



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:53 PM EDT

PDB ID : 3EBF / pdb\_00003ebf  
Title : Structure of inhibited murine iNOS oxygenase domain  
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Anderson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 2008-08-27  
Resolution : 2.29 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

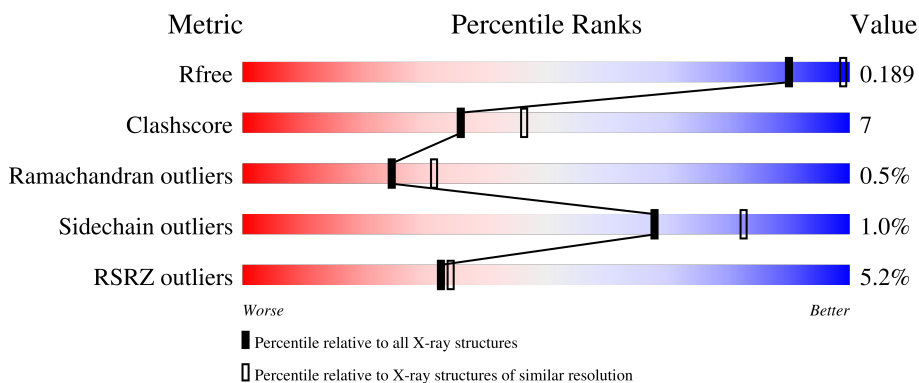
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	433	 5% 76% 20% ..
1	B	433	 5% 79% 17% ..

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
3	H4B	A	902	X	-	-	-
3	H4B	B	2902	X	-	-	-

## 2 Entry composition [i](#)

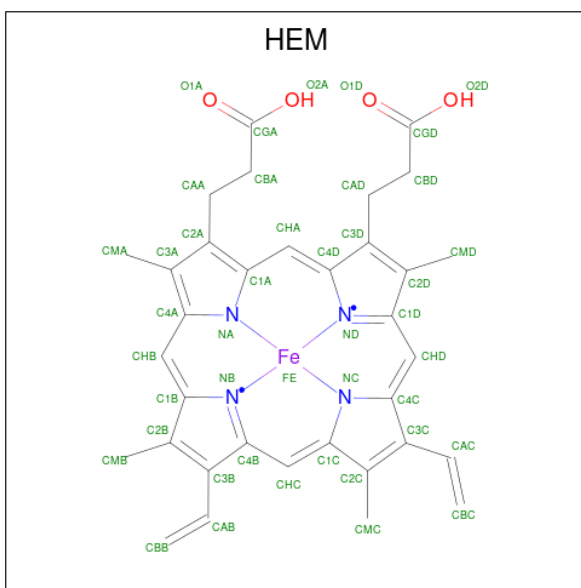
There are 6 unique types of molecules in this entry. The entry contains 7887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, inducible.

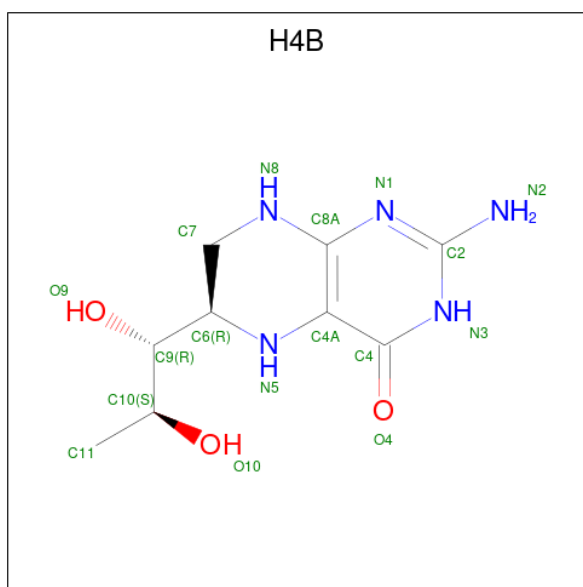
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	Total 3425	C 2195	N 590	O 619	S 21	0	0	0
1	B	421	Total 3421	C 2193	N 589	O 618	S 21	0	0	0

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



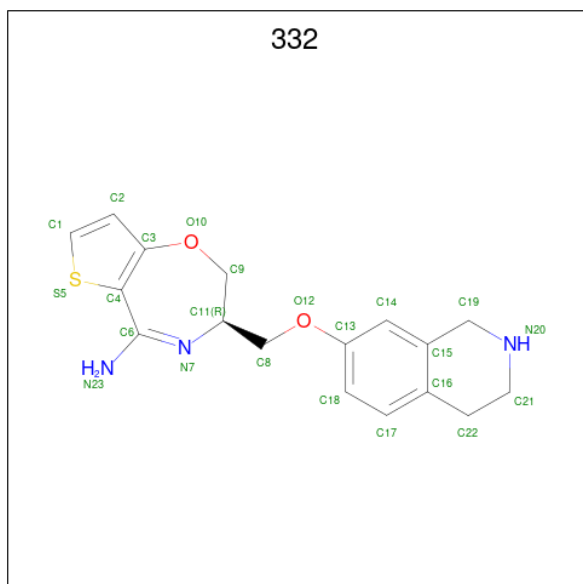
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 4 is (3R)-3-[(1,2,3,4-tetrahydroisquinolin-7-yloxy)methyl]-2,3-dihydrothieno[2,3-f][1,4]oxazepin-5-amine (CCD ID: 332) (formula: C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	23	17	3	2	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	23	17	3	2	1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

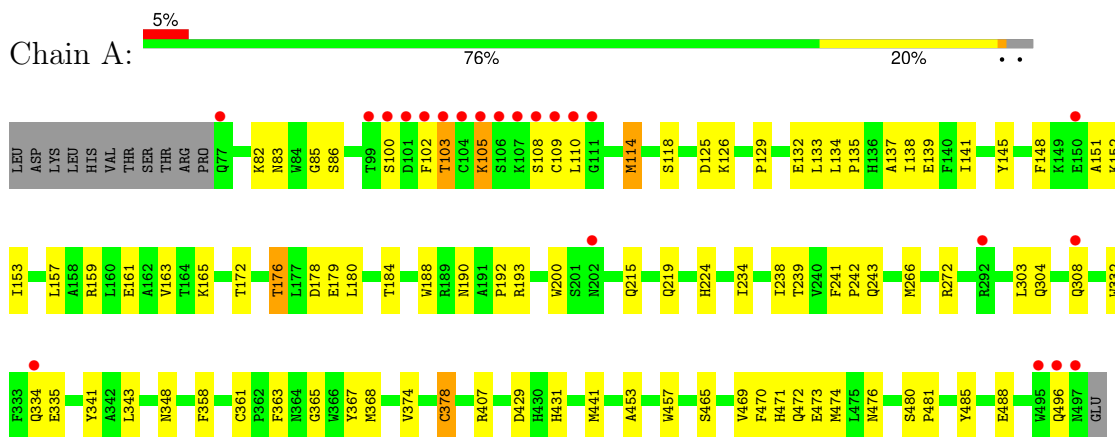
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	398	398	398	0	0
6	B	457	457	457	0	0

