



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:29 PM UTC

PDB ID : 6OOX / pdb_00006oox
Title : The crystal structure of 4-isopropylbenzoate bound to T252A mutant of CYP19A4
Authors : Coleman, T.; Bruning, J.B.; Bell, S.G.
Deposited on : 2019-04-23
Resolution : 1.77 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

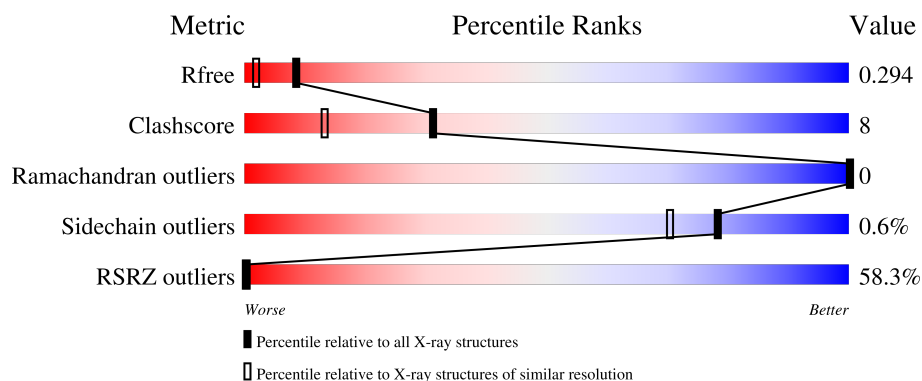
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	393	58% 88% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3267 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.

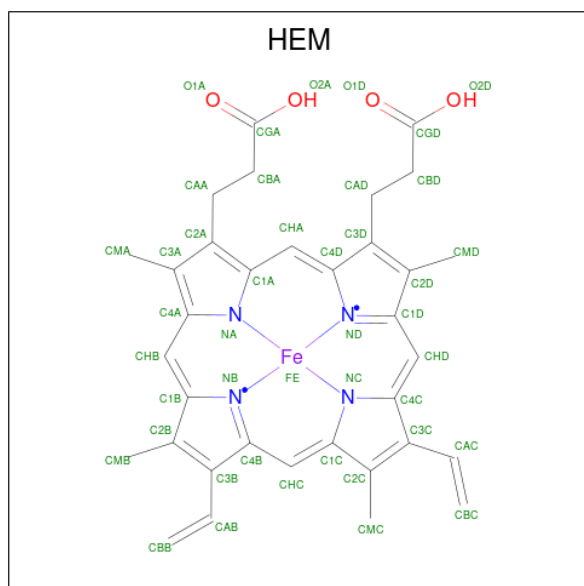
- Molecule 1 is a protein called Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	3061	1937	539	571	14	0	7	0

There is a discrepancy between the modelled and reference sequences:

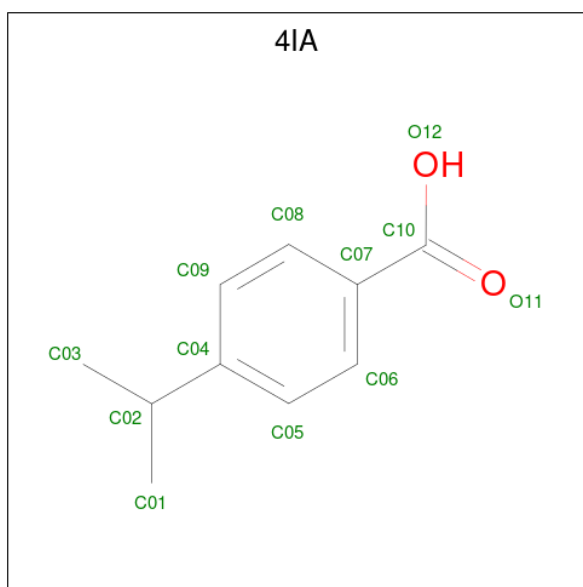
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	THR	engineered mutation	UNP Q2IU02

- 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	43	34	1	4	4	0	0

- Molecule 3 is 4-propan-2-ylbenzoic acid (CCD ID: 4IA) (formula: $C_{10}H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

