



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:43 AM UTC

PDB ID : 3E6O / pdb_00003e6o
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C124355
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, 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.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-15
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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](#) ①) 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

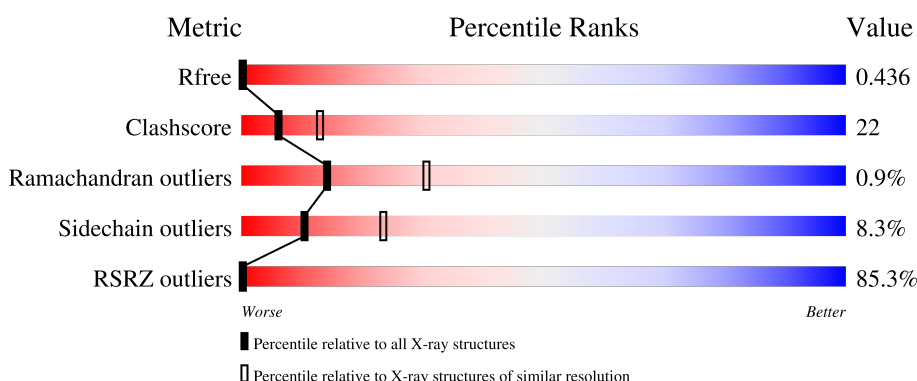
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	433	81% 53% 37% 5% • •
1	B	433	82% 58% 32% 5% 5%

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	-	-	-

2 Entry composition [i](#)

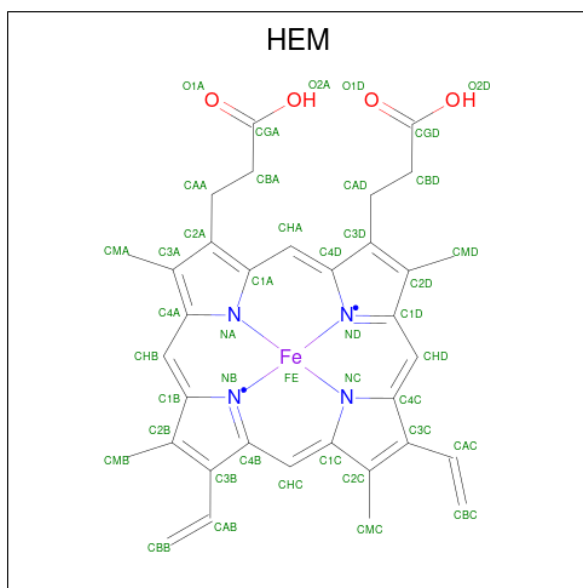
There are 5 unique types of molecules in this entry. The entry contains 7171 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

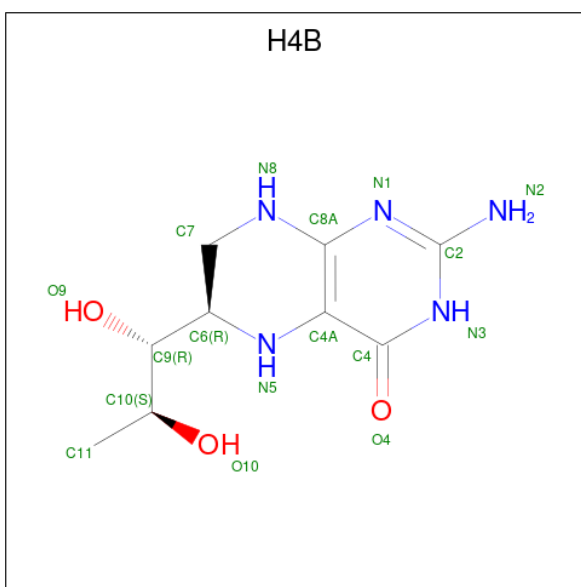
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3385	2171	582	612	20			
1	B	410	Total	C	N	O	S	0	0	0
			3347	2148	577	602	20			

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



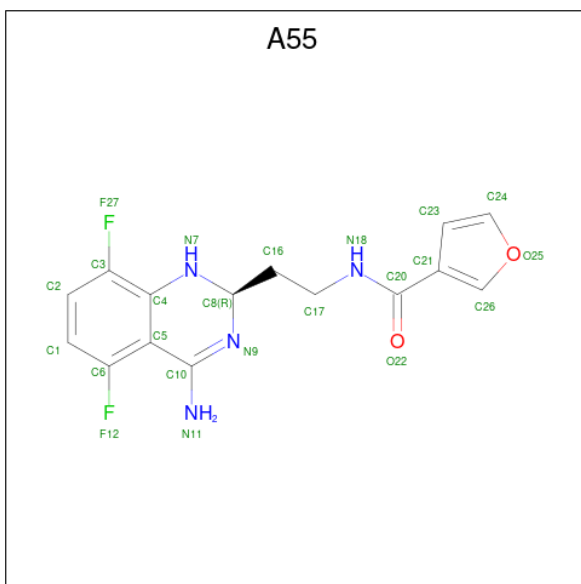
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is N-[2-(4-AMINO-5,8-DIFLUORO-1,2-DIHYDROQUINAZOLIN-2-YL)ETHYL]-3-FURAMIDE (CCD ID: A55) (formula: C₁₅H₁₄F₂N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			23	15	2	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			23	15	2	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	153	Total	O	0	0
			153	153		

