



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2020 – 02:44 PM EDT

PDB ID : 6OOX
Title : The crystal structure of 4-isopropylbenzoate bound to T252A mutant of CYP199A4
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 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 : 2.10.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
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) : 2.10.1

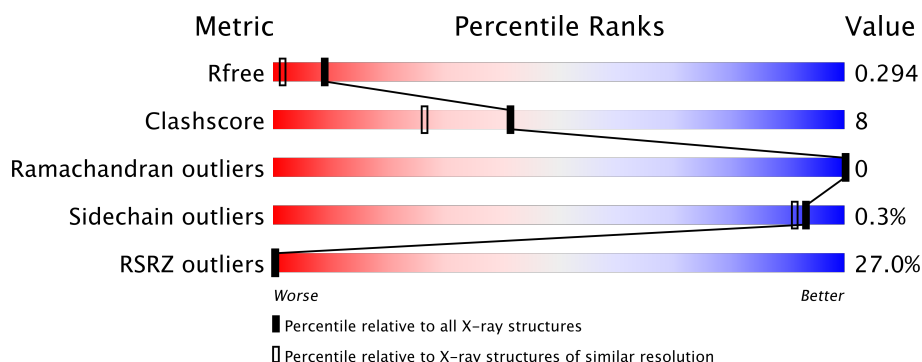
1 Overall quality at a glance

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}	111664	7886 (1.80-1.76)
Clashscore	122126	8858 (1.80-1.76)
Ramachandran outliers	120053	8764 (1.80-1.76)
Sidechain outliers	120020	8763 (1.80-1.76)
RSRZ outliers	108989	7741 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	

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:

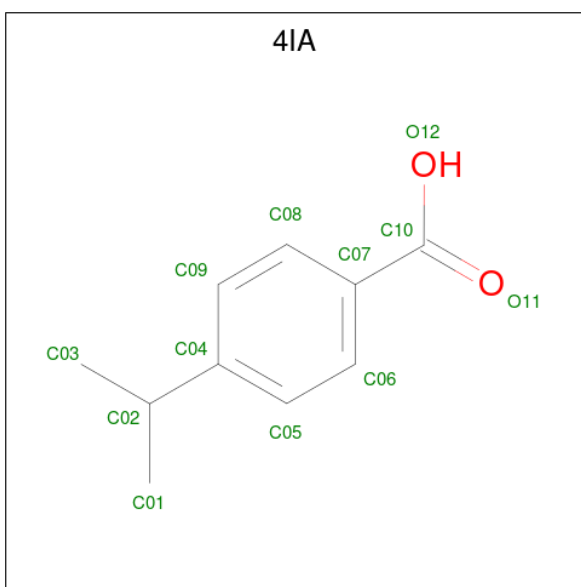
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	THR	engineered mutation	UNP Q2IU02

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (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	43	34	1	4	4	0	0

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



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

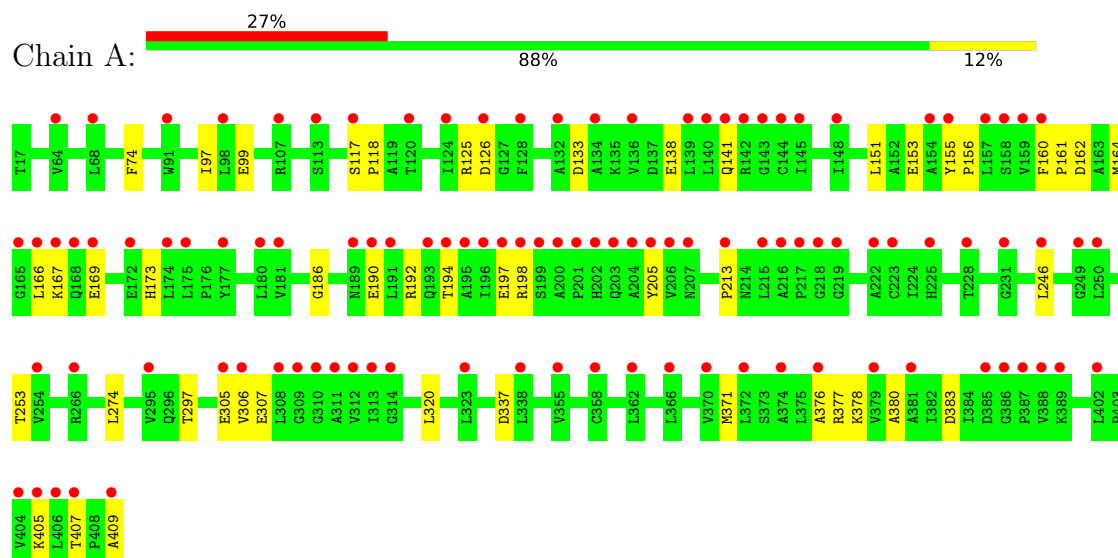
- Molecule 5 is water.