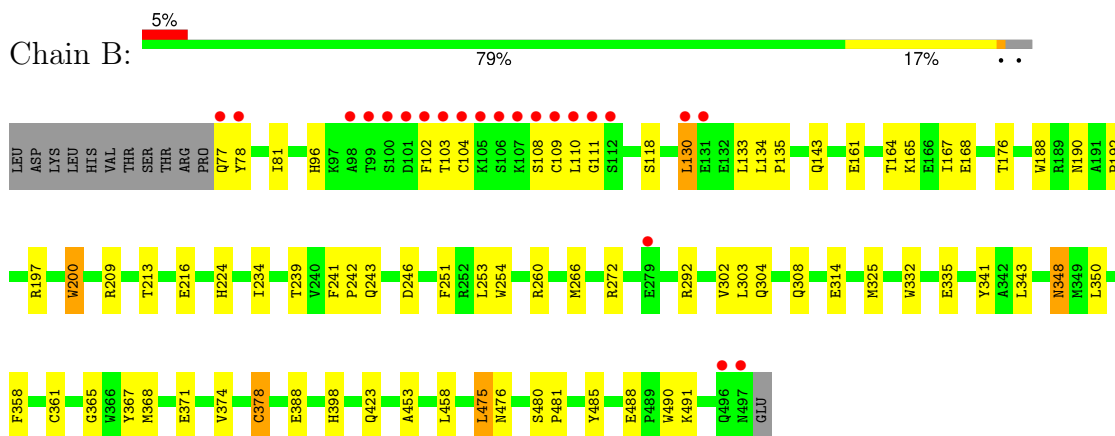
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	212.94Å 212.94Å 116.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.39 – 2.29 31.39 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.0 (31.39-2.29) 93.3 (31.39-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.203 , 0.242 0.194 , 0.189	Depositor DCC
$R_{free}$ test set	3291 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 332, SO4, H4B, 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	0.36	0/3525	0.88	10/4792 (0.2%)
1	B	0.36	0/3521	0.89	17/4787 (0.4%)
All	All	0.36	0/7046	0.89	27/9579 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	MET	N-CA-C	-7.52	96.96	109.07
1	B	348	ASN	N-CA-C	6.94	121.06	112.59
1	A	348	ASN	N-CA-C	6.49	120.51	112.59
1	B	368	MET	N-CA-C	-6.29	98.16	108.41
1	B	251	PHE	N-CA-C	-6.25	99.51	109.76
1	B	485	TYR	N-CA-C	-6.15	102.59	110.53
1	B	367	TYR	N-CA-C	6.10	118.79	110.55
1	A	365	GLY	N-CA-C	-6.06	98.81	113.18
1	B	197	ARG	N-CA-C	6.05	120.13	112.87
1	A	343	LEU	N-CA-C	5.92	120.41	109.10
1	B	303	LEU	N-CA-C	5.91	118.58	109.07
1	B	176	THR	N-CA-C	-5.87	102.96	110.53
1	B	253	LEU	N-CA-C	-5.70	99.90	109.07
1	B	234	ILE	N-CA-C	5.69	116.75	109.30
1	B	378	CYS	N-CA-C	5.60	120.39	113.50
1	A	485	TYR	N-CA-C	-5.57	102.52	110.59
1	B	111	GLY	N-CA-C	5.55	119.40	112.73
1	A	303	LEU	N-CA-C	5.49	117.92	109.07
1	A	234	ILE	N-CA-C	5.44	117.29	109.51
1	B	133	LEU	N-CA-C	5.36	116.81	110.97
1	B	343	LEU	N-CA-C	5.34	119.31	109.10
1	A	378	CYS	N-CA-C	5.32	119.92	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	TYR	N-CA-C	5.29	118.31	110.48
1	A	176	THR	N-CA-C	-5.24	103.47	110.55
1	B	325	MET	N-CA-C	5.21	117.22	109.25
1	B	200	TRP	N-CA-C	5.09	121.64	110.80
1	B	365	GLY	N-CA-C	-5.05	101.20	113.18