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



E487	E427	Y367	D306	D246	M186	K126
E488	E428	M368	Q307	G247	A187	T127
E489	E429	G369	Q308	G248	E188	T128
W490	H430	T370	D309	H249	R189	P129
E491	H431	E371	P310	D250	N190	L130
E492	T432	I372	E311	F251	A191	E131
E493	A433	G373	V312	L252	P192	E132
E494	E434	F374	F313	L253	R193	L133
W495	E435	R375	E314	W254	C194	L134
GLN	E436	D376	E315	N255	I195	P135
ASN	F437	F377	P316	S256	G196	H136
GLU	M438	G378	P317	Q257	R197	A137
	E439	D379	D318	L258	I198	I138
	H440	T380	L319	T259	Q199	E139
	M441	Q381	V320	R260	W200	F140
	Q442	R382		Y261	S201	I141
	N443	F383	V323	A262	N202	M142
	E444	N384	T324	G263	L203	Q143
	Y445	L385	M325	Y264	Q204	F144
	R446	L386	E326	Q265	V205	Y145
	A447	E387	H327	M266	F206	G146
	R448	E388	P328	F267	D207	S147
	G449	V389	K329	D268	A208	F148
	G450	G390	V330	G269	R209	K149
	C451	R391	E331	G270	N210	E150
	P452	R392	V332	I271	C211	A151
	A453	N393	F333	R272	S212	K152
	D454	G394	Q334	G273	T213	I153
	W455	L395	E335	D274	A214	F154
	T456	E396	L336	A275	Q215	E155
	W457	T397		A276	E216	H156
	L458	H398	L338	T277	M217	L157
	W459	T399	K339	L278	F218	A158
	P460	L400	V340	E279	Q219	R159
	P461	A401	V341	F280	H220	L160
	W462	S402	A342	T281	T221	E161
	S463	L403	L343	Q282	C222	A162
	G464	W404	P344	L283	V163	F163
	S465	K405	A345	C284	H224	T164
	I466	D406	V346	L285	L225	K165
	T467	R407	A347	D286	L226	F166
	P468	A408	R348	L287	Y227	I167
	W469	W409	F349	G288	A228	E168
	F470	T410	L350	W289	T229	T169
	H471	E411	L351	K290	N230	T170
	Q472	L412	V352	P291	N231	G171
	E473	W413	G353	R292	G232	T172
	W474	W414	G354	Y293	N233	Y173
	L475	A415	G355	G294	L234	Q174
	W476	W416	L356	R295	R235	L175
	T477	L417	E357	F296	S236	T176
	W478	H418	F358	D297	A237	L177
	L479	S419	P359	Y298	L238	D178
	S480	F420	A360	L299	T239	E179
	P481	Q421	C361	P300	V240	L180
	F482	K422	P362	L301	F241	I181
	Y483	Q423	V363	V302	P242	F182
	Y484	N424	N364	L303	Q243	A183
	W485	W425	G365	G304	R244	T184
	P486	T426	V366	A205	G245	F185

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.60) 93.4 (19.96-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.262 0.416 , 0.436	Depositor DCC
R_{free} test set	2686 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	7171	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: HEM, H4B, A55

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	0.44	0/3484	0.94	11/4737 (0.2%)
1	B	0.43	0/3445	0.92	9/4684 (0.2%)
All	All	0.44	0/6929	0.93	20/9421 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	N-CA-C	-9.61	97.93	110.33
1	A	365	GLY	N-CA-C	-7.88	98.25	110.77
1	A	367	TYR	N-CA-C	6.85	119.80	110.55
1	B	386	LEU	N-CA-C	6.67	119.16	111.02
1	A	485	TYR	N-CA-C	-6.64	100.69	110.52

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	3385	0	3278	167	4
1	B	3347	0	3248	135	4
2	A	43	0	30	3	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	14	0	1
3	B	17	0	14	0	0
4	A	23	0	14	0	0
4	B	23	0	14	0	0
5	A	120	0	0	12	1
5	B	153	0	0	10	1
All	All	7171	0	6642	304	8

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 22.

