



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:38 pm BST

PDB ID : 3EAI  
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 : 2008-08-25  
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

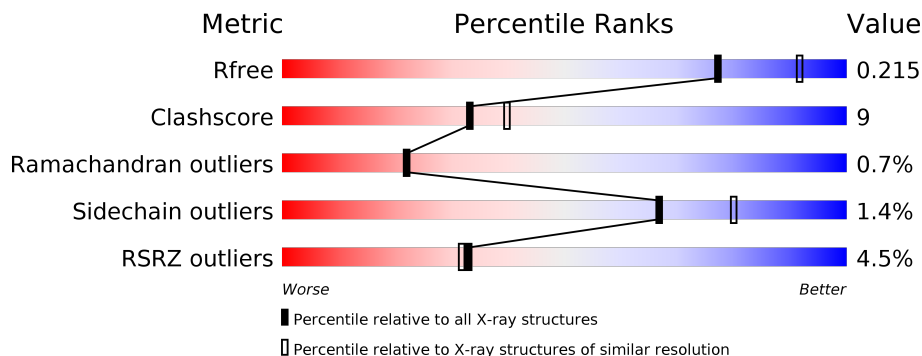
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	 4% 76% 21% •
1	B	433	 4% 80% 15% ••

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

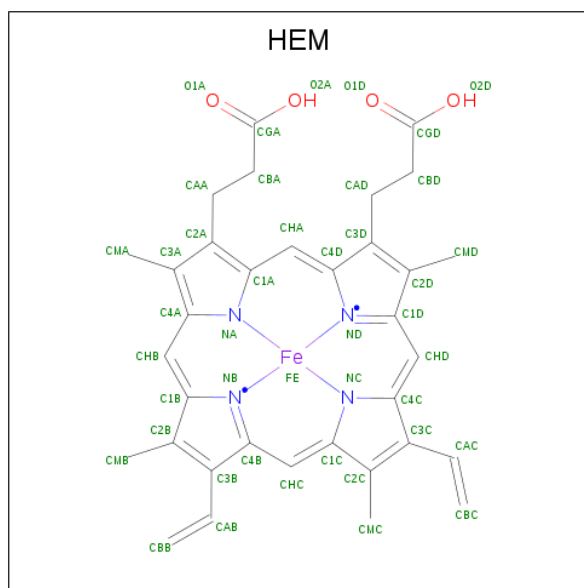
There are 6 unique types of molecules in this entry. The entry contains 7867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

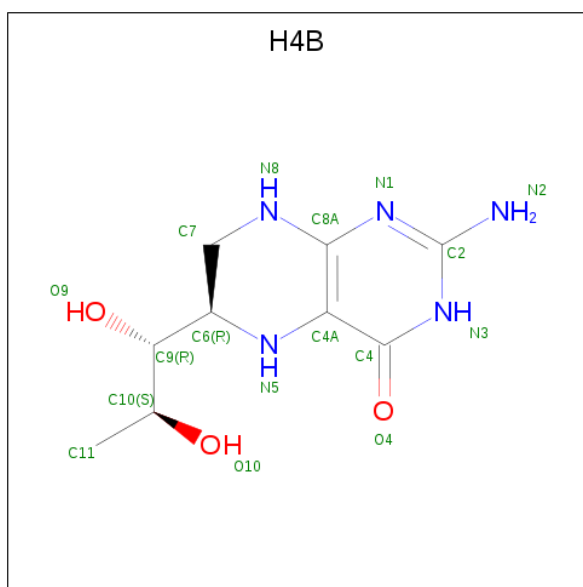
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	Total 3425	C 2195	N 590	O 619	S 21	0	0	0
1	B	421	Total 3421	C 2193	N 589	O 618	S 21	0	0	0

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



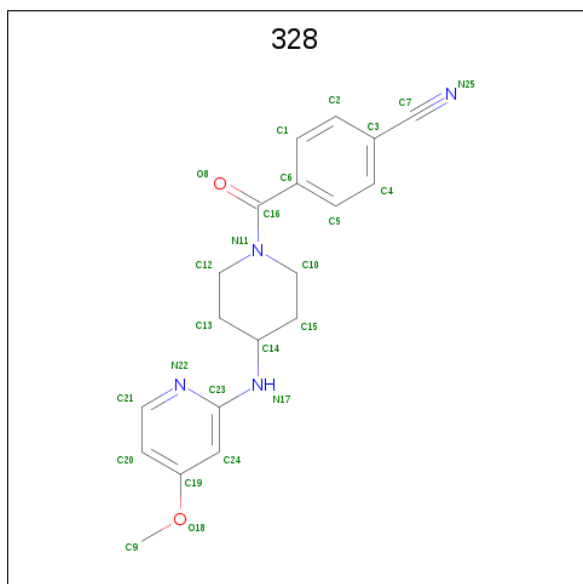
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: 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 4-({4-[(4-methoxypyridin-2-yl)amino]piperidin-1-yl}carbonyl)benzonitrile (three-letter code: 328) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>).



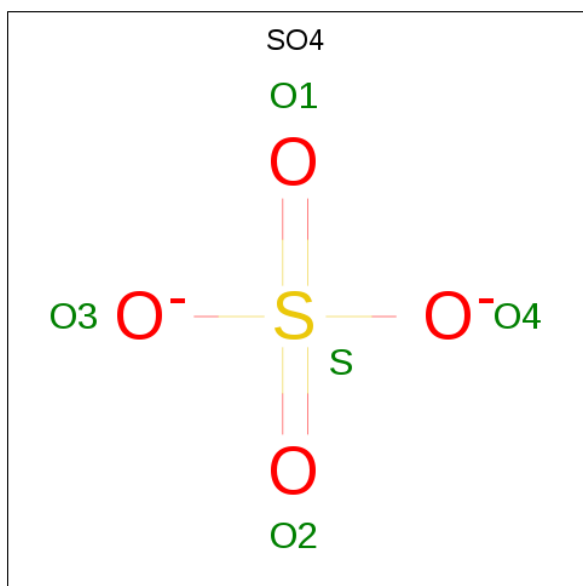
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	25	19	4	2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	25	19	4	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (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