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	3425	0	3318	57	0
1	B	3421	0	3312	42	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	17	0	14	0	0
3	B	17	0	14	0	0
4	A	23	0	19	1	0
4	B	23	0	19	4	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	398	0	0	3	0
6	B	457	0	0	6	0
All	All	7887	0	6756	101	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 (101) 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:81:ILE:HD11	1:B:475:LEU:HD13	1.42	0.97
1:A:103:THR:HG22	1:A:110:LEU:HB2	1.63	0.80
1:A:441:MET:HE1	1:A:472:GLN:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.94	0.67
1:A:83:ASN:HD22	1:A:86:SER:H	1.42	0.67
1:B:388:GLU:HG2	6:B:4814:HOH:O	1.96	0.66
1:A:215:GLN:O	1:A:219:GLN:HG3	1.96	0.65
1:B:190:ASN:O	1:B:192:PRO:HD3	1.97	0.64
1:A:441:MET:CE	1:A:472:GLN:HG2	2.26	0.64
1:A:83:ASN:ND2	1:A:85:GLY:H	1.98	0.62
1:B:77:GLN:O	1:B:96:HIS:HE1	1.85	0.60
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.84	0.59
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.85	0.58
1:A:103:THR:CG2	1:A:110:LEU:HB2	2.32	0.58
1:B:164:THR:O	1:B:168:GLU:HG3	2.04	0.57
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.39	0.57
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.27	0.57
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.85	0.57
1:B:104:CYS:HA	1:B:110:LEU:HD12	1.88	0.56
1:A:465:SER:O	1:A:471:HIS:HE1	1.89	0.55
1:A:161:GLU:O	1:A:165:LYS:HD3	2.07	0.55
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.06	0.55
1:A:469:VAL:HG13	1:A:474:MET:HE1	1.87	0.54
1:A:103:THR:H	1:A:118:SER:HB3	1.73	0.54
1:B:488:GLU:OE2	1:B:491:LYS:HE3	2.07	0.54
1:A:239:THR:O	1:A:361:CYS:HA	2.08	0.54
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.43	0.53
1:A:153:ILE:O	1:A:157:LEU:HD23	2.08	0.53
1:B:110:LEU:HD22	6:B:4647:HOH:O	2.09	0.53
1:A:105:LYS:HD2	1:A:108:SER:OG	2.08	0.53
1:B:332:TRP:O	1:B:335:GLU:HB2	2.08	0.53
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.44	0.52
1:A:152:LYS:HB2	1:A:152:LYS:NZ	2.24	0.52
1:A:332:TRP:O	1:A:335:GLU:HB2	2.10	0.52
1:A:407:ARG:HD2	6:A:4139:HOH:O	2.10	0.51
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.41	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.46	0.50
1:A:109:CYS:C	1:A:110:LEU:HD23	2.37	0.50
1:B:266:MET:HE2	1:B:272:ARG:CZ	2.42	0.50
1:A:135:PRO:O	1:A:139:GLU:HG3	2.11	0.50
1:A:266:MET:HE2	1:A:272:ARG:CZ	2.42	0.49
1:A:114:MET:HE1	6:A:4338:HOH:O	2.12	0.49
1:A:82:LYS:O	1:A:473:GLU:HG3	2.13	0.48
1:A:304:GLN:HG3	1:A:308:GLN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:O	1:A:192:PRO:HD3	2.14	0.48
1:B:78:TYR:C	1:B:78:TYR:CD1	2.92	0.47
1:A:134:LEU:O	1:A:138:ILE:HG12	2.15	0.47
1:A:469:VAL:HG13	1:A:474:MET:CE	2.45	0.47
1:B:254:TRP:HB2	1:B:302:VAL:HB	1.96	0.47
1:A:152:LYS:HB2	1:A:152:LYS:HZ2	1.80	0.47
1:A:308:GLN:HG2	1:A:496:GLN:HE22	1.78	0.47
1:B:304:GLN:HG3	1:B:308:GLN:O	2.15	0.47
1:A:83:ASN:ND2	1:A:86:SER:H	2.09	0.47
1:B:143:GLN:HG2	6:B:4660:HOH:O	2.15	0.47
1:A:103:THR:H	1:A:118:SER:CB	2.28	0.46
1:A:132:GLU:O	1:A:135:PRO:HD2	2.16	0.46
1:B:292:ARG:NH1	1:B:314:GLU:OE2	2.48	0.46
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.46	0.46
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.45	0.46
1:B:102:PHE:HZ	1:B:476:ASN:ND2	2.15	0.45
1:A:238:ILE:HG13	1:A:363:PHE:HB3	1.97	0.45
1:B:341:TYR:OH	4:B:2903:332:H17	2.17	0.45
1:B:350:LEU:C	1:B:350:LEU:HD23	2.42	0.45
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.46	0.45
1:B:371:GLU:OE1	4:B:2903:332:N7	2.49	0.45
1:B:239:THR:O	1:B:361:CYS:HA	2.17	0.45
1:A:480:SER:HA	1:A:481:PRO:C	2.42	0.45
1:B:374:VAL:O	1:B:378:CYS:HB2	2.18	0.44
2:B:2901:HEM:HBC2	2:B:2901:HEM:HMC1	1.99	0.44
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.18	0.44
1:B:161:GLU:HG2	1:B:165:LYS:HE3	2.00	0.44
1:B:246:ASP:HB3	6:B:4855:HOH:O	2.18	0.44
1:A:180:LEU:O	1:A:184:THR:HG23	2.18	0.43
1:B:103:THR:OG1	1:B:104:CYS:N	2.51	0.43
1:B:480:SER:HA	1:B:481:PRO:C	2.43	0.42
1:A:470:PHE:CD1	1:A:470:PHE:C	2.97	0.42
1:A:137:ALA:O	1:A:141:ILE:HG12	2.19	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.19	0.42
1:A:429:ASP:OD1	1:A:431:HIS:HB2	2.19	0.42
1:A:488:GLU:HG2	6:A:4254:HOH:O	2.19	0.42
1:A:165:LYS:N	1:A:165:LYS:HD2	2.34	0.42
1:A:341:TYR:OH	4:A:903:332:H17	2.20	0.42
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.54	0.42
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.01	0.42
1:A:133:LEU:HD21	1:A:172:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:HA	1:A:148:PHE:CD2	2.54	0.41
1:B:224:HIS:CD2	1:B:224:HIS:C	2.98	0.41
1:B:209:ARG:O	1:B:242:PRO:HG3	2.20	0.41
1:B:103:THR:HG22	1:B:118:SER:OG	2.20	0.41
1:A:241:PHE:HB3	1:A:242:PRO:HD2	2.03	0.41
1:A:453:ALA:HB3	1:A:474:MET:HB3	2.01	0.41
1:B:104:CYS:HG	1:B:109:CYS:HG	1.61	0.41
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.56	0.41
1:B:488:GLU:HB3	1:B:490:TRP:CE2	2.56	0.41
1:A:224:HIS:CD2	1:A:224:HIS:C	2.98	0.41
1:A:102:PHE:HZ	1:A:476:ASN:ND2	2.19	0.40
1:A:159:ARG:O	1:A:163:VAL:HG23	2.21	0.40
1:B:260:ARG:CZ	4:B:2903:332:H22A	2.51	0.40
1:B:398:HIS:HB2	6:B:4594:HOH:O	2.20	0.40
2:B:2901:HEM:HBA2	4:B:2903:332:H9A	2.02	0.40
1:B:108:SER:HB2	6:B:4582:HOH:O	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	419/433 (97%)	394 (94%)	21 (5%)	4 (1%)	12 15
1	B	419/433 (97%)	392 (94%)	27 (6%)	0	100 100
All	All	838/866 (97%)	786 (94%)	48 (6%)	4 (0%)	24 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	103	THR

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Mol	Chain	Res	Type
1	A	151	ALA
1	A	105	LYS

### 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	367/381 (96%)	364 (99%)	3 (1%)	73	86
1	B	366/381 (96%)	362 (99%)	4 (1%)	65	81
All	All	733/762 (96%)	726 (99%)	7 (1%)	68	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	MET
1	A	178	ASP
1	A	334	GLN
1	B	130	LEU
1	B	348	ASN
1	B	423	GLN
1	B	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	142	ASN
1	A	215	GLN
1	A	249	HIS
1	A	334	GLN
1	A	364	ASN
1	A	418	HIS
1	A	421	GLN

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Mol	Chain	Res	Type
1	A	442	GLN
1	A	471	HIS
1	A	476	ASN
1	A	486	GLN
1	A	496	GLN
1	B	96	HIS
1	B	143	GLN
1	B	199	GLN
1	B	202	ASN
1	B	215	GLN
1	B	265	GLN
1	B	334	GLN
1	B	348	ASN
1	B	418	HIS
1	B	421	GLN
1	B	486	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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
4	332	A	903	-	22,26,26	2.37	11 (50%)	24,36,36	1.47	3 (12%)
3	H4B	A	902	-	17,18,18	2.69	3 (17%)	14,26,26	5.00	10 (71%)
5	SO4	B	3004	-	4,4,4	0.38	0	6,6,6	0.10	0
4	332	B	2903	-	22,26,26	2.39	11 (50%)	24,36,36	1.52	3 (12%)
2	HEM	B	2901	1	50,50,50	1.46	8 (16%)	67,82,82	1.04	4 (5%)
5	SO4	A	3003	-	4,4,4	0.38	0	6,6,6	0.06	0
3	H4B	B	2902	-	17,18,18	2.71	3 (17%)	14,26,26	4.10	9 (64%)
5	SO4	A	3004	-	4,4,4	0.38	0	6,6,6	0.10	0
2	HEM	A	901	1	50,50,50	1.48	8 (16%)	67,82,82	1.06	6 (8%)
5	SO4	B	3003	-	4,4,4	0.38	0	6,6,6	0.08	0