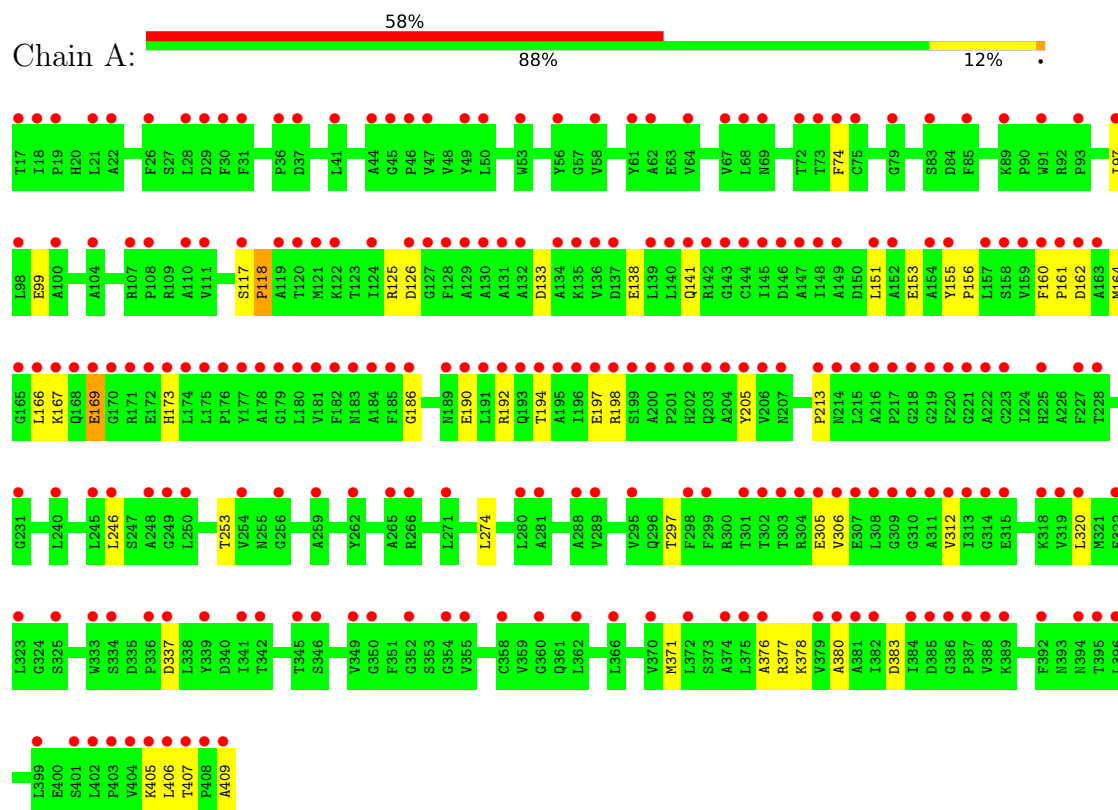
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		

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: Cytochrome P450



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.61Å 51.25Å 78.80Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	39.31 – 1.77 39.31 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.31-1.77) 99.0 (39.31-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.269 , 0.290 0.274 , 0.294	Depositor DCC
R_{free} test set	1519 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3267	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4IA, CL, 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	0.22	0/3142	0.57	0/4272

There are no bond length outliers.

There are no bond angle outliers.