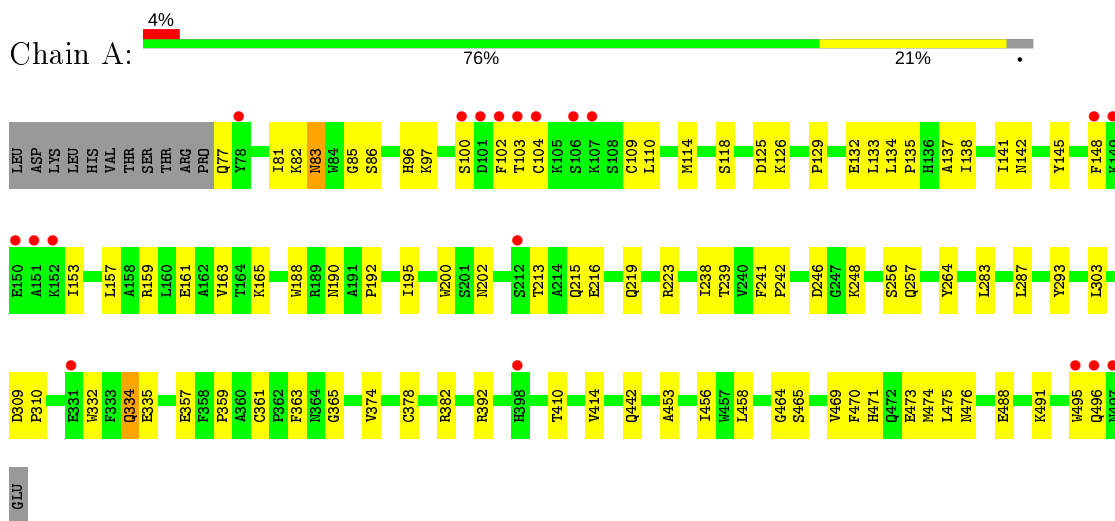
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	388	388	388	0	0
6	B	443	443	443	0	0

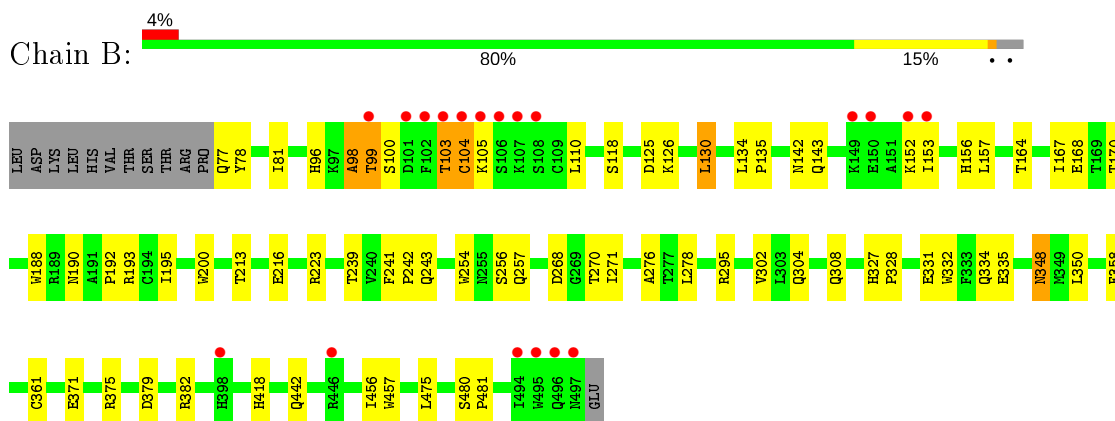
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	213.11Å 213.11Å 116.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.3 (19.95-2.20) 85.4 (19.95-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.19Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.223 , (Not available) 0.211 , 0.215	Depositor DCC
$R_{free}$ test set	3389 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 74.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: HEM, 328, H4B, 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	0.33	0/3525	0.59	1/4792 (0.0%)
1	B	0.34	0/3521	0.60	0/4787
All	All	0.34	0/7046	0.60	1/9579 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	-5.51	99.33	113.10

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	62	0
1	B	3421	0	3312	55	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	17	0	14	1	0
3	B	17	0	13	2	0
4	A	25	0	20	2	0
4	B	25	0	20	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	388	0	0	3	2
6	B	443	0	0	8	1
All	All	7867	0	6757	119	2

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 9.