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	332	A	903	-	-	1/4/25/25	0/3/4/4
3	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2
4	332	B	2903	-	-	1/4/25/25	0/3/4/4
2	HEM	B	2901	1	-	1/14/54/54	-
3	H4B	B	2902	-	1/1/3/5	3/8/17/17	0/2/2/2
2	HEM	A	901	1	-	1/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2902	H4B	C7-N8	-8.48	1.37	1.46
3	A	902	H4B	C7-N8	-8.33	1.38	1.46
3	A	902	H4B	C7-C6	-5.55	1.46	1.52
3	B	2902	H4B	C7-C6	-5.53	1.46	1.52
4	A	903	332	C14-C13	4.69	1.46	1.39
4	B	2903	332	C14-C13	4.65	1.46	1.39
4	A	903	332	C8-C11	4.44	1.62	1.51
4	B	2903	332	C8-C11	4.43	1.62	1.51
2	A	901	HEM	FE-NC	4.35	2.09	1.95
4	A	903	332	C17-C18	3.79	1.44	1.38
2	B	2901	HEM	FE-ND	3.72	2.06	1.94
2	B	2901	HEM	FE-NC	3.62	2.07	1.95
4	B	2903	332	C17-C18	3.58	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	FE-ND	3.51	2.05	1.94
2	B	2901	HEM	FE-NA	3.38	2.06	1.95
2	B	2901	HEM	FE-NB	3.30	2.05	1.94
2	A	901	HEM	FE-NB	3.17	2.04	1.94
4	A	903	332	C9-C11	3.12	1.56	1.51
4	B	2903	332	C18-C13	3.05	1.44	1.38
2	A	901	HEM	FE-NA	3.03	2.05	1.95
4	A	903	332	C21-C22	3.03	1.58	1.50
4	B	2903	332	C21-C22	2.99	1.57	1.50
4	A	903	332	C18-C13	2.96	1.44	1.38
4	B	2903	332	O12-C13	2.95	1.44	1.37
4	B	2903	332	C9-C11	2.93	1.55	1.51
3	A	902	H4B	C4-N3	-2.89	1.33	1.38
3	B	2902	H4B	C4-N3	-2.88	1.33	1.38
4	B	2903	332	C15-C16	2.71	1.45	1.40
4	A	903	332	C15-C16	2.69	1.45	1.40
4	A	903	332	O12-C13	2.68	1.43	1.37
2	A	901	HEM	CAC-C3C	-2.63	1.40	1.47
2	A	901	HEM	CAB-C3B	-2.54	1.40	1.47
2	A	901	HEM	C1B-NB	-2.50	1.35	1.40
4	B	2903	332	C22-C16	2.44	1.55	1.51
4	A	903	332	C17-C16	2.43	1.43	1.39
4	B	2903	332	C19-N20	2.42	1.49	1.46
2	B	2901	HEM	CAC-C3C	-2.35	1.41	1.47
4	B	2903	332	C17-C16	2.31	1.43	1.39
2	B	2901	HEM	CAB-C3B	-2.19	1.41	1.47
2	B	2901	HEM	CBC-CAC	2.16	1.40	1.30
4	A	903	332	C22-C16	2.16	1.54	1.51
4	A	903	332	C19-N20	2.15	1.49	1.46
2	B	2901	HEM	CBB-CAB	2.04	1.40	1.30
2	A	901	HEM	CBC-CAC	2.01	1.40	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	H4B	C2-N3-C4	-8.72	109.29	125.11
3	A	902	H4B	C4A-C4-N3	8.67	135.93	112.13
3	B	2902	H4B	O9-C9-C10	-8.37	93.21	109.14
3	A	902	H4B	O4-C4-C4A	-7.93	108.15	127.26
3	A	902	H4B	O9-C9-C6	-6.40	93.94	109.28
3	A	902	H4B	C4-C4A-N5	6.23	133.26	116.27
3	B	2902	H4B	C11-C10-C9	6.13	119.62	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2902	H4B	O4-C4-C4A	-5.53	113.92	127.26
3	B	2902	H4B	C4A-C4-N3	5.23	126.50	112.13
3	B	2902	H4B	C4-C4A-N5	4.37	128.19	116.27
3	A	902	H4B	O9-C9-C10	-4.34	100.89	109.14
3	B	2902	H4B	C2-N3-C4	-4.26	117.38	125.11
3	B	2902	H4B	C2-N1-C8A	-4.15	106.03	113.36
4	B	2903	332	C9-O10-C3	3.96	123.85	115.67
4	A	903	332	C9-O10-C3	3.89	123.71	115.67
4	B	2903	332	C8-C11-N7	3.85	115.64	109.46
3	A	902	H4B	N3-C2-N1	3.66	130.01	123.32
3	A	902	H4B	N2-C2-N1	-3.54	112.77	119.67
4	A	903	332	C8-C11-N7	3.51	115.09	109.46
2	A	901	HEM	CMD-C2D-C1D	2.86	129.51	125.03
4	B	2903	332	O12-C8-C11	2.81	114.37	108.29
2	A	901	HEM	C4B-C3B-C2B	-2.74	104.77	107.28
3	B	2902	H4B	N3-C2-N1	2.73	128.32	123.32
4	A	903	332	O12-C8-C11	2.69	114.11	108.29
2	B	2901	HEM	CMD-C2D-C1D	2.38	128.76	125.03
2	A	901	HEM	CAA-C2A-C1A	2.36	129.54	124.94
3	A	902	H4B	C2-N1-C8A	-2.30	109.30	113.36
2	A	901	HEM	C3B-C4B-NB	2.29	111.12	109.47
2	B	2901	HEM	CHC-C4B-NB	-2.25	122.00	124.42
3	A	902	H4B	O4-C4-N3	-2.23	115.92	120.11
2	B	2901	HEM	C4B-C3B-C2B	-2.22	105.23	107.28
2	A	901	HEM	CAD-C3D-C2D	-2.22	123.72	127.87
2	B	2901	HEM	CAA-C2A-C1A	2.15	129.14	124.94
2	A	901	HEM	CAD-C3D-C4D	2.14	128.43	124.70
3	B	2902	H4B	O10-C10-C11	-2.03	103.62	109.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6
3	B	2902	H4B	C6

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9
3	A	902	H4B	C7-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
3	B	2902	H4B	N5-C6-C9-O9