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	3061	0	3037	51	1
2	A	43	0	30	1	0
3	A	12	0	0	0	0
4	A	1	0	0	0	0
5	A	150	0	0	30	1
All	All	3267	0	3067	51	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 8.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LYS:N	5:A:601:HOH:O	1.86	1.04
1:A:383:ASP:O	5:A:601:HOH:O	1.88	0.89
1:A:126:ASP:N	5:A:604:HOH:O	2.07	0.87
1:A:213:PRO:O	5:A:602:HOH:O	1.94	0.84
1:A:99:GLU:OE2	5:A:603:HOH:O	2.01	0.78
1:A:125:ARG:NH1	5:A:609:HOH:O	2.19	0.75
1:A:377:ARG:NH1	5:A:611:HOH:O	2.20	0.74
1:A:167:LYS:HB2	5:A:608:HOH:O	1.89	0.72
1:A:190:GLU:N	5:A:612:HOH:O	2.22	0.71
1:A:305:GLU:OE2	5:A:605:HOH:O	2.10	0.69
1:A:190:GLU:CA	5:A:612:HOH:O	2.44	0.65
1:A:378:LYS:HE2	5:A:611:HOH:O	1.99	0.61
1:A:197:GLU:HG3	1:A:198:ARG:HG3	1.82	0.60
1:A:190:GLU:O	1:A:194:THR:OG1	2.20	0.58
1:A:74:PHE:CZ	1:A:306:VAL:HG11	2.38	0.58
1:A:166:LEU:HB3	5:A:629:HOH:O	2.02	0.58
1:A:405:LYS:CB	5:A:601:HOH:O	2.54	0.54
1:A:253:THR:HG23	5:A:682:HOH:O	2.06	0.54
1:A:405:LYS:HG2	5:A:613:HOH:O	2.06	0.54
1:A:169:GLU:CD	5:A:608:HOH:O	2.51	0.53
1:A:133:ASP:OD1	5:A:606:HOH:O	2.19	0.51
1:A:125:ARG:HB3	5:A:604:HOH:O	2.10	0.51
1:A:169:GLU:OE2	5:A:608:HOH:O	2.19	0.51
1:A:153:GLU:OE1	5:A:610:HOH:O	2.20	0.50
1:A:377:ARG:CZ	5:A:611:HOH:O	2.59	0.50
1:A:190:GLU:HB2	5:A:612:HOH:O	2.11	0.50
1:A:164[B]:MET:SD	1:A:246:LEU:HD23	2.53	0.48
1:A:274:LEU:HG	1:A:376:ALA:HB2	1.95	0.48
1:A:306:VAL:O	1:A:306:VAL:HG13	2.15	0.47
1:A:337:ASP:OD1	5:A:607:HOH:O	2.19	0.47
1:A:169:GLU:N	1:A:169:GLU:OE1	2.48	0.46
1:A:138:GLU:O	1:A:141:GLN:HB2	2.15	0.46
1:A:190:GLU:O	1:A:194:THR:CB	2.63	0.46
1:A:97:ILE:HG12	2:A:501:HEM:CGD	2.45	0.46
1:A:173:HIS:HB2	1:A:205:TYR:CD2	2.51	0.46
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.98	0.45
1:A:407:THR:N	5:A:613:HOH:O	2.49	0.45
1:A:153:GLU:CD	5:A:610:HOH:O	2.60	0.45
1:A:305:GLU:CD	1:A:312:VAL:HG13	2.43	0.44
1:A:169:GLU:CD	1:A:169:GLU:H	2.26	0.43
1:A:190:GLU:O	1:A:194:THR:HB	2.19	0.43
1:A:297:THR:HB	1:A:320:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HB3	1:A:161:PRO:HD3	2.01	0.42
1:A:162:ASP:CB	5:A:624:HOH:O	2.67	0.42
1:A:162:ASP:HB2	5:A:624:HOH:O	2.19	0.42
1:A:406:LEU:C	5:A:613:HOH:O	2.62	0.42
1:A:151:LEU:HG	1:A:371[B]:MET:HE2	2.02	0.42
1:A:213:PRO:C	5:A:602:HOH:O	2.52	0.41
1:A:186:GLY:O	1:A:192:ARG:HD2	2.20	0.41
1:A:117:SER:HB2	1:A:118:PRO:HD2	2.02	0.41
1:A:380:ALA:HB2	1:A:409:ALA:HA	2.02	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)
1:A:194:THR:OG1	1:A:305:GLU:OE1[1_655]	1.82	0.38
5:A:628:HOH:O	5:A:718:HOH:O[2_748]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

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	398/393 (101%)	392 (98%)	6 (2%)	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	325/318 (102%)	323 (99%)	2 (1%)	78	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	PRO
1	A	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	4IA	A	502	-	12,12,12	0.75	0	16,16,16	0.92	1 (6%)
2	HEM	A	501	1	50,50,50	1.43	7 (14%)	67,82,82	1.12	4 (5%)

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	4IA	A	502	-	-	0/8/8/8	0/1/1/1
2	HEM	A	501	1	-	4/14/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NA	4.18	2.09	1.95
2	A	501	HEM	FE-ND	4.00	2.07	1.94
2	A	501	HEM	CAC-C3C	3.14	1.55	1.47
2	A	501	HEM	CAB-C3B	3.14	1.55	1.47
2	A	501	HEM	CMC-C2C	2.20	1.55	1.50
2	A	501	HEM	CMB-C2B	2.08	1.55	1.50
2	A	501	HEM	FE-NC	2.07	2.02	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	2.44	108.10	105.21
2	A	501	HEM	C4D-ND-C1D	2.28	107.91	105.21
2	A	501	HEM	C3B-C2B-C1B	2.22	108.08	106.41
2	A	501	HEM	C3D-C4D-ND	-2.15	107.82	110.17
3	A	502	4IA	O12-C10-C07	2.09	120.20	114.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