All (119) 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	1.49	0.93
1:A:153:ILE:HD12	1:A:153:ILE:H	1.50	0.76
1:A:83:ASN:ND2	1:A:85:GLY:H	1.85	0.74
1:B:77:GLN:O	1:B:96:HIS:HE1	1.75	0.69
1:A:488:GLU:HB2	1:A:491:LYS:HE2	1.74	0.68
1:B:152:LYS:HB3	1:B:152:LYS:HZ2	1.58	0.68
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.23	0.67
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.78	0.66
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.97	0.64
1:A:309:ASP:OD1	1:A:496:GLN:HG2	1.98	0.62
1:B:105:LYS:HD3	6:B:4610:HOH:O	2.00	0.61
1:A:83:ASN:HD22	1:A:86:SER:H	1.48	0.61
1:A:195:ILE:HD12	6:A:4332:HOH:O	2.00	0.60
1:B:190:ASN:O	1:B:192:PRO:HD3	2.01	0.60
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.83	0.60
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.37	0.60
1:B:304:GLN:HG3	1:B:308:GLN:O	2.02	0.59
1:A:103:THR:HG22	1:A:118:SER:OG	2.03	0.58
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.33	0.58
1:B:125:ASP:OD2	1:B:126:LYS:HG3	2.04	0.58
1:B:170:THR:HG21	6:B:4493:HOH:O	2.03	0.58
1:A:213:THR:OG1	1:A:216:GLU:HG3	2.04	0.58
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.39	0.57
1:A:239:THR:O	1:A:361:CYS:HA	2.04	0.57
1:B:152:LYS:HB3	1:B:152:LYS:NZ	2.19	0.57
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.38	0.57
1:A:153:ILE:HD12	1:A:153:ILE:N	2.19	0.57
1:B:382:ARG:NH2	4:B:2905:328:H2	2.20	0.56
1:A:97:LYS:N	1:A:97:LYS:HD2	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:O	1:A:310:PRO:HA	2.06	0.56
1:A:83:ASN:HD22	1:A:85:GLY:H	1.51	0.55
1:A:357:GLU:O	1:A:359:PRO:HD3	2.06	0.55
1:A:465:SER:O	1:A:471:HIS:HE1	1.89	0.55
1:B:256:SER:HB3	1:B:257:GLN:NE2	2.21	0.55
1:B:110:LEU:HD22	6:B:4611:HOH:O	2.06	0.55
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.42	0.54
1:B:334:GLN:NE2	1:B:335:GLU:HG3	2.22	0.54
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.07	0.54
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.38	0.54
1:B:239:THR:O	1:B:361:CYS:HA	2.07	0.54
1:B:99:THR:HG22	6:B:4825:HOH:O	2.09	0.53
1:A:190:ASN:O	1:A:192:PRO:HD3	2.09	0.52
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.91	0.52
1:B:348:ASN:HB2	6:B:4535:HOH:O	2.09	0.52
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.46	0.51
1:A:153:ILE:H	1:A:153:ILE:CD1	2.19	0.51
1:A:246:ASP:OD1	1:A:248:LYS:HB2	2.10	0.51
1:B:331:GLU:O	1:B:334:GLN:HG3	2.10	0.51
1:A:83:ASN:ND2	1:A:86:SER:H	2.08	0.51
1:B:98:ALA:O	1:B:100:SER:N	2.44	0.51
1:A:382:ARG:NH2	4:A:905:328:H2	2.26	0.50
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.94	0.50
1:B:153:ILE:O	1:B:157:LEU:HG	2.12	0.50
1:A:134:LEU:O	1:A:138:ILE:HG12	2.12	0.50
1:A:215:GLN:O	1:A:219:GLN:HG3	2.11	0.50
1:A:137:ALA:O	1:A:141:ILE:HG12	2.12	0.49
1:B:103:THR:HG22	1:B:118:SER:OG	2.12	0.49
1:B:456:ILE:HG22	3:B:2902:H4B:H71	1.94	0.49
1:B:110:LEU:N	1:B:110:LEU:HD12	2.27	0.49
1:A:159:ARG:O	1:A:163:VAL:HG23	2.12	0.49
1:A:110:LEU:HD12	1:A:110:LEU:N	2.28	0.49
1:A:334:GLN:OE1	1:A:335:GLU:N	2.45	0.49
1:B:375:ARG:O	1:B:379:ASP:HB2	2.12	0.49
1:B:104:CYS:HA	1:B:110:LEU:CD1	2.43	0.49
1:B:142:ASN:OD1	1:B:156:HIS:NE2	2.45	0.48
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.43	0.48
1:A:161:GLU:O	1:A:165:LYS:HD3	2.12	0.48
1:B:295:ARG:HD2	6:B:4545:HOH:O	2.13	0.48
1:B:143:GLN:HG3	6:B:4624:HOH:O	2.15	0.47
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:HB3	1:B:457:TRP:CE3	2.51	0.46
1:B:271:ILE:HD12	1:B:278:LEU:HD11	1.98	0.46
1:A:104:CYS:HG	1:A:109:CYS:HG	1.58	0.46
2:A:901:HEM:HBC2	2:A:901:HEM:HMC1	1.98	0.46
1:A:82:LYS:O	1:A:473:GLU:HG3	2.16	0.45
1:A:102:PHE:HA	6:A:4343:HOH:O	2.16	0.45
1:B:332:TRP:O	1:B:335:GLU:HB2	2.16	0.45
1:B:456:ILE:CG2	3:B:2902:H4B:H71	2.47	0.45
1:A:374:VAL:O	1:A:378:CYS:HB2	2.17	0.45
1:B:480:SER:HA	1:B:481:PRO:C	2.36	0.45
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.51	0.45
1:B:104:CYS:HA	1:B:110:LEU:HD13	1.98	0.45
1:A:81:ILE:HD11	1:A:475:LEU:CD1	2.48	0.44
1:A:382:ARG:CZ	4:A:905:328:H2	2.48	0.44
1:B:195:ILE:O	1:B:195:ILE:HG13	2.18	0.44
1:B:98:ALA:O	1:B:99:THR:C	2.56	0.44
1:A:453:ALA:HB1	1:A:458:LEU:CD1	2.48	0.44
1:A:77:GLN:O	1:A:96:HIS:HE1	2.00	0.44
1:B:98:ALA:O	1:B:100:SER:O	2.36	0.43
1:B:164:THR:O	1:B:168:GLU:HG3	2.19	0.43
1:B:418:HIS:HD2	6:B:4721:HOH:O	2.01	0.43
1:A:256:SER:HB3	1:A:257:GLN:HE22	1.84	0.43
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.00	0.43
1:A:195:ILE:HG12	1:A:195:ILE:O	2.18	0.43
1:A:256:SER:HB3	1:A:257:GLN:NE2	2.33	0.42
1:A:334:GLN:OE1	1:A:335:GLU:HG3	2.19	0.42
1:B:78:TYR:CD1	1:B:78:TYR:C	2.92	0.42
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.01	0.42
1:A:133:LEU:HD22	6:A:4180:HOH:O	2.18	0.42
1:A:470:PHE:C	1:A:470:PHE:CD1	2.93	0.42
1:A:309:ASP:OD2	1:A:495:TRP:HE3	2.03	0.42
1:B:276:ALA:HB2	1:B:382:ARG:HD2	2.01	0.42
1:B:81:ILE:HD13	1:B:81:ILE:HA	1.85	0.42
1:A:283:LEU:O	1:A:287:LEU:HG	2.19	0.42
1:A:469:VAL:HG13	1:A:474:MET:CE	2.49	0.42
1:A:410:THR:O	1:A:414:VAL:HG23	2.20	0.41
1:B:350:LEU:C	1:B:350:LEU:HD23	2.40	0.41
1:A:165:LYS:HD2	1:A:165:LYS:N	2.34	0.41
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.55	0.41
1:A:153:ILE:HG22	1:A:157:LEU:HD23	2.03	0.41
1:B:371:GLU:OE2	4:B:2905:328:N22	2.53	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HZ	1:A:476:ASN:ND2	2.18	0.41
1:A:97:LYS:N	1:A:97:LYS:CD	2.84	0.41
1:B:268:ASP:OD1	1:B:270:THR:HG23	2.21	0.41
1:A:238:ILE:HG13	1:A:363:PHE:HB3	2.02	0.40
2:B:2901:HEM:HBC2	2:B:2901:HEM:HMC1	2.03	0.40
1:B:254:TRP:HB2	1:B:302:VAL:HB	2.02	0.40
1:A:138:ILE:O	1:A:142:ASN:ND2	2.54	0.40
1:A:456:ILE:CG2	3:A:902:H4B:H71	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:4789:HOH:O	6:B:4330:HOH:O[12_556]	1.94	0.26
6:A:4196:HOH:O	6:A:4210:HOH:O[11_655]	2.06	0.14

## 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%)	389 (93%)	28 (7%)	2 (0%)	29 31
1	B	419/433 (97%)	388 (93%)	27 (6%)	4 (1%)	15 14
All	All	838/866 (97%)	777 (93%)	55 (7%)	6 (1%)	22 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	B	99	THR
1	B	104	CYS
1	A	464	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	103	THR
1	B	98	ALA

### 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%)	361 (98%)	6 (2%)	62	76
1	B	366/381 (96%)	362 (99%)	4 (1%)	73	85
All	All	733/762 (96%)	723 (99%)	10 (1%)	67	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	114	MET
1	A	202	ASN
1	A	223	ARG
1	A	334	GLN
1	A	442	GLN
1	B	130	LEU
1	B	223	ARG
1	B	348	ASN
1	B	442	GLN