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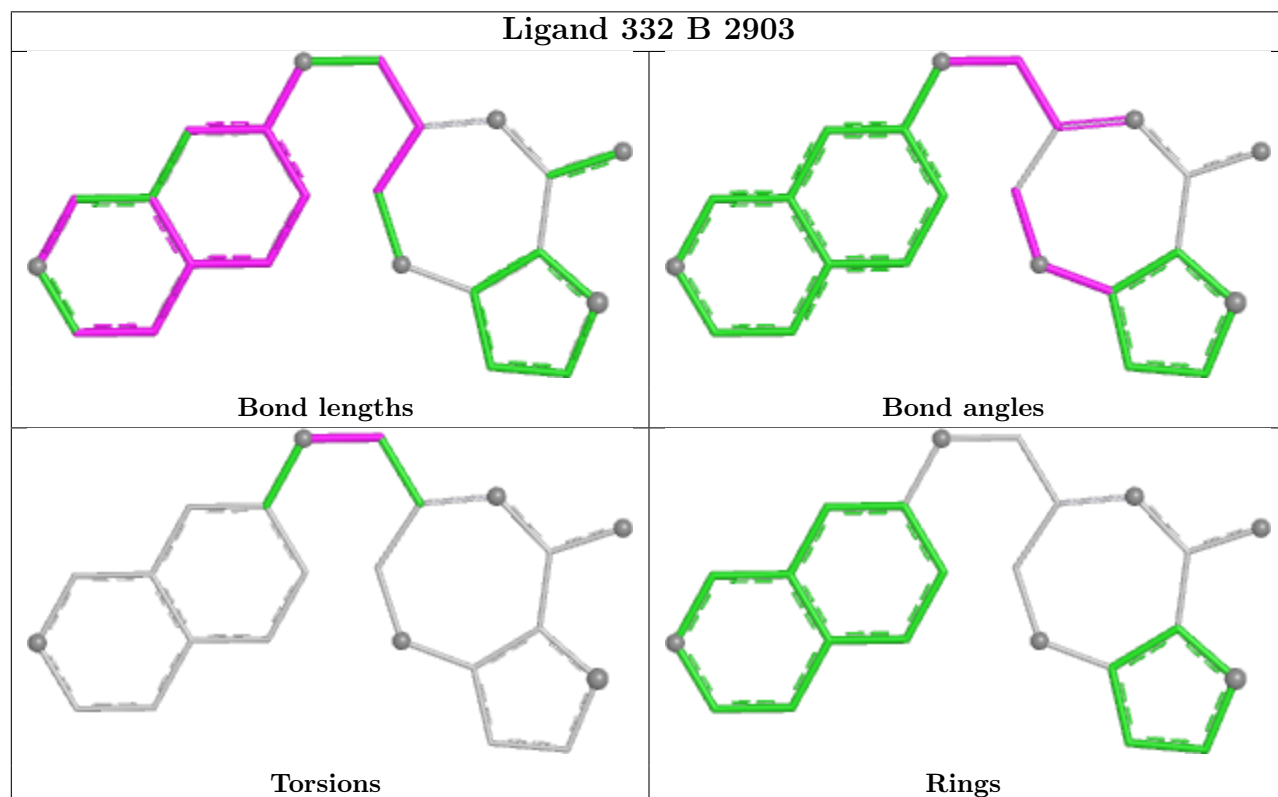
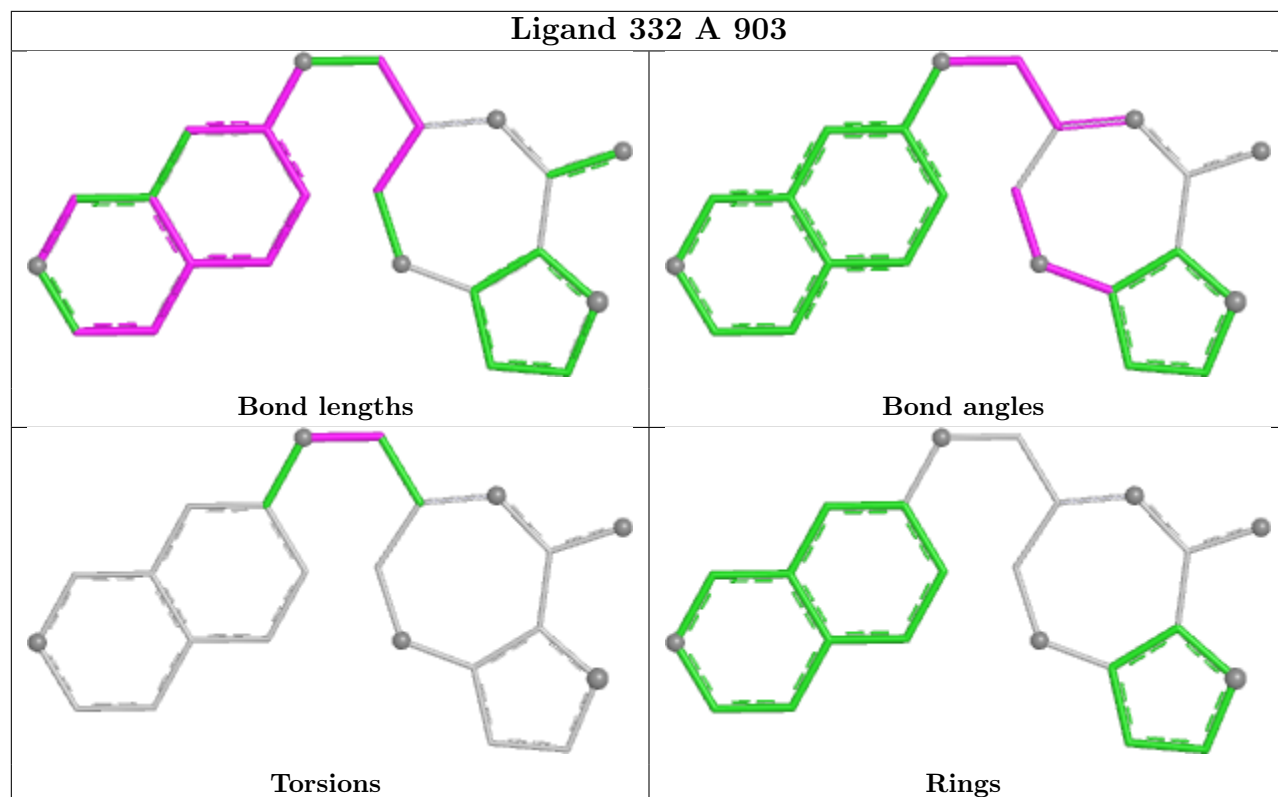
Mol	Chain	Res	Type	Atoms
3	B	2902	H4B	C7-C6-C9-O9
3	B	2902	H4B	C7-C6-C9-C10
4	A	903	332	C11-C8-O12-C13
4	B	2903	332	C11-C8-O12-C13
2	B	2901	HEM	C4B-C3B-CAB-CBB
3	A	902	H4B	O10-C10-C9-C6
2	A	901	HEM	CAA-CBA-CGA-O2A