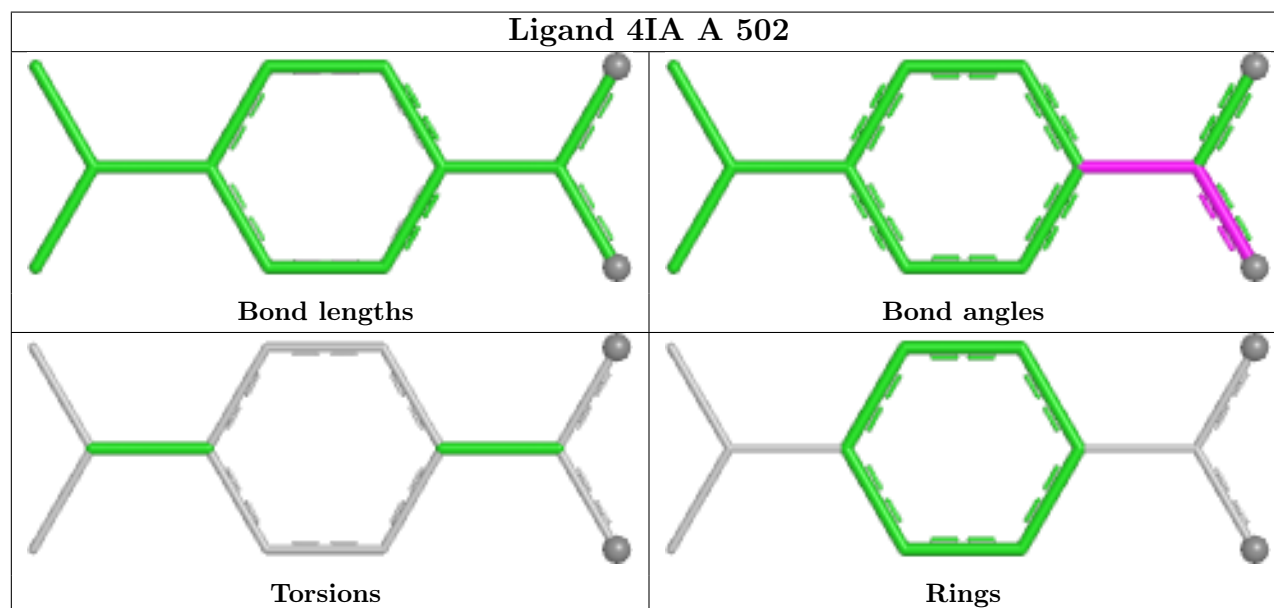
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D