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

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	142	ASN
1	A	202	ASN
1	A	215	GLN
1	A	219	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS
1	B	96	HIS
1	B	215	GLN
1	B	334	GLN
1	B	348	ASN
1	B	421	GLN
1	B	493	HIS

### 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](#)

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	$\# Z  > 2$
5	SO4	A	3001	-	4,4,4	0.29	0	6,6,6	0.10	0
3	H4B	B	2902	-	16,18,18	1.85	3 (18%)	11,26,26	5.85	9 (81%)
5	SO4	B	3003	-	4,4,4	0.27	0	6,6,6	0.09	0
4	328	B	2905	-	27,27,27	1.85	6 (22%)	35,36,36	1.74	12 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	2901	1	27,50,50	1.61	4 (14%)	17,82,82	1.09	2 (11%)
4	328	A	905	-	27,27,27	1.80	6 (22%)	35,36,36	1.85	11 (31%)
2	HEM	A	901	1	27,50,50	1.53	3 (11%)	17,82,82	1.05	1 (5%)
3	H4B	A	902	-	16,18,18	1.87	3 (18%)	11,26,26	9.26	8 (72%)
5	SO4	A	3002	-	4,4,4	0.25	0	6,6,6	0.09	0
5	SO4	B	3004	-	4,4,4	0.25	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
3	H4B	B	2902	-	1/1/3/5	2/8/17/17	0/2/2/2
4	328	B	2905	-	-	2/16/26/26	0/3/3/3
2	HEM	B	2901	1	-	0/6/54/54	-
4	328	A	905	-	-	3/16/26/26	0/3/3/3
2	HEM	A	901	1	-	0/6/54/54	-
3	H4B	A	902	-	1/1/3/5	5/8/17/17	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	H4B	C7-C6	-5.70	1.46	1.52
3	B	2902	H4B	C7-C6	-5.61	1.46	1.52
2	B	2901	HEM	C3B-C2B	-3.98	1.34	1.40
3	B	2902	H4B	C7-N8	-3.96	1.38	1.44
2	A	901	HEM	C3C-CAC	-3.89	1.39	1.47
4	A	905	328	C15-C14	3.89	1.61	1.52
3	A	902	H4B	C7-N8	-3.89	1.38	1.44
2	A	901	HEM	C3B-CAB	-3.79	1.40	1.47
2	B	2901	HEM	C3C-CAC	-3.72	1.40	1.47
4	B	2905	328	C15-C14	3.63	1.60	1.52
4	B	2905	328	C5-C6	3.52	1.45	1.39
2	B	2901	HEM	C3B-CAB	-3.44	1.40	1.47
4	A	905	328	C5-C6	3.28	1.44	1.39
4	B	2905	328	C2-C1	3.20	1.44	1.38
4	A	905	328	C2-C1	3.18	1.44	1.38
4	B	2905	328	C2-C3	2.84	1.45	1.39
2	A	901	HEM	C3B-C2B	-2.84	1.36	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2905	328	C16-N11	2.72	1.40	1.34
4	A	905	328	C2-C3	2.67	1.45	1.39
4	A	905	328	C1-C6	2.66	1.43	1.39
4	B	2905	328	C1-C6	2.64	1.43	1.39
4	A	905	328	C16-N11	2.55	1.40	1.34
2	B	2901	HEM	C1C-C2C	2.39	1.48	1.42
3	B	2902	H4B	C4A-N5	-2.08	1.33	1.38
3	A	902	H4B	C4A-N5	-2.05	1.33	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	H4B	C4-C4A-N5	21.16	136.88	119.12
3	A	902	H4B	C4-C4A-C8A	-18.39	98.23	114.57
3	B	2902	H4B	C4-C4A-N5	11.76	128.99	119.12
3	B	2902	H4B	C4-C4A-C8A	-11.16	104.65	114.57
3	A	902	H4B	O10-C10-C11	-7.31	88.09	109.74
3	B	2902	H4B	N2-C2-N1	-6.66	106.90	117.25
3	A	902	H4B	N2-C2-N1	-5.95	107.99	117.25
4	A	905	328	C15-C10-N11	-4.55	103.91	110.82
3	A	902	H4B	N2-C2-N3	4.42	124.13	117.25
3	B	2902	H4B	C2-N1-C8A	-4.38	104.71	114.54
3	A	902	H4B	C4A-C4-N3	4.20	135.95	124.01
3	B	2902	H4B	N2-C2-N3	4.05	123.56	117.25
4	B	2905	328	C15-C10-N11	-3.99	104.76	110.82
4	B	2905	328	C21-N22-C23	3.74	122.53	117.22
4	A	905	328	C21-N22-C23	3.74	122.52	117.22
3	A	902	H4B	O9-C9-C6	-3.70	100.14	108.98
4	A	905	328	C20-C21-N22	-3.69	119.38	123.96
3	B	2902	H4B	O10-C10-C11	-3.56	99.19	109.74
4	B	2905	328	C20-C21-N22	-3.55	119.55	123.96
4	A	905	328	C15-C14-N17	3.26	115.67	110.60
4	A	905	328	C13-C12-N11	-3.18	105.98	110.82
3	A	902	H4B	C4-N3-C2	-3.17	110.88	115.93
4	B	2905	328	C15-C14-N17	3.03	115.32	110.60
4	A	905	328	C6-C16-N11	2.86	122.34	118.72
3	B	2902	H4B	C4A-N5-C6	-2.64	113.97	121.16
3	B	2902	H4B	N3-C2-N1	2.63	129.54	125.42
4	A	905	328	C21-C20-C19	2.48	120.42	118.02
4	B	2905	328	C13-C12-N11	-2.47	107.07	110.82
4	B	2905	328	C24-C23-N22	-2.41	119.39	122.75
4	A	905	328	C13-C14-N17	-2.40	106.85	110.60

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2901	HEM	C4C-C3C-C2C	-2.40	105.22	106.90
4	B	2905	328	C6-C16-N11	2.40	121.76	118.72
4	A	905	328	O8-C16-C6	-2.40	115.56	120.23
4	B	2905	328	C9-O18-C19	2.36	122.63	117.51
3	B	2902	H4B	O9-C9-C6	2.25	114.36	108.98
4	A	905	328	C9-O18-C19	2.21	122.31	117.51
4	B	2905	328	C21-C20-C19	2.19	120.15	118.02
4	A	905	328	C24-C23-N22	-2.19	119.70	122.75
2	A	901	HEM	C1D-C2D-C3D	-2.19	105.47	107.00
4	B	2905	328	O8-C16-C6	-2.17	116.01	120.23
4	B	2905	328	C13-C14-N17	-2.16	107.23	110.60
2	B	2901	HEM	CBD-CAD-C3D	-2.09	108.62	112.48
4	B	2905	328	C12-N11-C10	2.05	116.57	112.62

All (2) chirality outliers are listed below:

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

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2902	H4B	N5-C6-C9-O9
3	B	2902	H4B	C7-C6-C9-C10
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	A	902	H4B	O10-C10-C9-C6
4	A	905	328	N22-C23-N17-C14
4	B	2905	328	C13-C14-N17-C23
4	B	2905	328	C15-C14-N17-C23
4	A	905	328	C13-C14-N17-C23
4	A	905	328	C15-C14-N17-C23
3	A	902	H4B	O10-C10-C9-O9

There are no ring outliers.