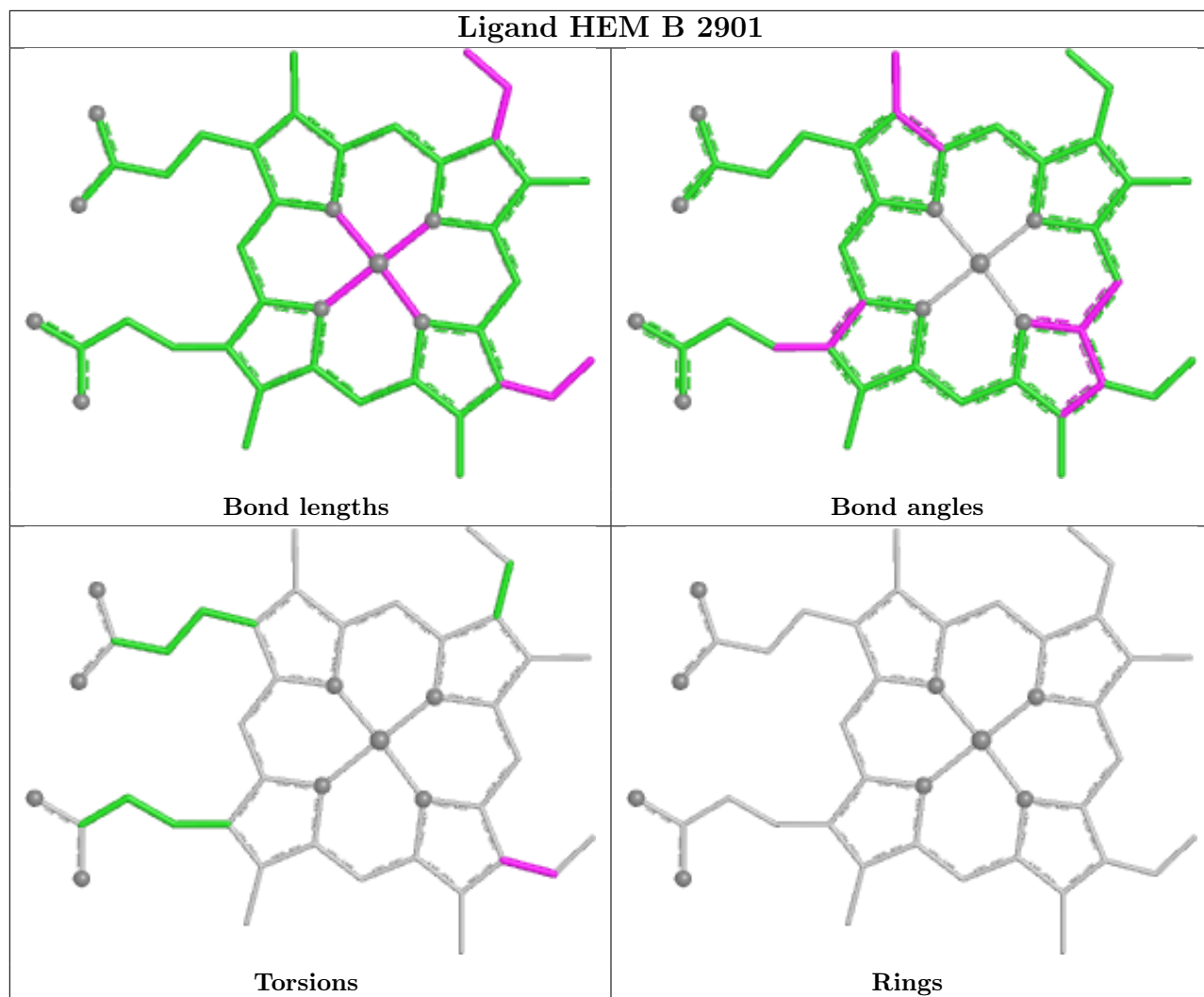
There are no ring outliers.

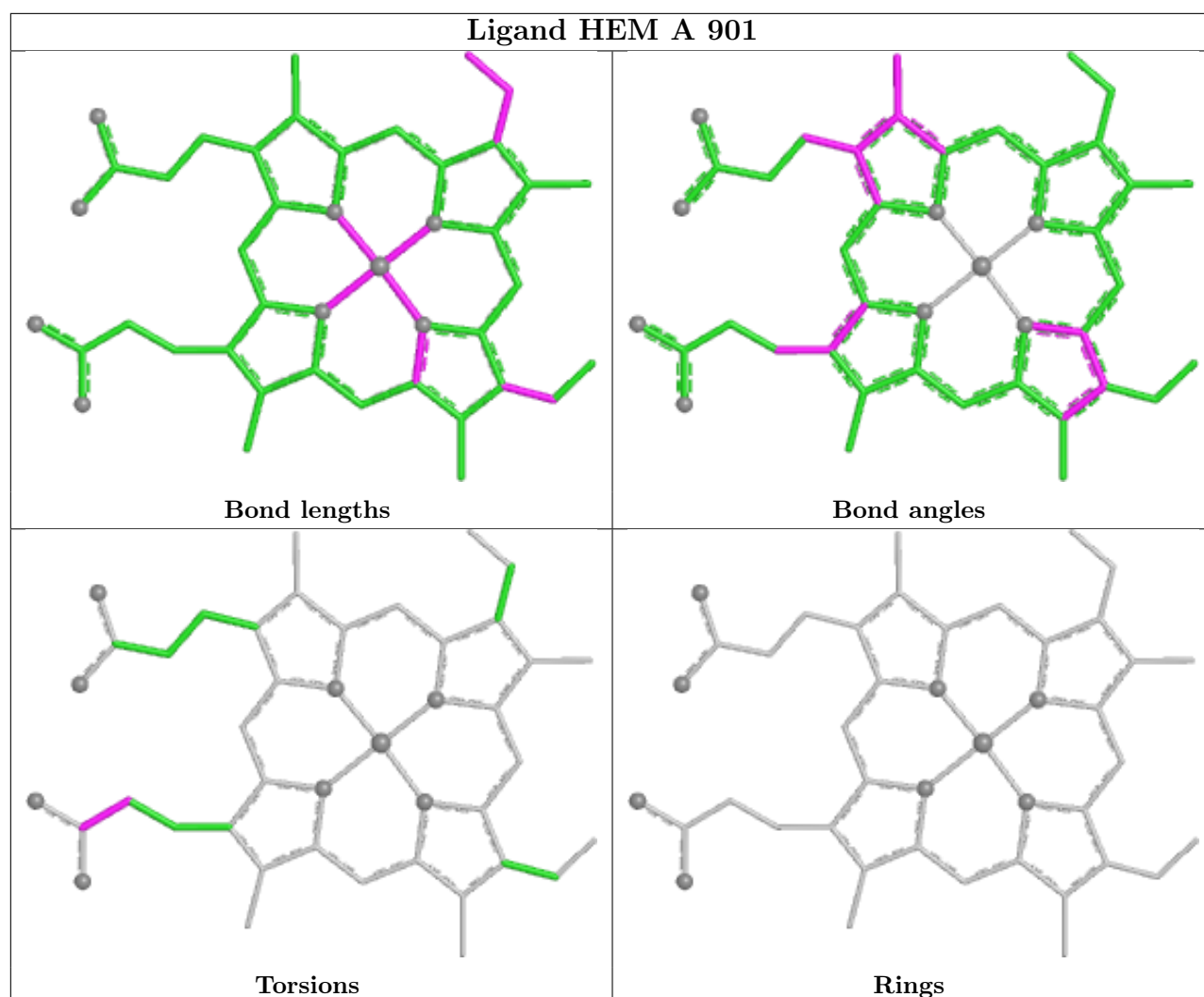
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	332	1	0
4	B	2903	332	4	0
2	B	2901	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/433 (97%)	0.16	22 (5%) 33 34	17, 32, 56, 86	0
1	B	421/433 (97%)	0.07	22 (5%) 33 34	16, 29, 55, 84	0
All	All	842/866 (97%)	0.12	44 (5%) 33 34	16, 30, 56, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	THR	8.8
1	A	103	THR	8.0
1	A	102	PHE	6.5
1	B	102	PHE	6.1
1	B	99	THR	5.9
1	B	100	SER	5.4
1	B	108	SER	5.2
1	A	497	ASN	5.1
1	B	497	ASN	4.9
1	B	111	GLY	4.5
1	B	105	LYS	4.4
1	B	130	LEU	4.3
1	A	106	SER	4.3
1	A	108	SER	4.3
1	B	98	ALA	4.3
1	A	105	LYS	4.3
1	A	110	LEU	4.3
1	A	107	LYS	4.2
1	A	77	GLN	4.0
1	B	106	SER	4.0
1	A	104	CYS	3.8
1	B	107	LYS	3.7
1	B	101	ASP	3.7
1	B	104	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	496	GLN	3.4
1	A	111	GLY	3.3
1	B	77	GLN	3.2
1	A	109	CYS	2.9
1	B	109	CYS	2.8
1	B	496	GLN	2.7
1	B	110	LEU	2.6
1	A	495	TRP	2.6
1	A	308	GLN	2.5
1	A	202	ASN	2.5
1	A	334	GLN	2.4
1	A	99	THR	2.3
1	B	131	GLU	2.3
1	B	112	SER	2.3
1	A	100	SER	2.2
1	B	78	TYR	2.1
1	A	101	ASP	2.1
1	A	150	GLU	2.0
1	B	279	GLU	2.0
1	A	292	ARG	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, 95<sup>th</sup> 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.