The worst 5 of 304 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:195:ILE:HB	5:B:1937:HOH:O	1.33	1.26
1:A:195:ILE:HB	5:A:1043:HOH:O	1.43	1.18
1:B:438:MET:HE3	1:B:469:VAL:HG12	1.45	0.96
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.47	0.94
1:A:153:ILE:HD12	1:A:153:ILE:H	1.31	0.94

The worst 5 of 8 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)
1:B:406:ASP:OD2	1:B:463:SER:OG[9_766]	1.72	0.48
1:A:103:THR:CG2	1:A:118:SER:OG[11_655]	1.87	0.33
1:B:231:ASN:N	1:B:318:ASP:OD2[11_656]	1.99	0.21
1:B:318:ASP:N	5:B:1954:HOH:O[11_656]	1.99	0.21
1:A:470:PHE:O	3:A:902:H4B:O9[11_655]	2.00	0.20

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	411/433 (95%)	370 (90%)	35 (8%)	6 (2%)	8	18
1	B	406/433 (94%)	367 (90%)	38 (9%)	1 (0%)	43	66
All	All	817/866 (94%)	737 (90%)	73 (9%)	7 (1%)	14	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	200	TRP
1	A	306	ASP
1	B	306	ASP
1	A	307	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/381 (95%)	334 (92%)	29 (8%)	11	25
1	B	358/381 (94%)	327 (91%)	31 (9%)	9	21
All	All	721/762 (95%)	661 (92%)	60 (8%)	10	23

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	LEU
1	B	417	LEU
1	B	134	LEU
1	B	414	VAL
1	B	467	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	HIS

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Mol	Chain	Res	Type
1	B	143	GLN
1	B	423	GLN
1	B	115	ASN
1	B	199	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](#)

6 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	$\# Z > 2$
3	H4B	B	1902	-	17,18,18	2.77	3 (17%)	14,26,26	1.95	5 (35%)
4	A55	B	904	-	23,25,25	1.59	5 (21%)	25,35,35	2.04	10 (40%)
4	A55	A	903	-	23,25,25	1.62	5 (21%)	25,35,35	2.04	10 (40%)
2	HEM	B	1901	-	50,50,50	1.60	6 (12%)	67,82,82	1.14	5 (7%)
2	HEM	A	901	-	50,50,50	1.49	7 (14%)	67,82,82	1.32	8 (11%)
3	H4B	A	902	-	17,18,18	2.53	4 (23%)	14,26,26	1.97	4 (28%)

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	1902	-	-	0/8/17/17	0/2/2/2
4	A55	B	904	-	-	3/9/22/22	0/2/3/3
4	A55	A	903	-	-	2/9/22/22	0/2/3/3
2	HEM	B	1901	-	-	2/14/54/54	-
2	HEM	A	901	-	-	1/14/54/54	-
3	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1902	H4B	C7-N8	-7.89	1.38	1.46
3	A	902	H4B	C7-N8	-7.37	1.39	1.46
3	B	1902	H4B	C7-C6	-6.81	1.45	1.52
3	A	902	H4B	C7-C6	-5.75	1.46	1.52
2	B	1901	HEM	FE-NB	4.71	2.09	1.94

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	904	A55	O25-C26-C21	5.36	115.48	110.81
4	A	903	A55	O25-C26-C21	5.15	115.31	110.81
2	A	901	HEM	CMD-C2D-C1D	4.24	131.65	125.03
3	A	902	H4B	O4-C4-C4A	-4.14	117.27	127.26
2	A	901	HEM	C4B-C3B-C2B	-4.09	103.52	107.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6

5 of 12 torsion outliers are listed below:

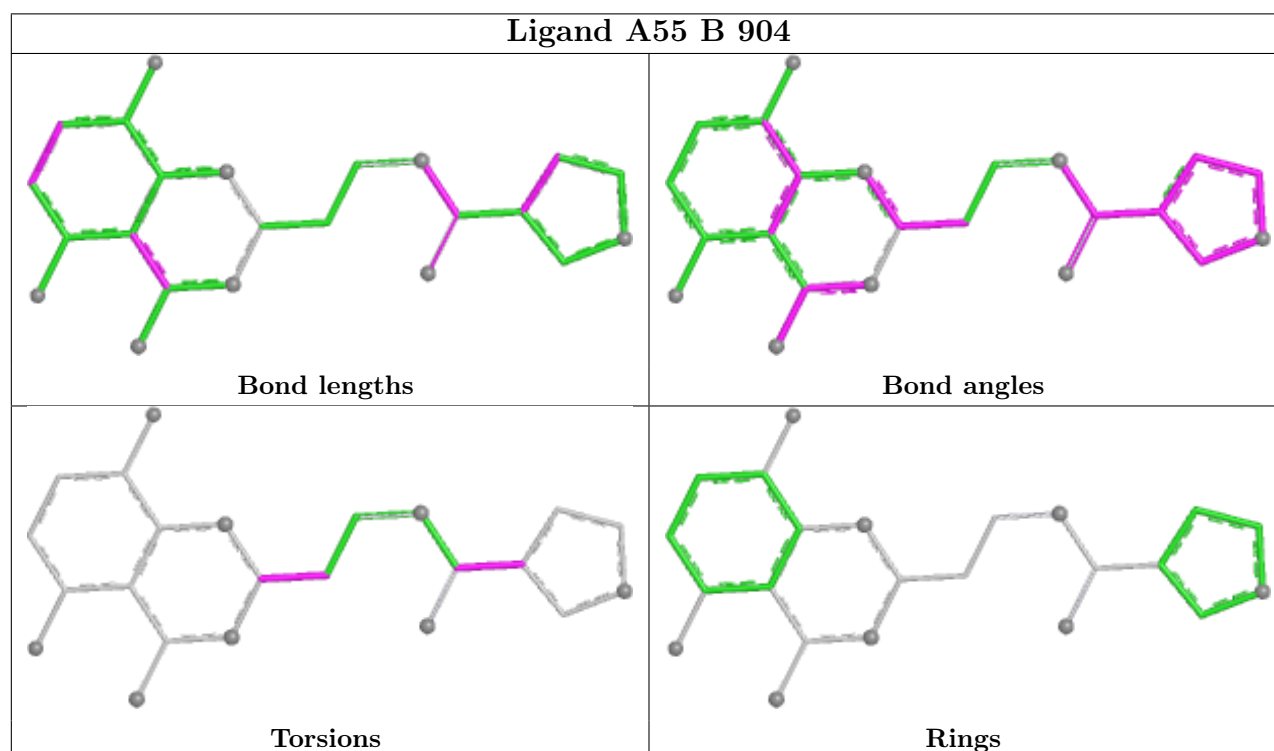
Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9
3	A	902	H4B	C7-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
4	B	904	A55	C17-C16-C8-N7
2	B	1901	HEM	C2B-C3B-CAB-CBB

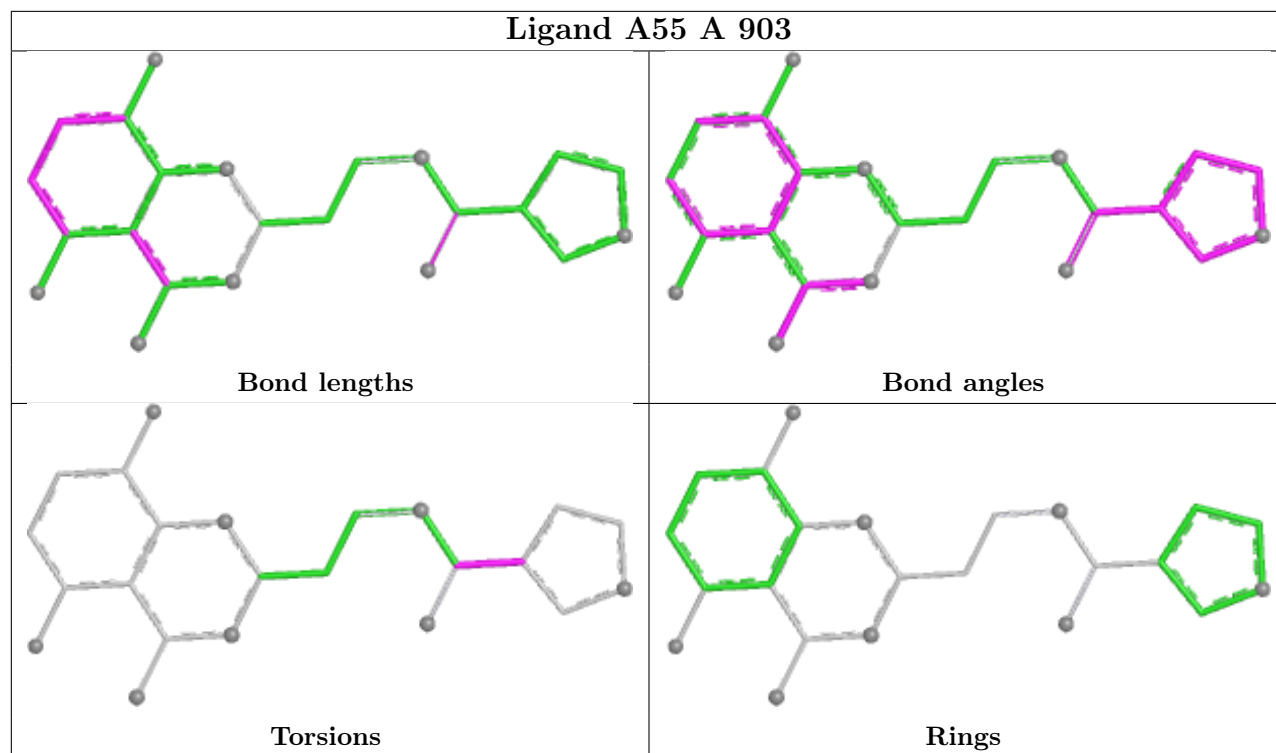
There are no ring outliers.