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 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: 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 0.273 , 0.294	Depositor DCC
R_{free} test set	1517 reflections (4.99%)	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 , 45.2	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: HEM, 4IA, CL

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	0.30	0/3142	0.55	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	47	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	28	1
All	All	3267	0	3067	47	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 (47) 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:166:LEU:HB3	5:A:629:HOH:O	2.02	0.58
1:A:74:PHE:CZ	1:A:306:VAL:HG11	2.38	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: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:169:GLU:CD	5:A:608:HOH:O	2.51	0.49
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:OE1	1:A:169:GLU:N	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:173:HIS:HB2	1:A:205:TYR:CD2	2.51	0.46
1:A:97:ILE:HG12	2:A:501:HEM:CGD	2.45	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HG	1:A:371[B]:MET:HE2	2.02	0.42
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:153:GLU:CD	5:A:610:HOH:O	2.60	0.40
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 [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	398/393 (101%)	392 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	325/318 (102%)	324 (100%)	1 (0%)	93	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	GLU

Some 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 carbohydrates 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	$\# Z > 2$
2	HEM	A	501	1	27,50,50	1.82	5 (18%)	17,82,82	1.69	5 (29%)
3	4IA	A	502	-	10,12,12	1.84	1 (10%)	13,16,16	0.75	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
2	HEM	A	501	1	-	0/6/54/54	-
3	4IA	A	502	-	-	0/4/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	4IA	C07-C10	5.79	1.53	1.47
2	A	501	HEM	C3C-CAC	3.89	1.55	1.47
2	A	501	HEM	C3B-CAB	3.84	1.55	1.47
2	A	501	HEM	C3B-C2B	-3.51	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.51	1.35	1.40
2	A	501	HEM	CAA-C2A	2.41	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CMC-C2C-C3C	3.41	131.05	124.68
2	A	501	HEM	CMB-C2B-C3B	2.75	129.83	124.68
2	A	501	HEM	C4A-C3A-C2A	2.46	108.71	107.00
2	A	501	HEM	CAD-CBD-CGD	-2.30	108.80	112.67
2	A	501	HEM	CBD-CAD-C3D	-2.08	108.65	112.48

There are no chirality outliers.

There are no torsion outliers.