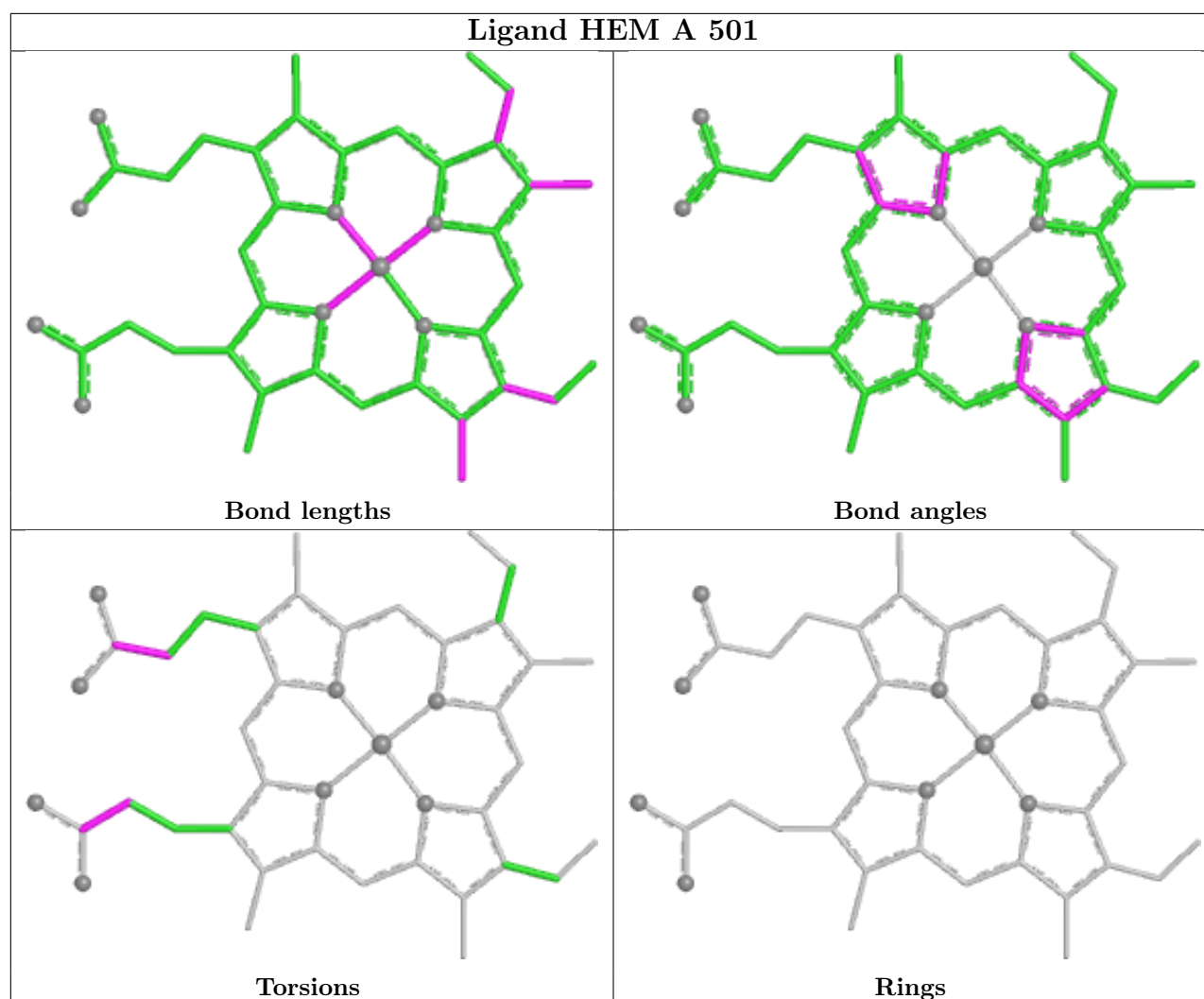
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	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, 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	393/393 (100%)	2.37	229 (58%) 0 0	14, 29, 55, 77	7 (1%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	7.4
1	A	312	VAL	6.6
1	A	180	LEU	6.1
1	A	306	VAL	5.9
1	A	198	ARG	5.6
1	A	314	GLY	5.6
1	A	194	THR	5.4
1	A	145	ILE	5.4
1	A	148	ILE	5.4
1	A	197	GLU	5.0
1	A	381	ALA	5.0
1	A	206	VAL	5.0
1	A	311	ALA	5.0
1	A	91	TRP	4.7
1	A	28	LEU	4.7
1	A	215	LEU	4.7
1	A	216	ALA	4.6
1	A	139	LEU	4.6
1	A	406	LEU	4.6
1	A	204	ALA	4.5
1	A	305	GLU	4.5
1	A	205	TYR	4.4
1	A	159	VAL	4.4
1	A	196	ILE	4.4
1	A	203	GLN	4.4
1	A	308	LEU	4.4
1	A	201	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	144	CYS	4.3
1	A	193	GLN	4.3
1	A	68	LEU	4.2
1	A	136	VAL	4.2
1	A	207	ASN	4.2
1	A	140	LEU	4.2
1	A	313	ILE	4.1
1	A	175	LEU	4.1
1	A	250	LEU	4.1
1	A	128	PHE	4.1
1	A	246	LEU	4.1
1	A	149	ALA	4.0
1	A	17	THR	4.0
1	A	200	ALA	4.0
1	A	386	GLY	4.0
1	A	202	HIS	4.0
1	A	166	LEU	3.9
1	A	181	VAL	3.9
1	A	169	GLU	3.9
1	A	402	LEU	3.9
1	A	404	VAL	3.8
1	A	219	GLY	3.8
1	A	165	GLY	3.8
1	A	217	PRO	3.8
1	A	160	PHE	3.8
1	A	384	ILE	3.8
1	A	374	ALA	3.7
1	A	143	GLY	3.7
1	A	98	LEU	3.7
1	A	403	PRO	3.7
1	A	199	SER	3.7
1	A	124	ILE	3.6
1	A	387	PRO	3.6
1	A	405	LYS	3.6
1	A	174	LEU	3.6
1	A	302	THR	3.5
1	A	409	ALA	3.5
1	A	191	LEU	3.5
1	A	223[A]	CYS	3.5
1	A	376	ALA	3.4
1	A	189	ASN	3.4
1	A	74	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	3.4
1	A	379	VAL	3.3
1	A	26	PHE	3.3
1	A	190	GLU	3.3
1	A	167	LYS	3.3
1	A	131	ALA	3.3
1	A	132	ALA	3.3
1	A	213	PRO	3.3
1	A	399	LEU	3.3
1	A	249	GLY	3.2
1	A	295	VAL	3.2
1	A	107	ARG	3.2
1	A	375	LEU	3.2
1	A	304	ARG	3.2
1	A	228	THR	3.2
1	A	392	PHE	3.1
1	A	370	VAL	3.1
1	A	46	PRO	3.1
1	A	44	ALA	3.1
1	A	134	ALA	3.1
1	A	254	VAL	3.1
1	A	231	GLY	3.1
1	A	245	LEU	3.1
1	A	372	LEU	3.1
1	A	355	VAL	3.0
1	A	31	PHE	3.0
1	A	58	VAL	3.0
1	A	352	GLY	3.0
1	A	259	ALA	3.0
1	A	380	ALA	3.0
1	A	126	ASP	3.0
1	A	161	PRO	3.0
1	A	176	PRO	3.0
1	A	137	ASP	2.9
1	A	21	LEU	2.9
1	A	157	LEU	2.9
1	A	218	GLY	2.9
1	A	154	ALA	2.9