6 monomers are involved in 9 short contacts:

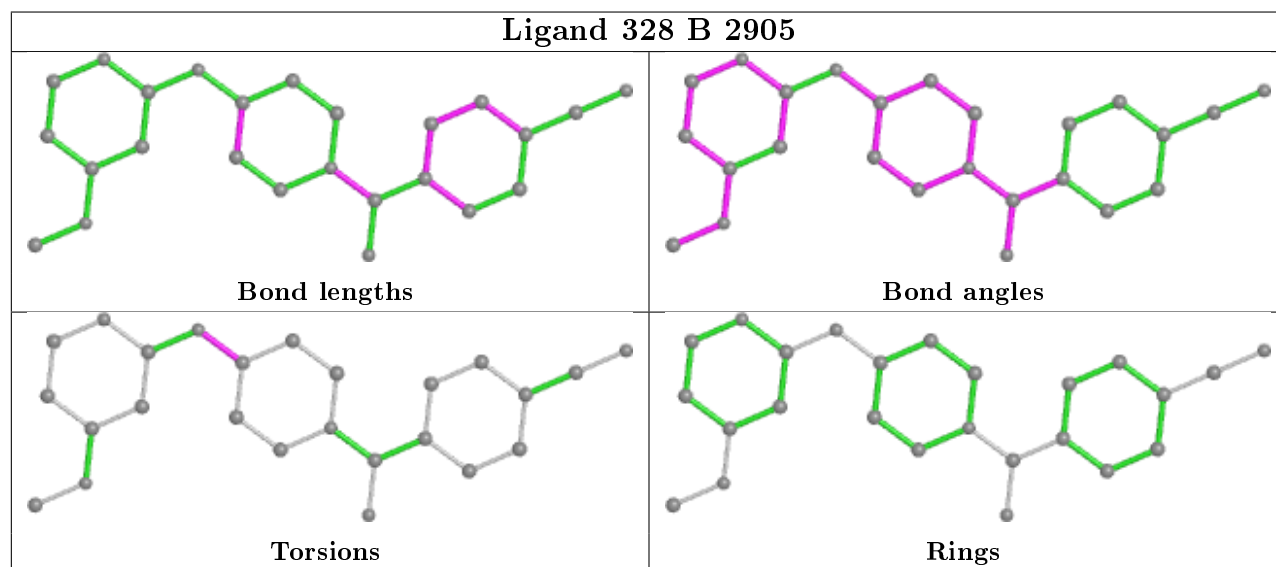
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2902	H4B	2	0

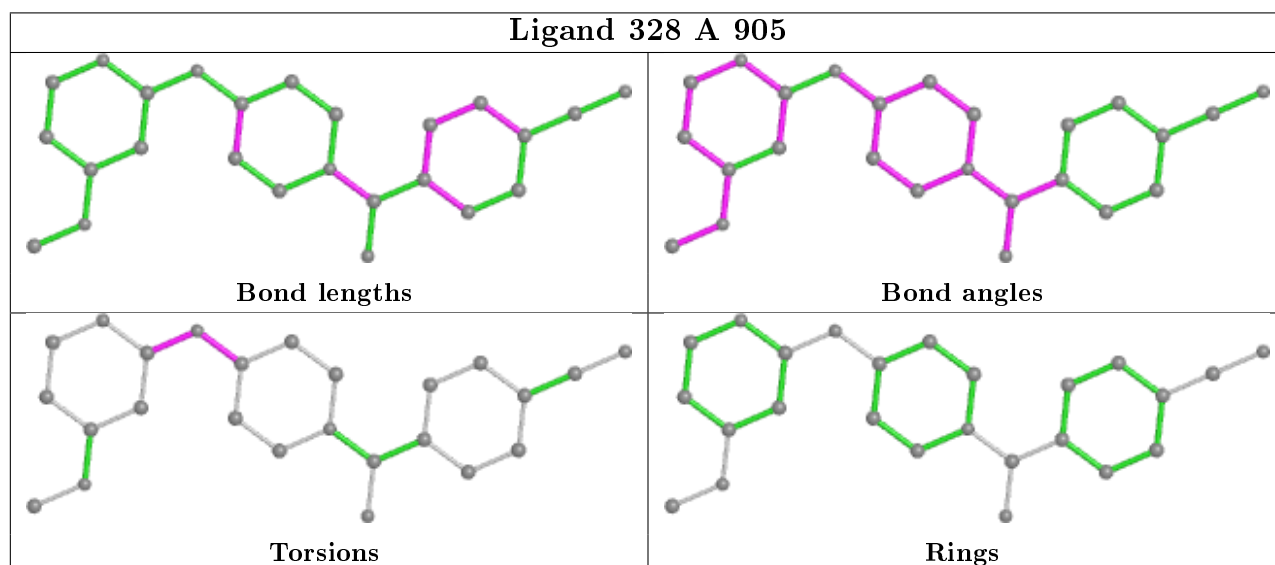
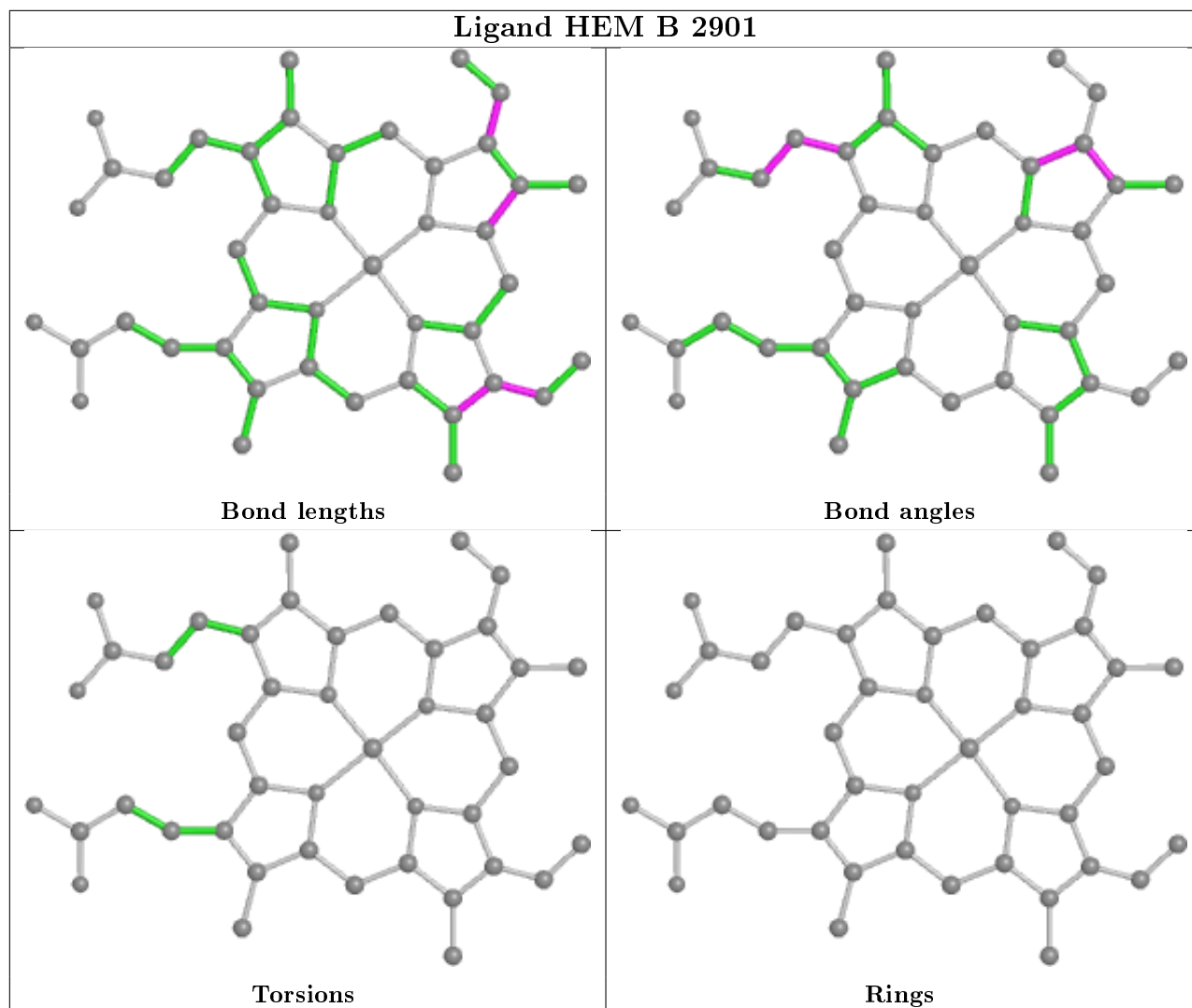
Continued on next page...