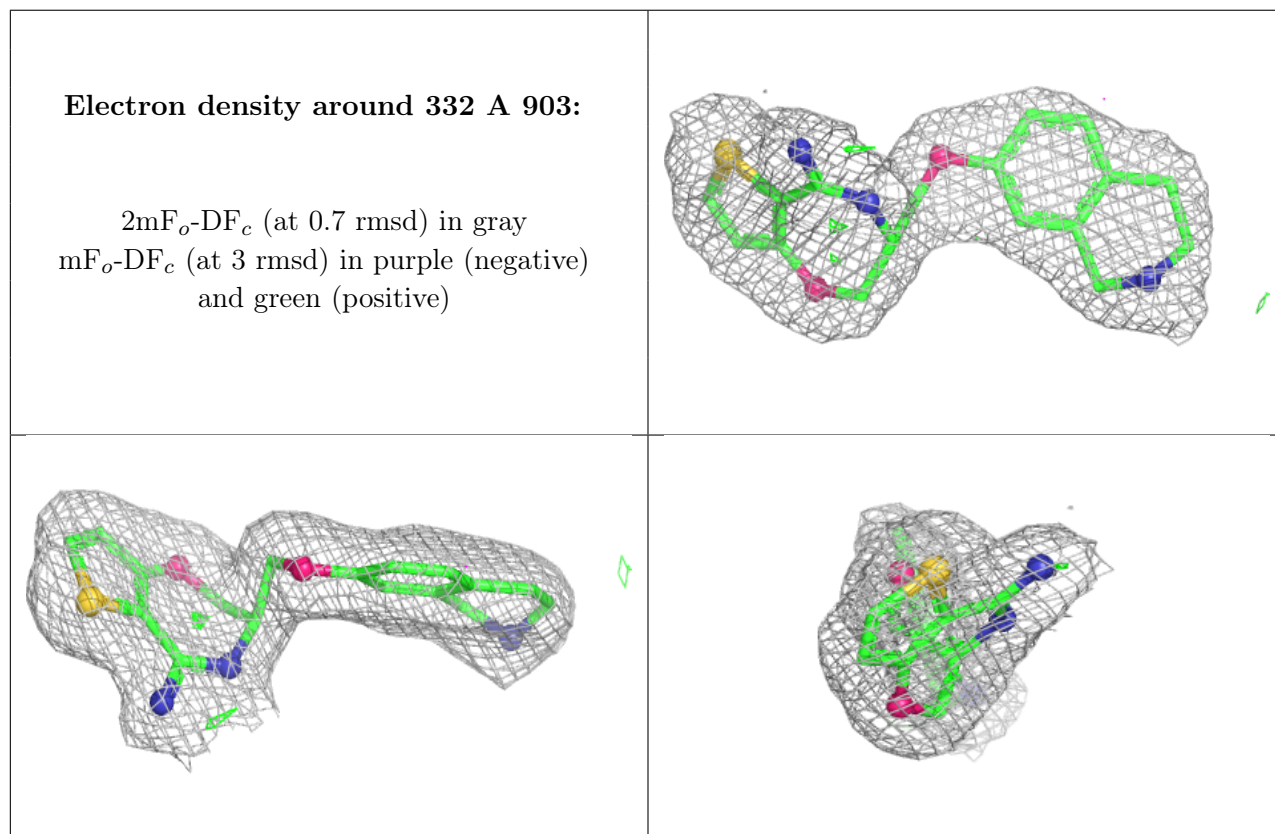
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	B	3003	5/5	0.72	0.15	89,89,89,90	0
5	SO4	A	3004	5/5	0.75	0.14	82,83,84,84	0
5	SO4	A	3003	5/5	0.77	0.13	87,87,88,88	0

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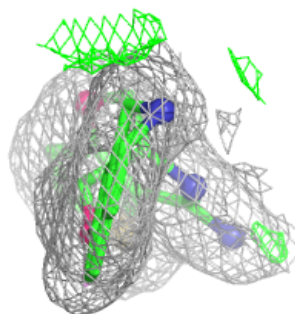
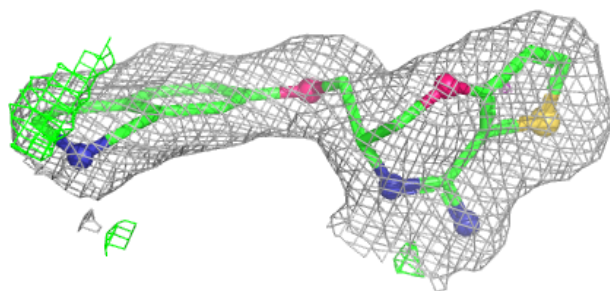
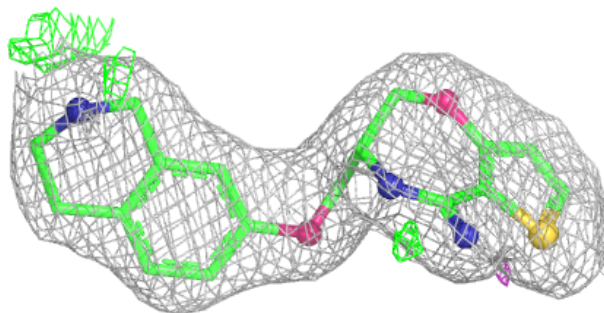
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	3004	5/5	0.77	0.15	84,84,85,85	0
4	332	A	903	23/23	0.97	0.06	16,20,22,24	0
4	332	B	2903	23/23	0.97	0.06	13,18,22,23	0
3	H4B	A	902	17/17	0.97	0.05	13,23,26,26	0
3	H4B	B	2902	17/17	0.98	0.04	14,19,22,23	0
2	HEM	A	901	43/43	0.99	0.05	15,19,22,24	0
2	HEM	B	2901	43/43	0.99	0.05	13,16,18,19	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.