1	A	56	TYR	2.9
1	A	67	VAL	2.8
1	A	349	VAL	2.8
1	A	170	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	151	LEU	2.8
1	A	271	LEU	2.8
1	A	18	ILE	2.8
1	A	303	THR	2.8
1	A	119	ALA	2.8
1	A	36	PRO	2.8
1	A	323	LEU	2.8
1	A	298	PHE	2.8
1	A	346	SER	2.8
1	A	318	LYS	2.8
1	A	389	LYS	2.8
1	A	171	ARG	2.7
1	A	366	LEU	2.7
1	A	72	THR	2.7
1	A	122	LYS	2.7
1	A	30	PHE	2.7
1	A	29[A]	ASP	2.7
1	A	146	ASP	2.7
1	A	117	SER	2.7
1	A	127	GLY	2.7
1	A	89	LYS	2.7
1	A	225	HIS	2.7
1	A	155	TYR	2.7
1	A	186	GLY	2.7
1	A	382	ILE	2.7
1	A	110	ALA	2.7
1	A	75	CYS	2.6
1	A	158	SER	2.6
1	A	221	GLY	2.6
1	A	395	THR	2.6
1	A	41	LEU	2.6
1	A	341	ILE	2.6
1	A	53	TRP	2.6
1	A	222	ALA	2.6
1	A	120	THR	2.6
1	A	266	ARG	2.6
1	A	319	VAL	2.6
1	A	129	ALA	2.6
1	A	152	ALA	2.6
1	A	50	LEU	2.5
1	A	177	TYR	2.5
1	A	47	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	2.5
1	A	163	ALA	2.5
1	A	309	GLY	2.5
1	A	141	GLN	2.5
1	A	358	CYS	2.5
1	A	147	ALA	2.5
1	A	301	THR	2.5
1	A	183	ASN	2.4
1	A	168	GLN	2.4
1	A	280	LEU	2.4
1	A	108	PRO	2.4
1	A	79	GLY	2.4
1	A	396	LEU	2.4
1	A	408	PRO	2.4
1	A	62	ALA	2.4
1	A	401	SER	2.4
1	A	362	LEU	2.4
1	A	265	ALA	2.4
1	A	307	GLU	2.4
1	A	310	GLY	2.3
1	A	325	SER	2.3
1	A	93	PRO	2.3
1	A	184	ALA	2.3
1	A	385	ASP	2.3
1	A	350	GLY	2.3
1	A	142	ARG	2.3
1	A	336	PRO	2.3
1	A	100	ALA	2.3
1	A	240	LEU	2.3
1	A	179	GLY	2.3
1	A	214	ASN	2.3
1	A	49	TYR	2.3
1	A	61	TYR	2.3
1	A	345	THR	2.2
1	A	315	GLU	2.2
1	A	130	ALA	2.2
1	A	320	LEU	2.2
1	A	337	ASP	2.2
1	A	185	PHE	2.2
1	A	299	PHE	2.2
1	A	354	GLY	2.2
1	A	97	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	VAL	2.2
1	A	22	ALA	2.2
1	A	135	LYS	2.2
1	A	342	THR	2.2
1	A	394	ASN	2.2
1	A	288	ALA	2.2
1	A	19	PRO	2.2
1	A	334	SER	2.2
1	A	37	ASP	2.1
1	A	121	MET	2.1
1	A	248	ALA	2.1
1	A	69	ASN	2.1
1	A	322	PHE	2.1
1	A	262	TYR	2.1
1	A	339	TYR	2.1
1	A	360	GLY	2.1
1	A	162	ASP	2.1
1	A	333	TRP	2.1
1	A	407	THR	2.1
1	A	173	HIS	2.1
1	A	45	GLY	2.1
1	A	256	GLY	2.1
1	A	281	ALA	2.1
1	A	64	VAL	2.1
1	A	289	VAL	2.1
1	A	388	VAL	2.1
1	A	220	PHE	2.1
1	A	178	ALA	2.0
1	A	73	THR	2.0
1	A	85	PHE	2.0
1	A	182	PHE	2.0
1	A	192	ARG	2.0
1	A	104	ALA	2.0
1	A	83	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