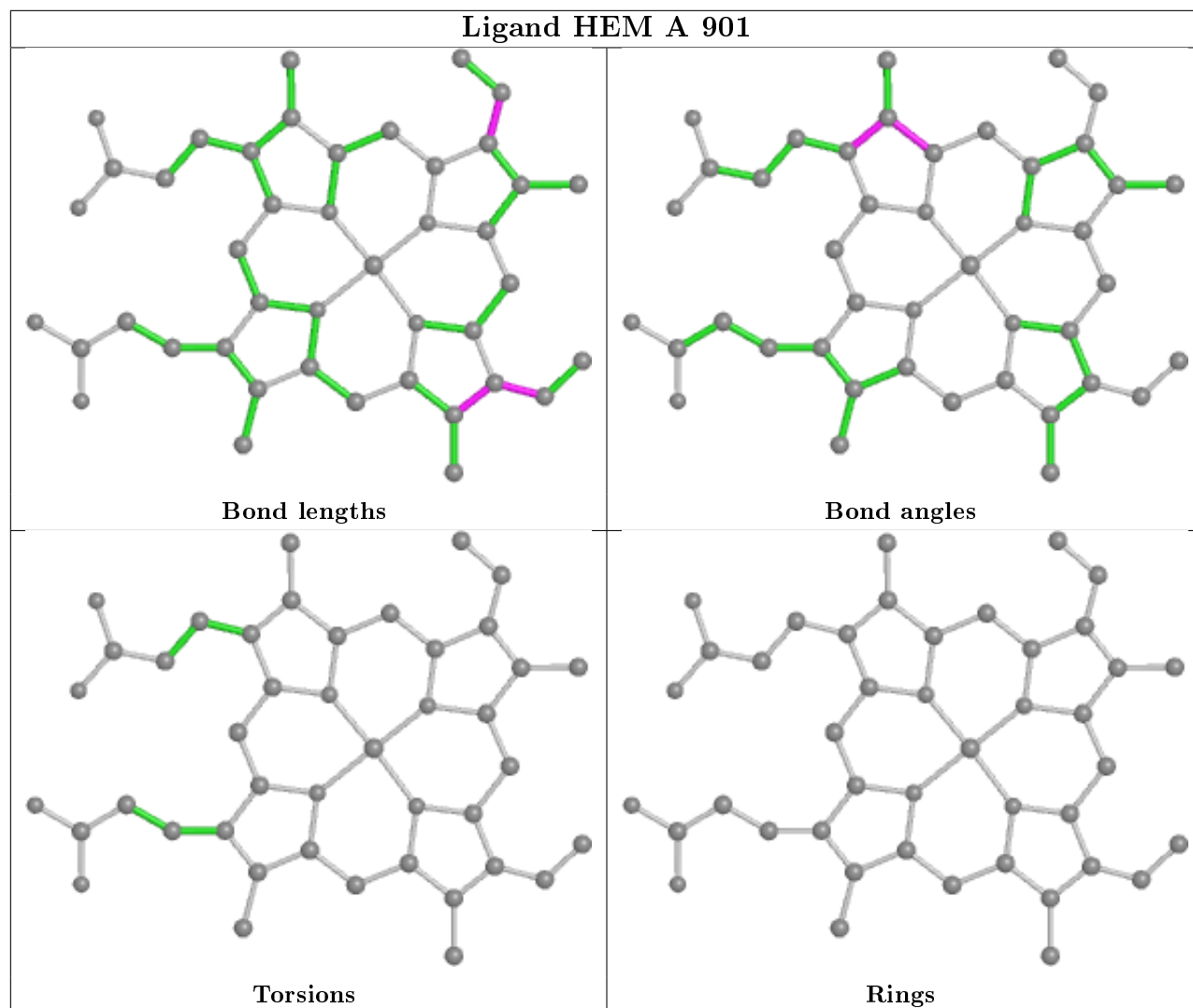
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2905	328	2	0
2	B	2901	HEM	1	0
4	A	905	328	2	0
2	A	901	HEM	1	0
3	A	902	H4B	1	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%)	-0.05	19 (4%) 33 32	27, 45, 70, 95	0
1	B	421/433 (97%)	-0.08	19 (4%) 33 32	25, 42, 67, 96	0
All	All	842/866 (97%)	-0.06	38 (4%) 33 32	25, 44, 70, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	THR	9.4
1	B	101	ASP	5.8
1	A	104	CYS	5.7
1	B	103	THR	5.5
1	B	104	CYS	5.3
1	B	497	ASN	5.1
1	A	149	LYS	5.0
1	A	107	LYS	4.8
1	A	100	SER	4.7
1	A	106	SER	4.5
1	B	107	LYS	4.5
1	B	106	SER	4.3
1	B	149	LYS	4.3
1	A	103	THR	4.2
1	A	101	ASP	4.2
1	B	102	PHE	4.1
1	A	151	ALA	4.1
1	B	494	ILE	3.9
1	A	496	GLN	3.5
1	A	102	PHE	3.3
1	A	150	GLU	3.3
1	A	78	TYR	3.2
1	A	497	ASN	3.1
1	B	495	TRP	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	150	GLU	2.9
1	B	108	SER	2.9
1	A	398	HIS	2.8
1	B	105	LYS	2.7
1	B	153	ILE	2.7
1	A	331	GLU	2.6
1	A	495	TRP	2.5
1	A	148	PHE	2.5
1	B	152	LYS	2.4
1	B	446	ARG	2.3
1	A	212	SER	2.2
1	B	496	GLN	2.2
1	A	152	LYS	2.2
1	B	398	HIS	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. 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.