3 monomers are involved in 5 short contacts:

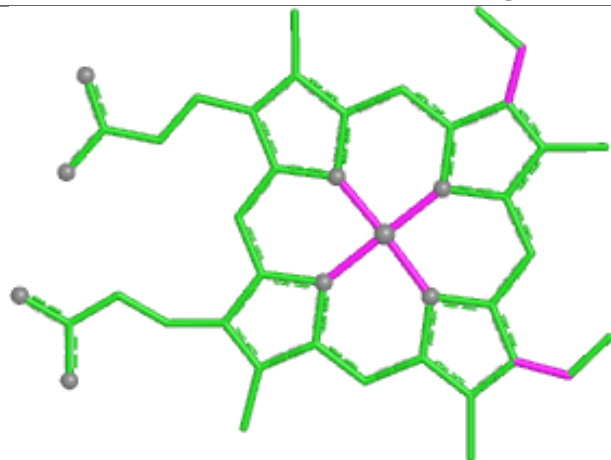
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1901	HEM	1	0
2	A	901	HEM	3	0
3	A	902	H4B	0	1

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.

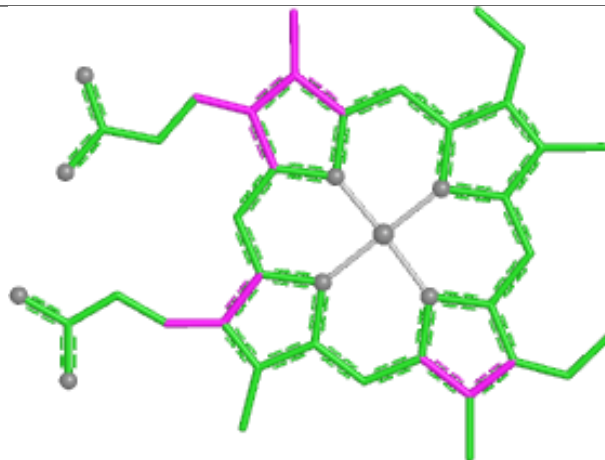




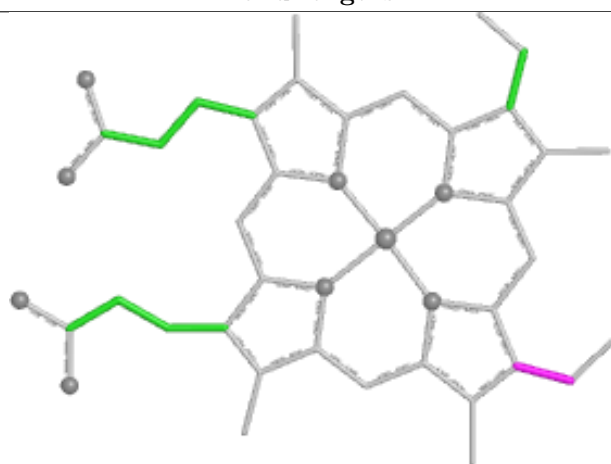
Ligand HEM B 1901



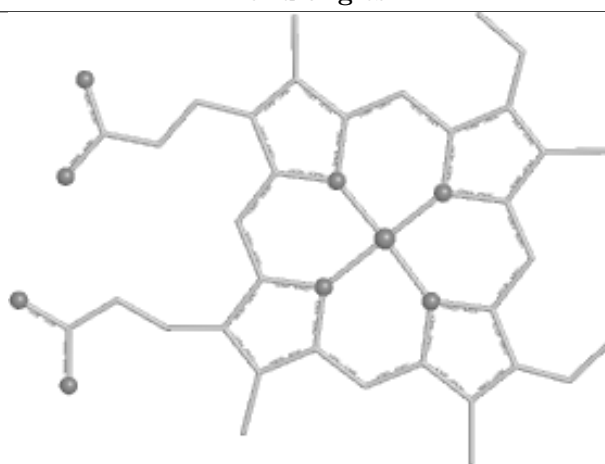
Bond lengths



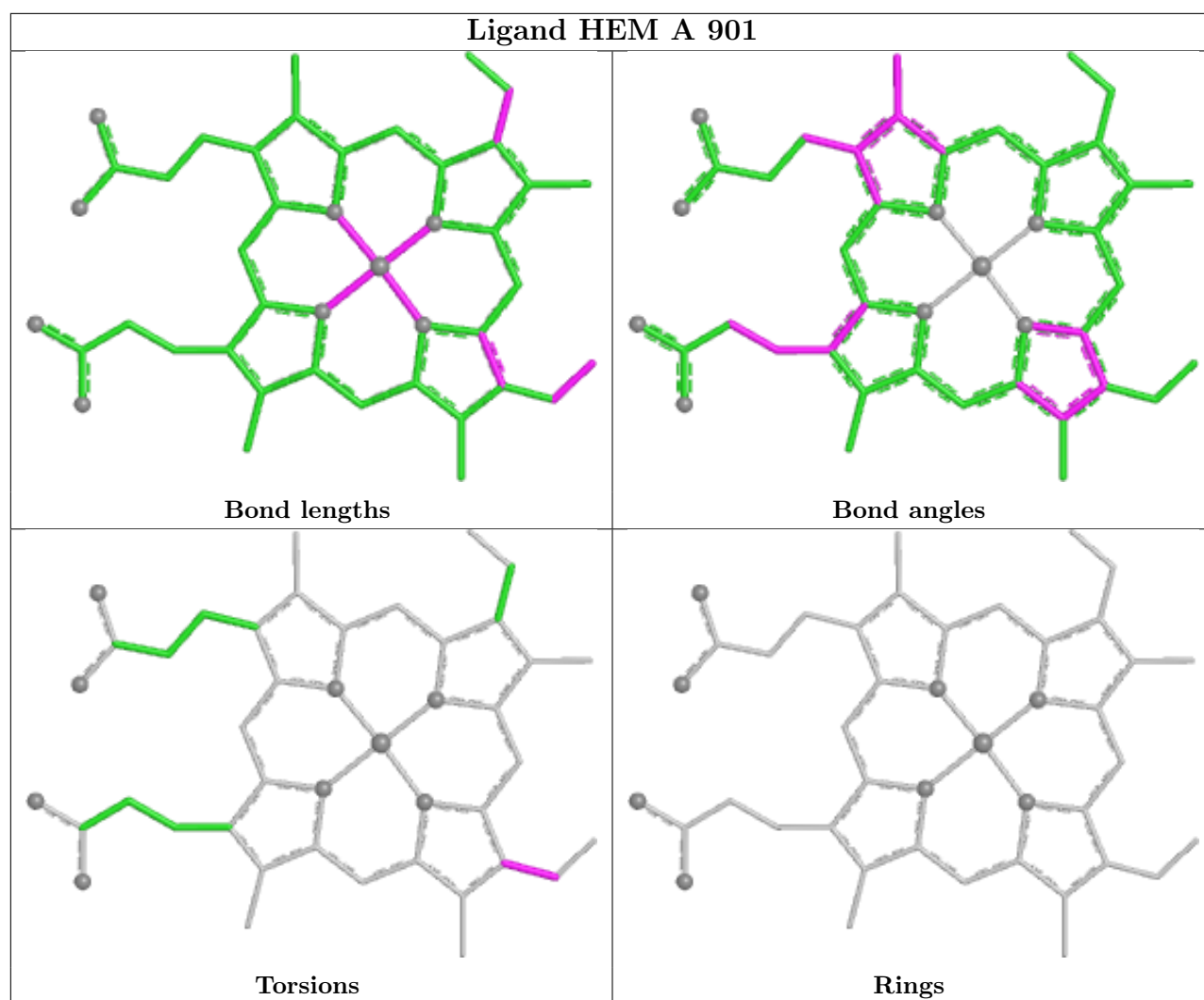
Bond angles



Torsions



Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	415/433 (95%)	3.07	349 (84%) 0 0	26, 45, 74, 99	0
1	B	410/433 (94%)	3.16	355 (86%) 0 0	25, 43, 68, 94	0
All	All	825/866 (95%)	3.12	704 (85%) 0 0	25, 44, 70, 99	0

The worst 5 of 704 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	CYS	7.8
1	A	102	PHE	7.3
1	B	494	ILE	6.8
1	B	112	SER	6.4
1	A	171	GLY	6.3

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](#)