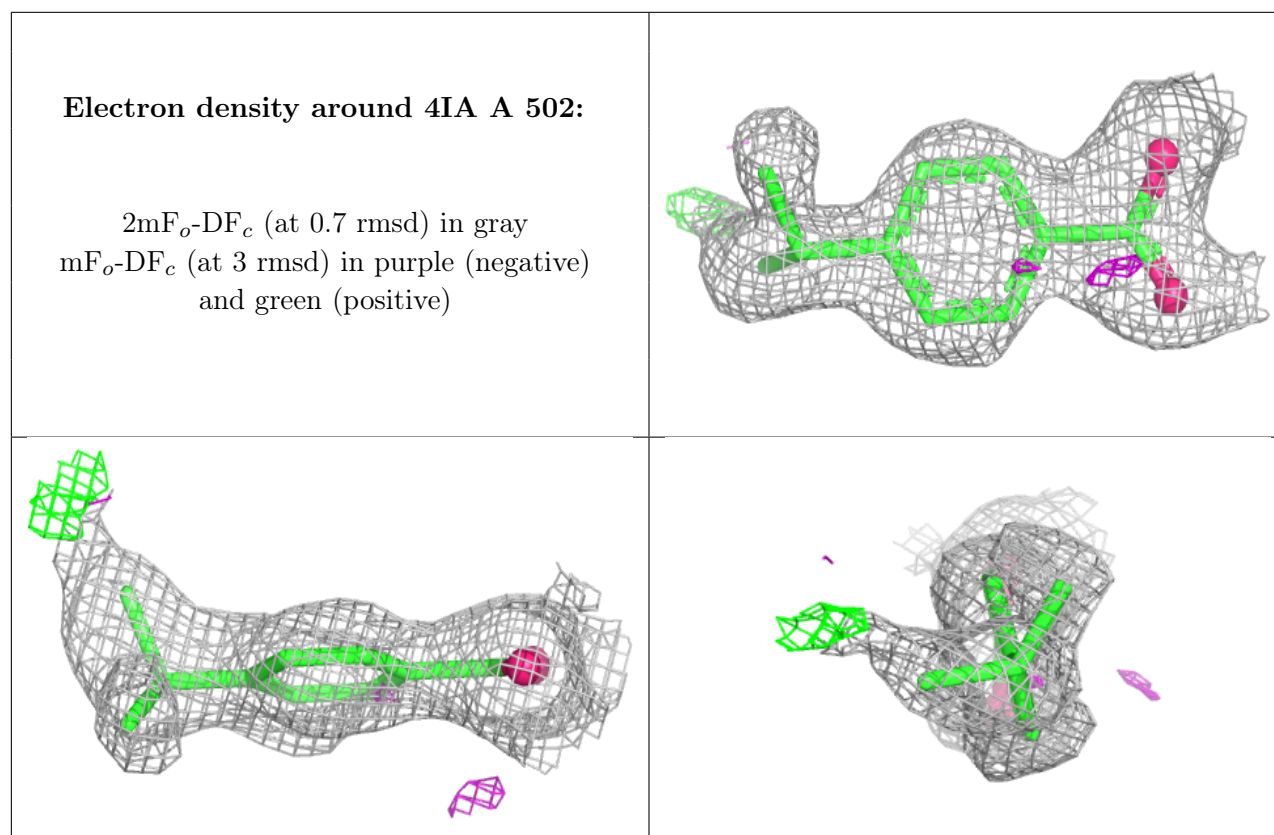
There are no oligosaccharides in this entry.