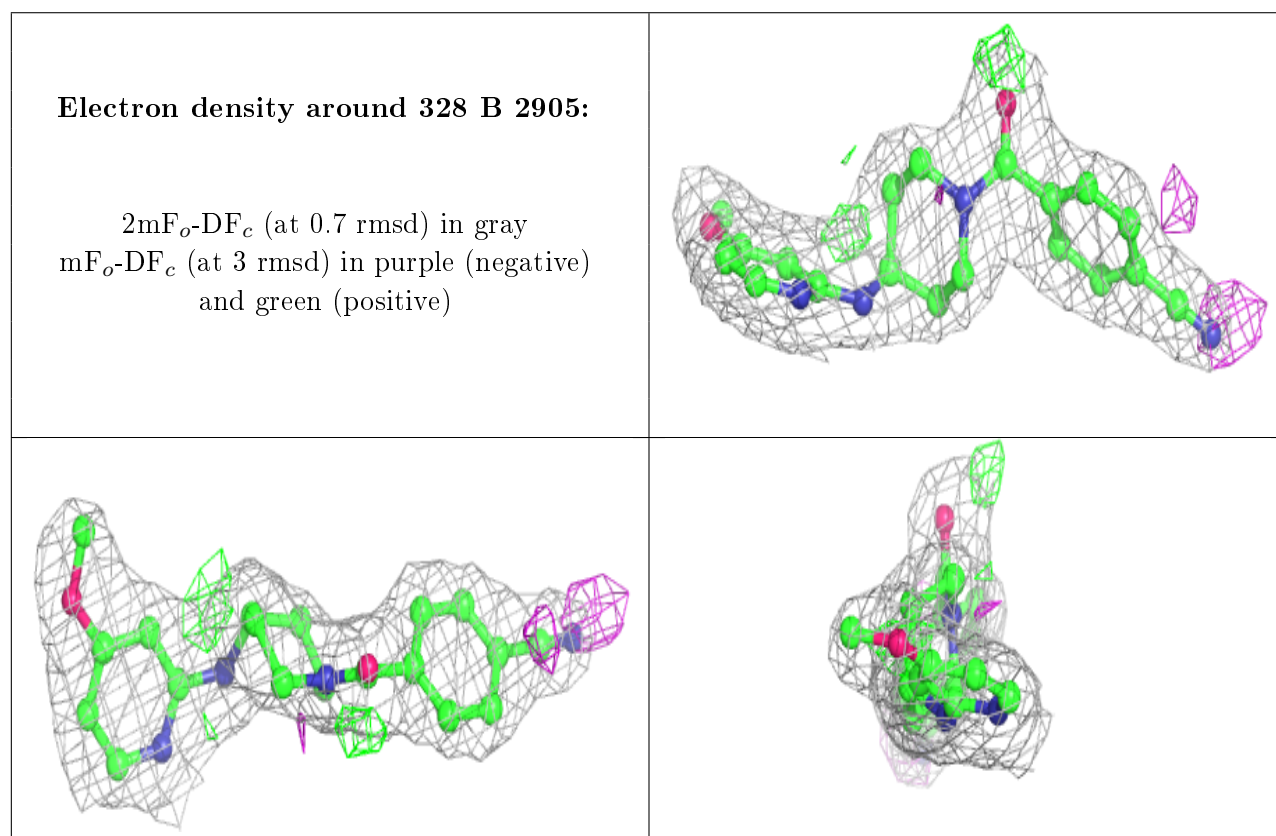
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	B	3004	5/5	0.85	0.29	97,98,99,100	0
5	SO4	A	3002	5/5	0.89	0.25	93,94,94,94	0
5	SO4	A	3001	5/5	0.89	0.27	106,106,106,106	0
5	SO4	B	3003	5/5	0.91	0.27	104,104,105,106	0
4	328	B	2905	25/25	0.95	0.11	21,26,28,32	0
4	328	A	905	25/25	0.95	0.11	24,28,31,37	0
3	H4B	A	902	17/17	0.97	0.06	23,30,35,35	0
2	HEM	B	2901	43/43	0.98	0.08	19,25,29,30	0
3	H4B	B	2902	17/17	0.98	0.06	23,28,33,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	901	43/43	0.98	0.09	25,28,30,33	0

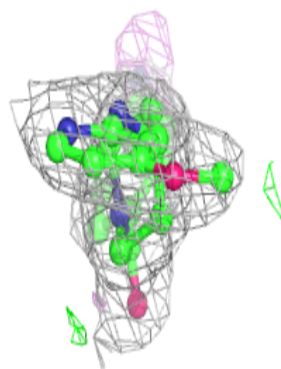
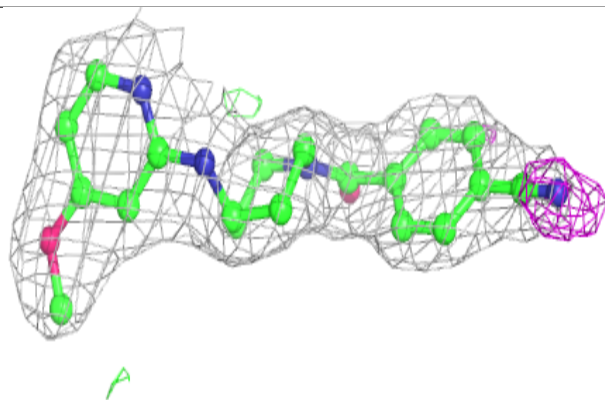
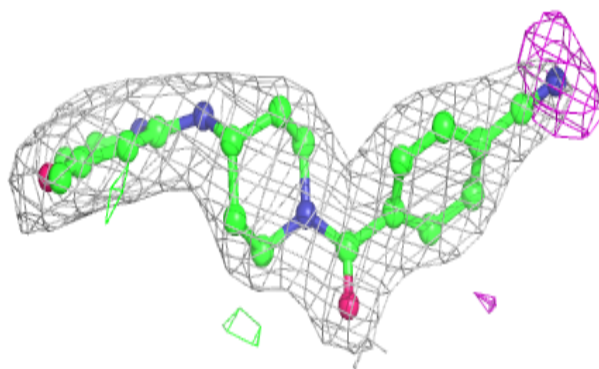
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