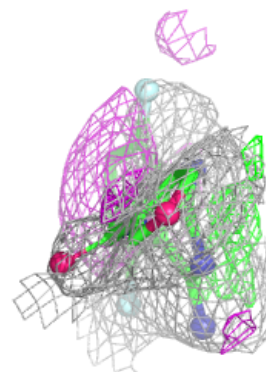
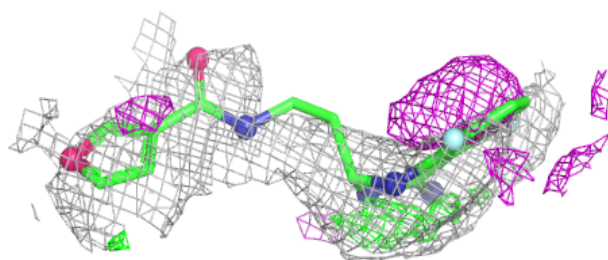
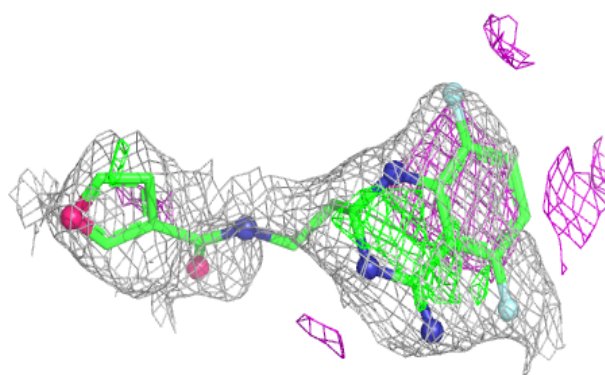
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	A55	B	904	23/23	0.51	0.27	23,31,54,56	0
3	H4B	B	1902	17/17	0.67	0.24	26,29,34,34	0
4	A55	A	903	23/23	0.71	0.21	28,32,46,48	0
2	HEM	B	1901	43/43	0.76	0.25	23,25,29,37	0
2	HEM	A	901	43/43	0.79	0.22	24,26,30,30	0
3	H4B	A	902	17/17	0.80	0.16	28,30,31,32	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.

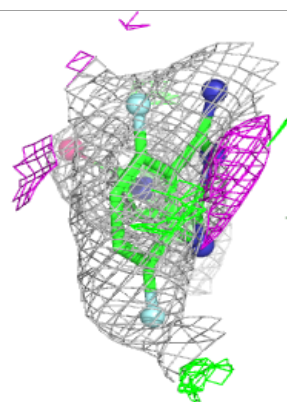
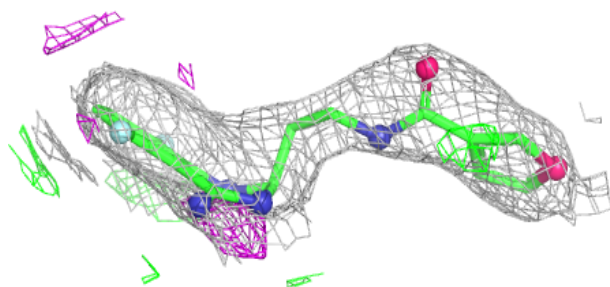
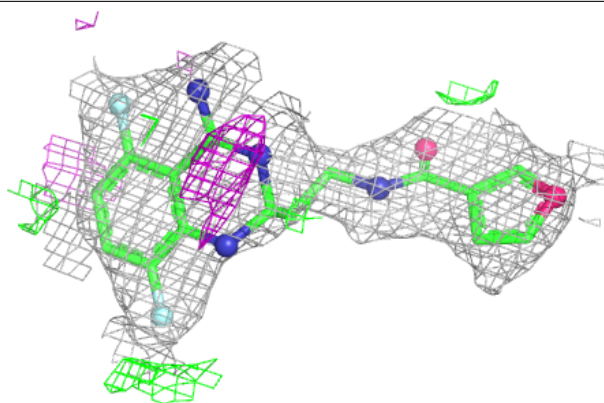
Electron density around A55 B 904:

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

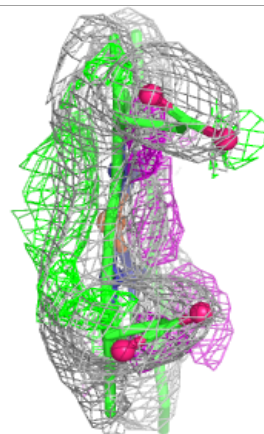
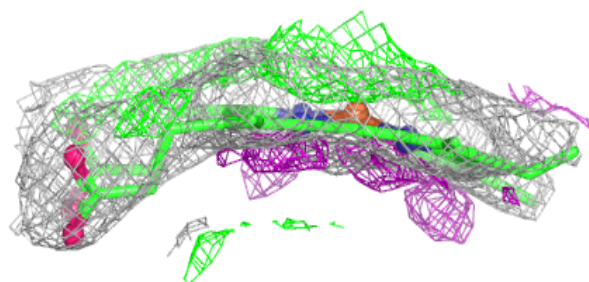
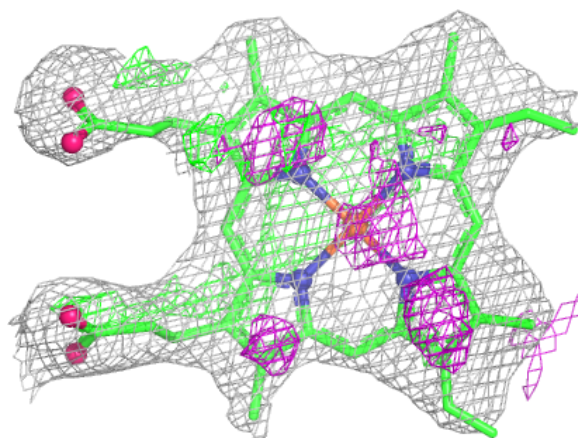