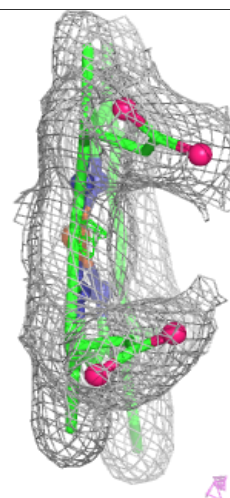
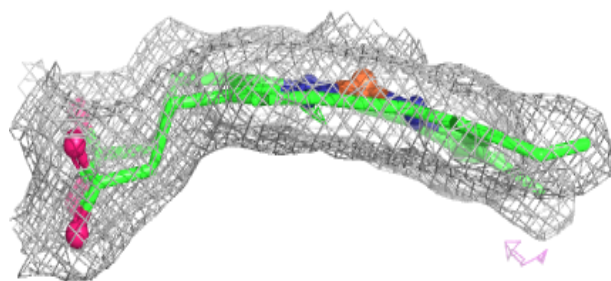
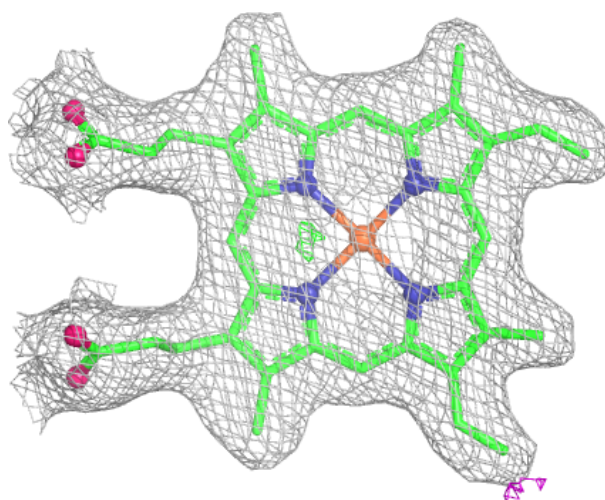
**Electron density around 332 B 2903:**

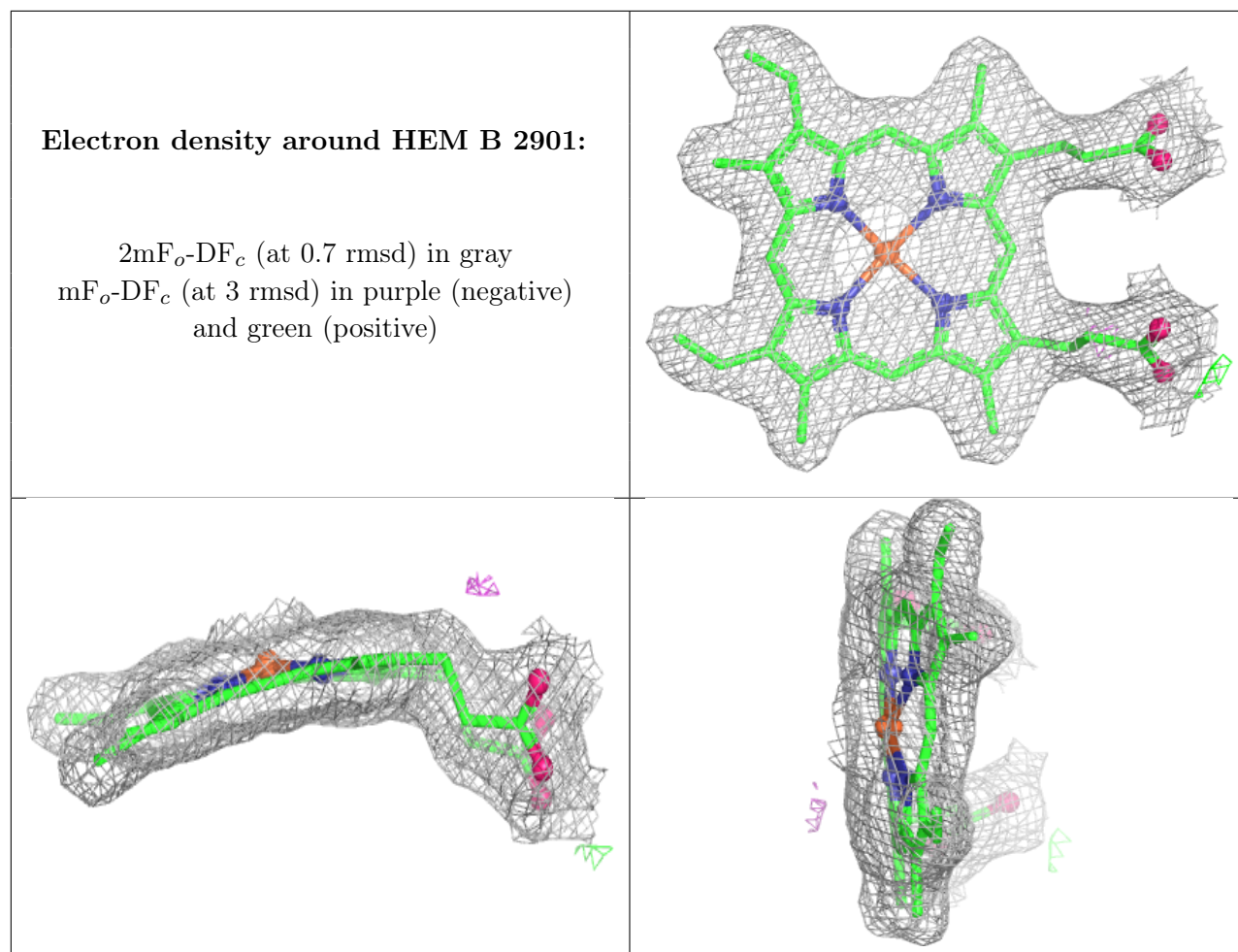
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 901:**

$2mF_o-DF_c$  (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.