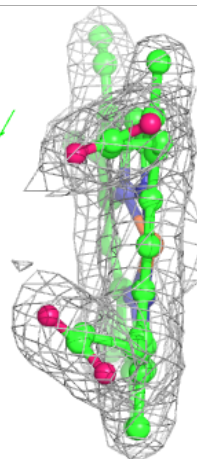
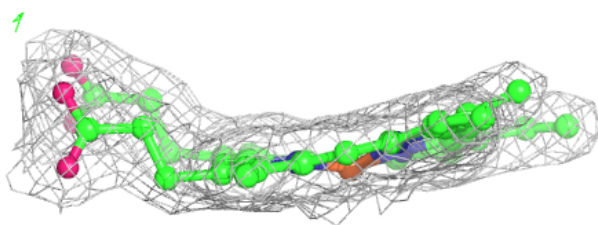
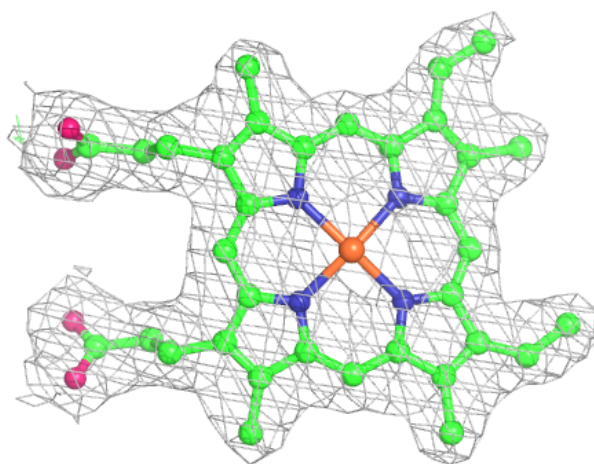
**Electron density around 328 A 905:**

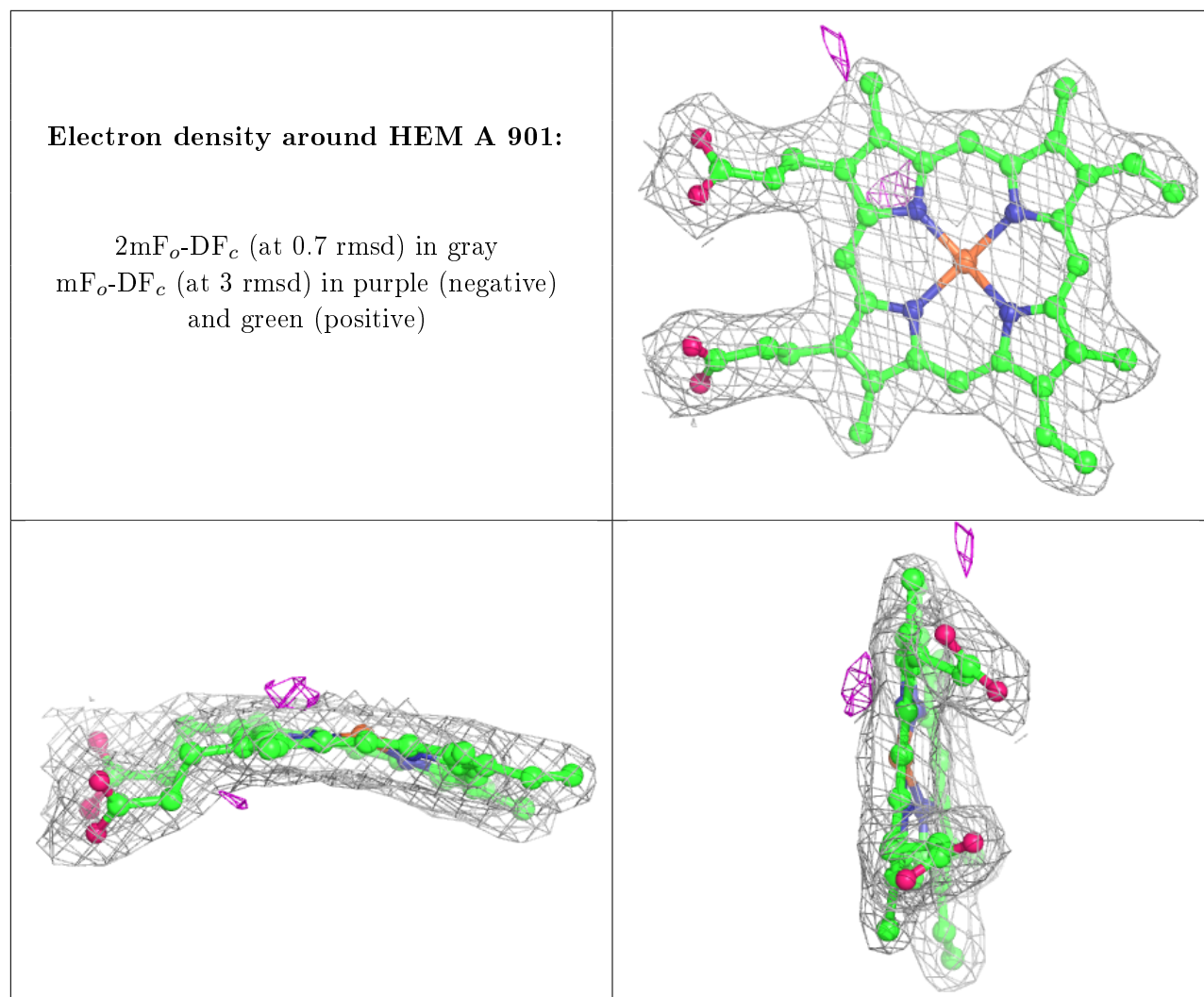
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 2901:**

$2mF_o-DF_c$  (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.