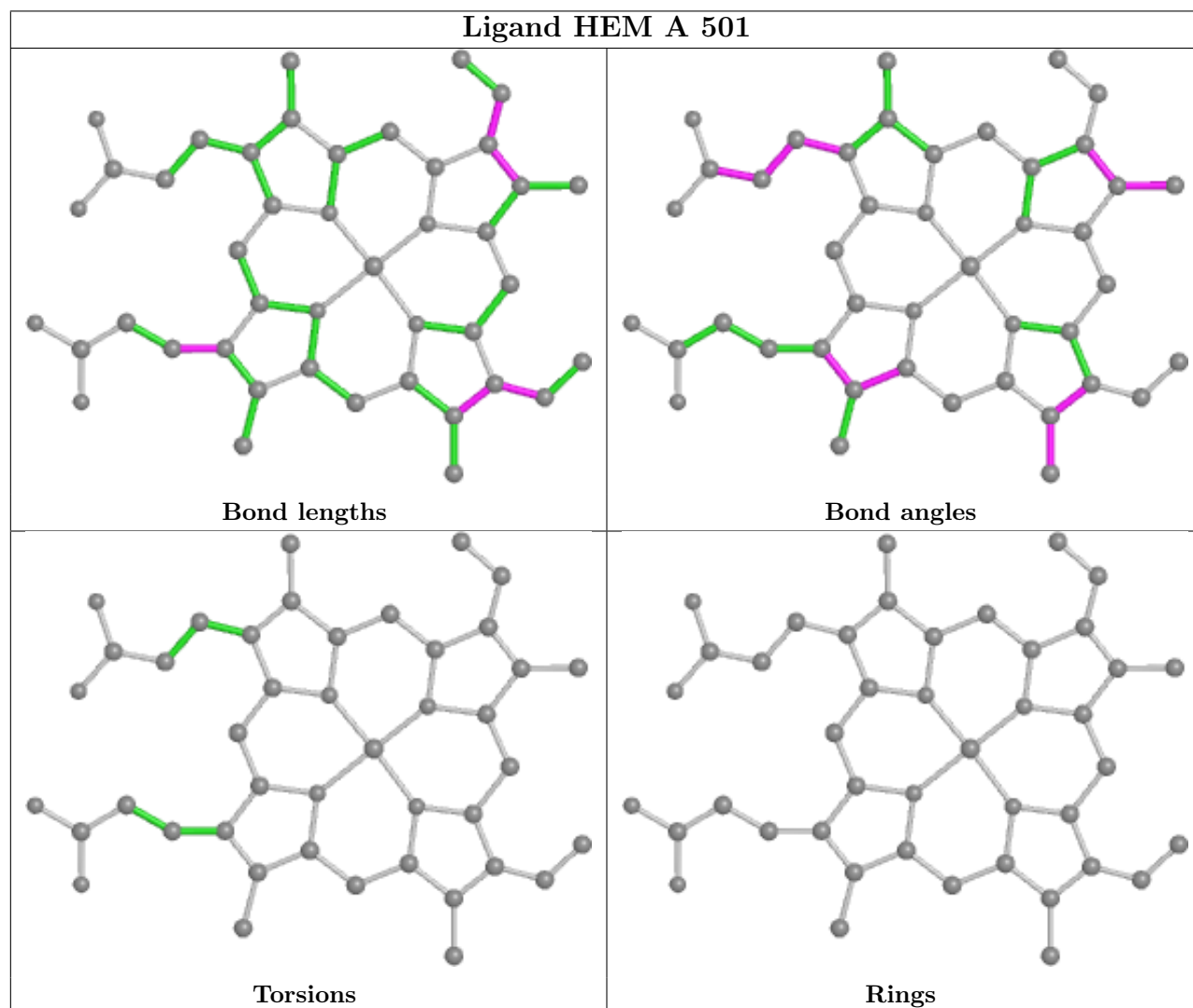
There are no ring outliers.

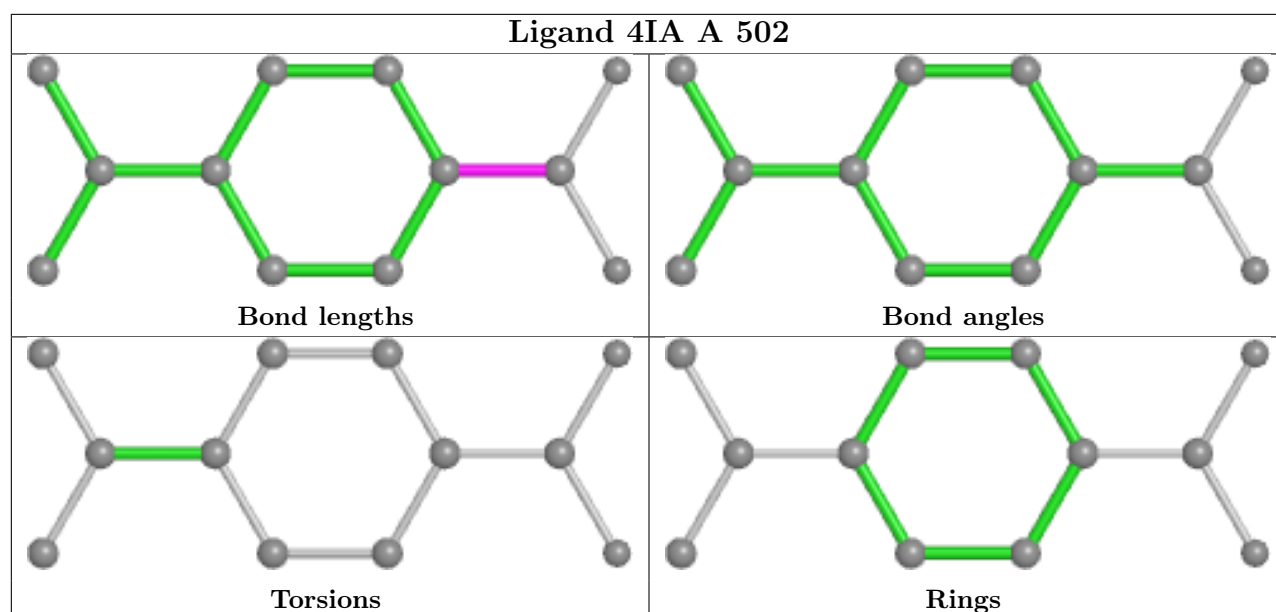
1 monomer is involved in 1 short contact:

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%)	1.71	106 (26%) 0 0	18, 29, 55, 77	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	13.8
1	A	198	ARG	13.2
1	A	197	GLU	11.1
1	A	312	VAL	8.5
1	A	200	ALA	8.1
1	A	194	THR	7.5
1	A	203	GLN	6.0
1	A	143	GLY	5.3
1	A	196	ILE	5.3
1	A	180	LEU	5.2
1	A	205	TYR	5.1
1	A	144	CYS	5.0
1	A	193	GLN	5.0
1	A	306	VAL	5.0
1	A	406	LEU	4.9
1	A	215	LEU	4.9
1	A	386	GLY	4.9
1	A	128	PHE	4.8
1	A	201	PRO	4.8
1	A	202	HIS	4.8
1	A	199	SER	4.6
1	A	166	LEU	4.5
1	A	381	ALA	4.5
1	A	206	VAL	4.5
1	A	207	ASN	4.4
1	A	409	ALA	4.4
1	A	175	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	405	LYS	4.3
1	A	148	ILE	4.1
1	A	308	LEU	4.0
1	A	246	LEU	4.0
1	A	145	ILE	3.9
1	A	314	GLY	3.9
1	A	305	GLU	3.8
1	A	219	GLY	3.8
1	A	213	PRO	3.8
1	A	372	LEU	3.8
1	A	190	GLU	3.6
1	A	126	ASP	3.5
1	A	204	ALA	3.5
1	A	376	ALA	3.3
1	A	313	ILE	3.3
1	A	167	LYS	3.3
1	A	159	VAL	3.3
1	A	358	CYS	3.2
1	A	98	LEU	3.2
1	A	139	LEU	3.2
1	A	216	ALA	3.1
1	A	91	TRP	3.1
1	A	169	GLU	3.1
1	A	250	LEU	3.1
1	A	311	ALA	3.1
1	A	374	ALA	3.0
1	A	174	LEU	3.0
1	A	136	VAL	3.0
1	A	366	LEU	3.0
1	A	191	LEU	2.9
1	A	254	VAL	2.9
1	A	404	VAL	2.9
1	A	217	PRO	2.8
1	A	407	THR	2.8
1	A	165	GLY	2.7
1	A	228	THR	2.7
1	A	295	VAL	2.7
1	A	160	PHE	2.7
1	A	132	ALA	2.7
1	A	64	VAL	2.7
1	A	172	GLU	2.6
1	A	168	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	189	ASN	2.5
1	A	141	GLN	2.5
1	A	140	LEU	2.5
1	A	223[A]	CYS	2.5
1	A	266	ARG	2.5
1	A	157	LEU	2.5
1	A	107	ARG	2.4
1	A	142	ARG	2.4
1	A	249	GLY	2.4
1	A	388	VAL	2.4
1	A	124	ILE	2.4
1	A	379	VAL	2.4
1	A	231	GLY	2.4
1	A	362	LEU	2.3
1	A	134	ALA	2.3
1	A	385	ASP	2.3
1	A	370	VAL	2.3
1	A	387	PRO	2.2
1	A	222	ALA	2.2
1	A	177	TYR	2.2
1	A	68	LEU	2.2
1	A	310	GLY	2.2
1	A	309	GLY	2.2
1	A	158	SER	2.1
1	A	402	LEU	2.1
1	A	113[A]	SER	2.1
1	A	117	SER	2.1
1	A	389	LYS	2.1
1	A	225	HIS	2.1
1	A	120	THR	2.1
1	A	323	LEU	2.1
1	A	355	VAL	2.0
1	A	218	GLY	2.0
1	A	154	ALA	2.0
1	A	155	TYR	2.0
1	A	181	VAL	2.0
1	A	338	LEU	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](#)

