D	6.93	1.51	1.36
2	B	900	MH0	C3D-C2D	6.84	1.51	1.36
2	A	501	MH0	CBB-CAB	-3.44	1.36	1.51
2	B	900	MH0	CBB-CAB	-3.34	1.37	1.51
2	B	900	MH0	CBC-CAC	-3.20	1.37	1.51
2	A	501	MH0	CBC-CAC	-3.15	1.38	1.51
2	B	900	MH0	C3B-C2B	-3.04	1.30	1.36
3	B	901	H4B	C7-N8	2.48	1.48	1.46
3	A	502	H4B	C7-C6	2.42	1.54	1.52
2	B	900	MH0	C2A-C3A	-2.35	1.31	1.36
2	A	501	MH0	C2A-C3A	-2.33	1.31	1.36
3	A	502	H4B	C7-N8	2.25	1.48	1.46
2	A	501	MH0	O1D-CGD	-2.18	1.23	1.30
2	B	900	MH0	O2A-CGA	-2.16	1.23	1.30
2	B	900	MH0	O1D-CGD	-2.14	1.23	1.30
2	A	501	MH0	C3B-C2B	-2.13	1.32	1.36
2	A	501	MH0	O2A-CGA	-2.07	1.24	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	MH0	C1D-ND-C4D	5.43	111.64	105.21
2	A	501	MH0	C1D-ND-C4D	5.23	111.41	105.21
3	B	901	H4B	O4-C4-C4A	-3.93	117.79	127.26
3	A	502	H4B	C2-N1-C8A	3.92	120.27	113.36
3	B	901	H4B	C2-N1-C8A	3.63	119.77	113.36
3	A	502	H4B	O4-C4-C4A	-3.62	118.52	127.26
2	B	900	MH0	CAB-C3B-C4B	3.58	129.45	124.79
2	B	900	MH0	CHA-C4D-ND	3.22	127.89	124.42
3	A	502	H4B	C11-C10-C9	-3.08	108.34	112.11
3	B	901	H4B	C2-N3-C4	-3.03	119.62	125.11
2	B	900	MH0	CAB-C3B-C2B	-2.90	122.23	127.56
3	A	502	H4B	C2-N3-C4	-2.89	119.87	125.11
2	B	900	MH0	CBD-CAD-C3D	-2.84	104.68	112.53
3	B	901	H4B	O10-C10-C9	-2.78	105.17	109.77
2	B	900	MH0	C3B-C4B-NB	-2.78	107.67	110.35