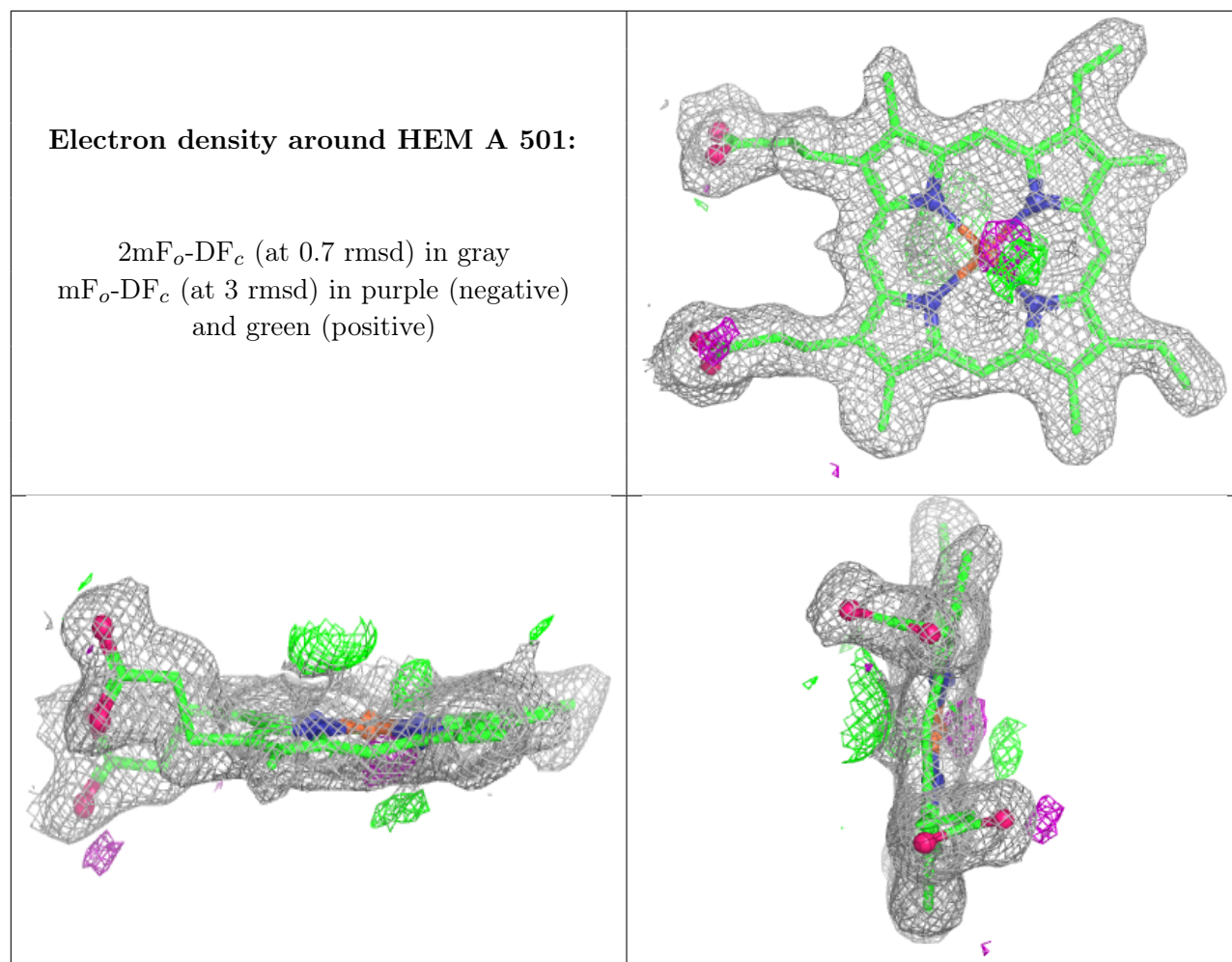
6.4 Ligands [i](#)

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	CL	A	503	1/1	0.72	0.17	61,61,61,61	0
3	4IA	A	502	12/12	0.83	0.12	21,25,28,29	0
2	HEM	A	501	43/43	0.93	0.09	16,22,25,28	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.