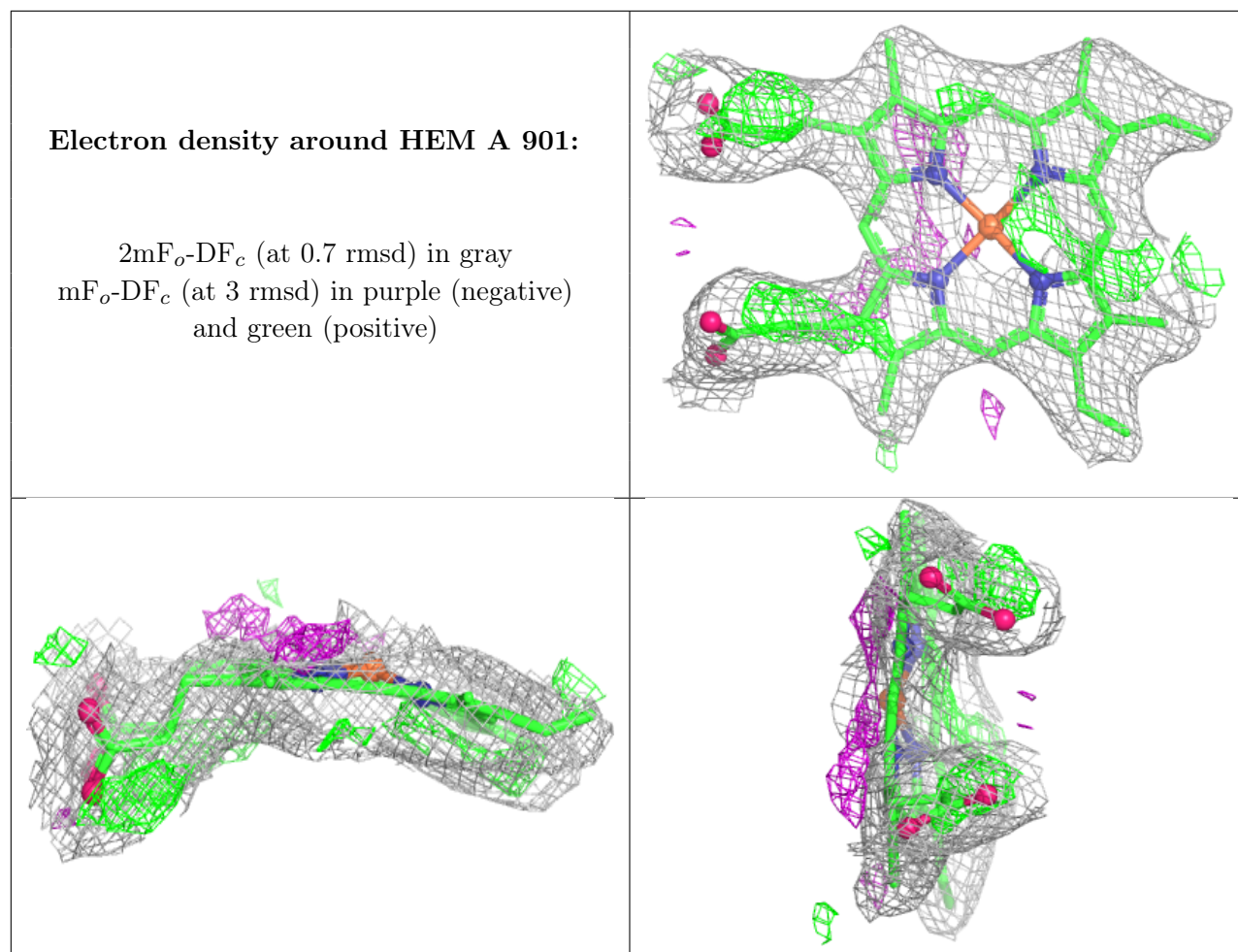
Electron density around A55 A 903:

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

**Electron density around HEM B 1901:**

$2mF_o-DF_c$ (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.