2	A	501	MH0	CAD-CBD-CGD	-2.74	106.39	113.67
2	A	501	MH0	C3B-C4B-NB	-2.69	107.75	110.35
2	A	501	MH0	C1B-NB-C4B	2.57	108.26	105.21
3	A	502	H4B	O10-C10-C9	-2.55	105.55	109.77
2	B	900	MH0	C3C-C4C-NC	-2.47	107.96	110.35
3	B	901	H4B	C4A-C4-N3	2.46	118.88	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MH0	C3D-C4D-ND	-2.45	107.99	110.35
2	A	501	MH0	C1D-C2D-C3D	-2.37	104.48	106.98
2	B	900	MH0	CMD-C2D-C1D	2.34	128.70	125.03
2	A	501	MH0	CHA-C4D-ND	2.32	126.92	124.42
3	A	502	H4B	C4A-C4-N3	2.29	118.42	112.13
2	A	501	MH0	CBD-CAD-C3D	-2.28	106.23	112.53
2	A	501	MH0	CAA-C2A-C3A	-2.19	123.76	127.87
2	A	501	MH0	C2A-C1A-NA	-2.18	107.78	110.17
2	A	501	MH0	C3C-C4C-NC	-2.14	108.29	110.35
2	A	501	MH0	CAA-C2A-C1A	2.13	128.42	124.70
2	B	900	MH0	CHD-C4C-C3C	2.11	127.84	124.77
2	A	501	MH0	C1A-NA-C4A	2.08	107.67	105.21
2	A	501	MH0	C2B-C1B-NB	-2.07	107.46	109.84
2	B	900	MH0	C3D-C4D-ND	-2.07	108.35	110.35
2	B	900	MH0	C1C-NC-C4C	2.04	107.63	105.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MH0	C2C-C3C-CAC-CBC
2	B	900	MH0	C2C-C3C-CAC-CBC
2	A	501	MH0	C4C-C3C-CAC-CBC
2	B	900	MH0	C4C-C3C-CAC-CBC
2	A	501	MH0	CAD-CBD-CGD-O2D
2	A	501	MH0	CAD-CBD-CGD-O1D
2	B	900	MH0	CAD-CBD-CGD-O1D
2	B	900	MH0	CAD-CBD-CGD-O2D
2	B	900	MH0	C3D-CAD-CBD-CGD

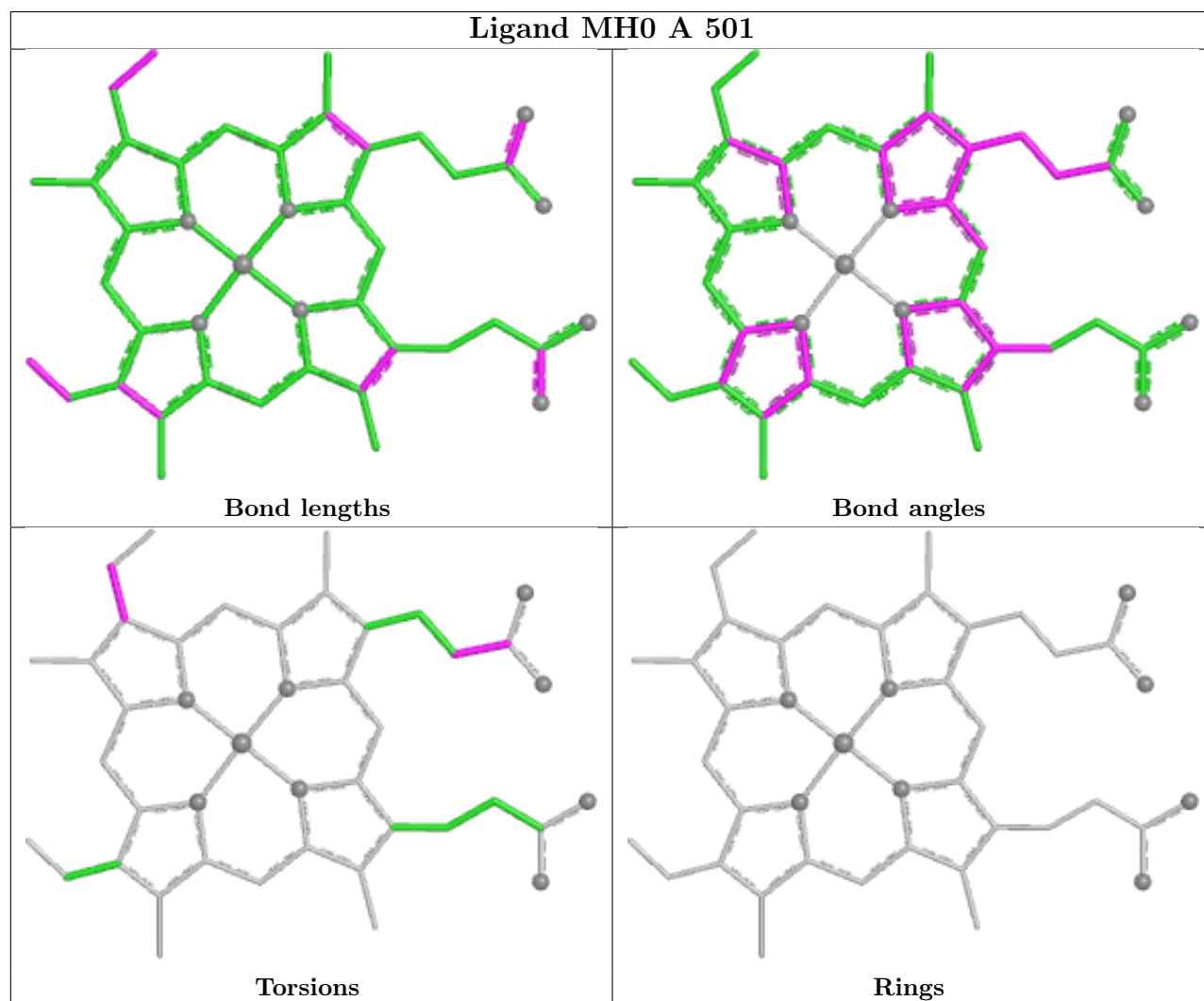
There are no ring outliers.

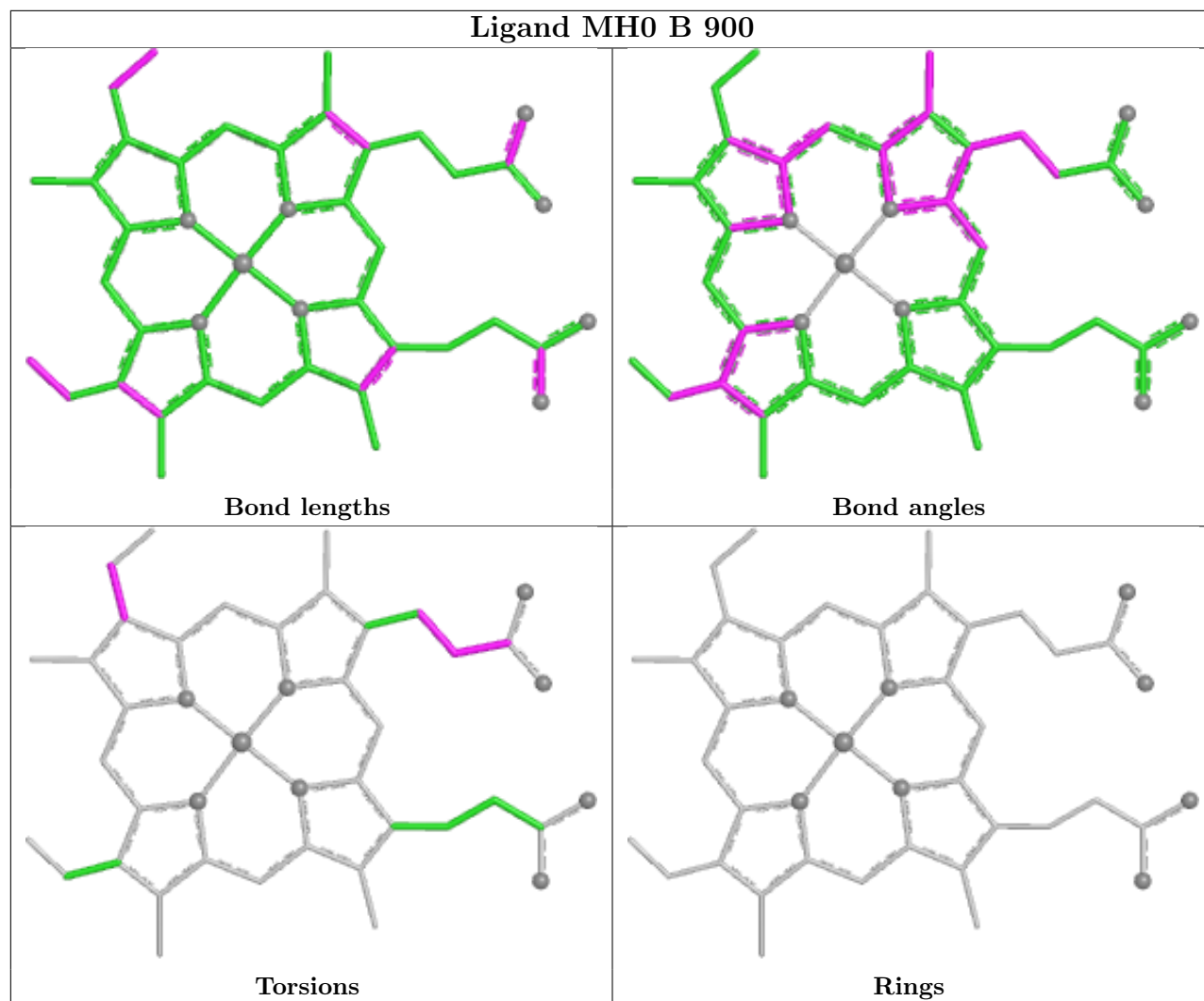
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MH0	7	0
3	B	901	H4B	1	0
2	B	900	MH0	7	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

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	405/431 (93%)	0.82	38 (9%) 14 11	27, 43, 67, 85	0
1	B	402/431 (93%)	0.73	32 (7%) 18 14	29, 43, 67, 84	0
All	All	807/862 (93%)	0.77	70 (8%) 16 13	27, 43, 67, 85	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ILE	6.7
1	A	267	PRO	5.8
1	B	111	GLY	5.0
1	A	171	GLY	4.4
1	A	148	PHE	4.1
1	B	266	MET	4.1
1	A	292	ARG	3.9
1	B	293	TYR	3.8
1	B	270	THR	3.6
1	A	270	THR	3.5
1	B	80	ARG	3.4
1	A	493	HIS	3.3
1	A	78	TYR	3.3
1	B	78	TYR	3.2
1	A	290	LYS	3.1
1	A	112	SER	3.1
1	A	293	TYR	3.0
1	B	271	ILE	3.0
1	B	334	GLN	3.0
1	B	292	ARG	3.0
1	B	148	PHE	3.0
1	A	303	LEU	2.9
1	A	153	ILE	2.8
1	B	130	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	271	ILE	2.7
1	B	91	HIS	2.7
1	B	335	GLU	2.7
1	A	147	SER	2.7
1	B	153	ILE	2.7
1	B	330	TYR	2.6
1	A	442	GLN	2.6
1	A	213	THR	2.6
1	B	265	GLN	2.6
1	B	331	GLU	2.5
1	A	266	MET	2.5
1	A	150	GLU	2.5
1	B	123	PRO	2.5
1	B	213	THR	2.4
1	A	124	ARG	2.4
1	B	442	GLN	2.4
1	B	291	PRO	2.4
1	A	151	ALA	2.4
1	B	210	ASN	2.4
1	A	331	GLU	2.4
1	A	80	ARG	2.4
1	A	337	GLY	2.4
1	A	330	TYR	2.3
1	B	277	THR	2.3
1	B	125	ASP	2.3
1	B	249	HIS	2.3
1	A	149	LYS	2.3
1	B	100	SER	2.3
1	A	308	GLN	2.3
1	B	131	GLU	2.3
1	A	291	PRO	2.3
1	B	171	GLY	2.3
1	B	149	LYS	2.2
1	A	485	TYR	2.2
1	A	223	ARG	2.2
1	A	294	GLY	2.2
1	A	77	GLN	2.1
1	B	165	LYS	2.1
1	B	279	GLU	2.1
1	A	394	GLY	2.1
1	B	383	TYR	2.1
1	A	100	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	391	ARG	2.1
1	A	428	MET	2.1
1	A	146	GLY	2.0
1	A	285	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

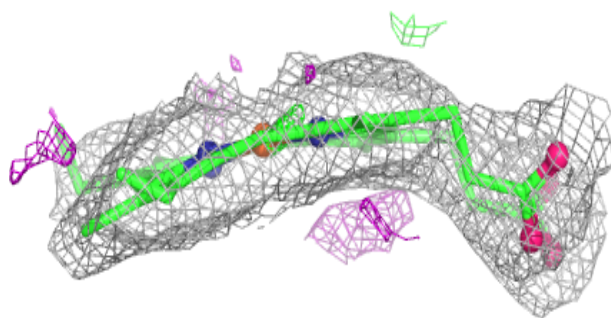
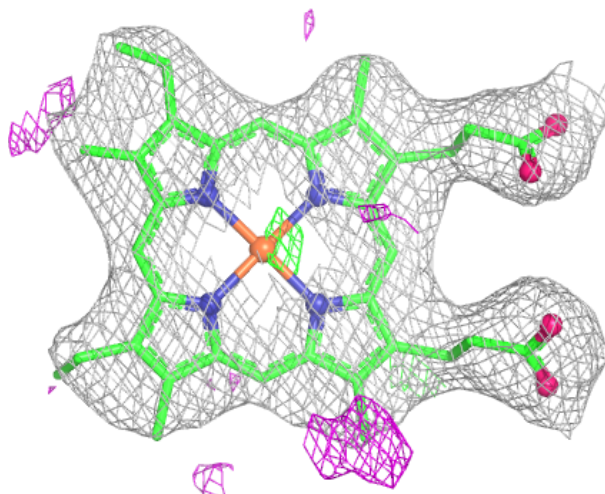
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	503	5/5	0.78	0.22	62,64,83,87	0
3	H4B	B	901	17/17	0.94	0.11	29,30,40,40	0
3	H4B	A	502	17/17	0.94	0.09	26,28,33,38	0
2	MH0	B	900	43/43	0.96	0.11	23,33,40,43	0
2	MH0	A	501	43/43	0.96	0.11	21,33,40,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

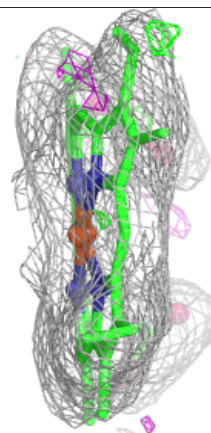
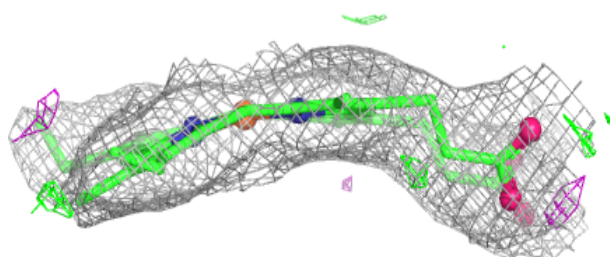
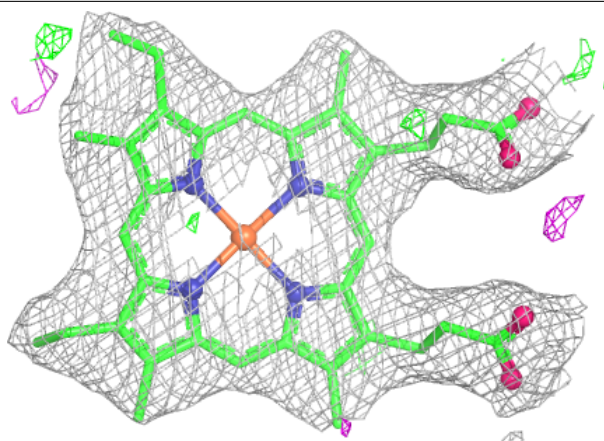
Electron density around MH0 B 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MH0 A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.