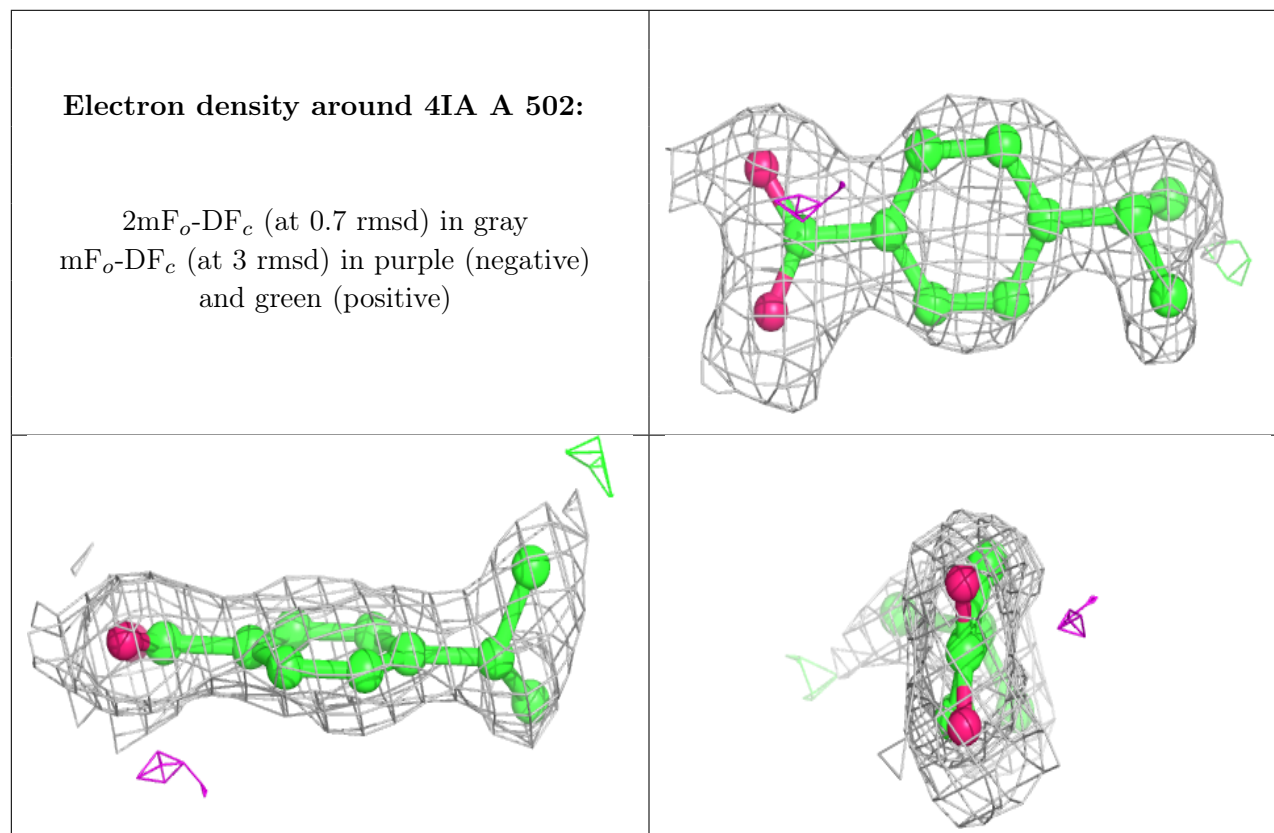
There are no carbohydrates in this entry.

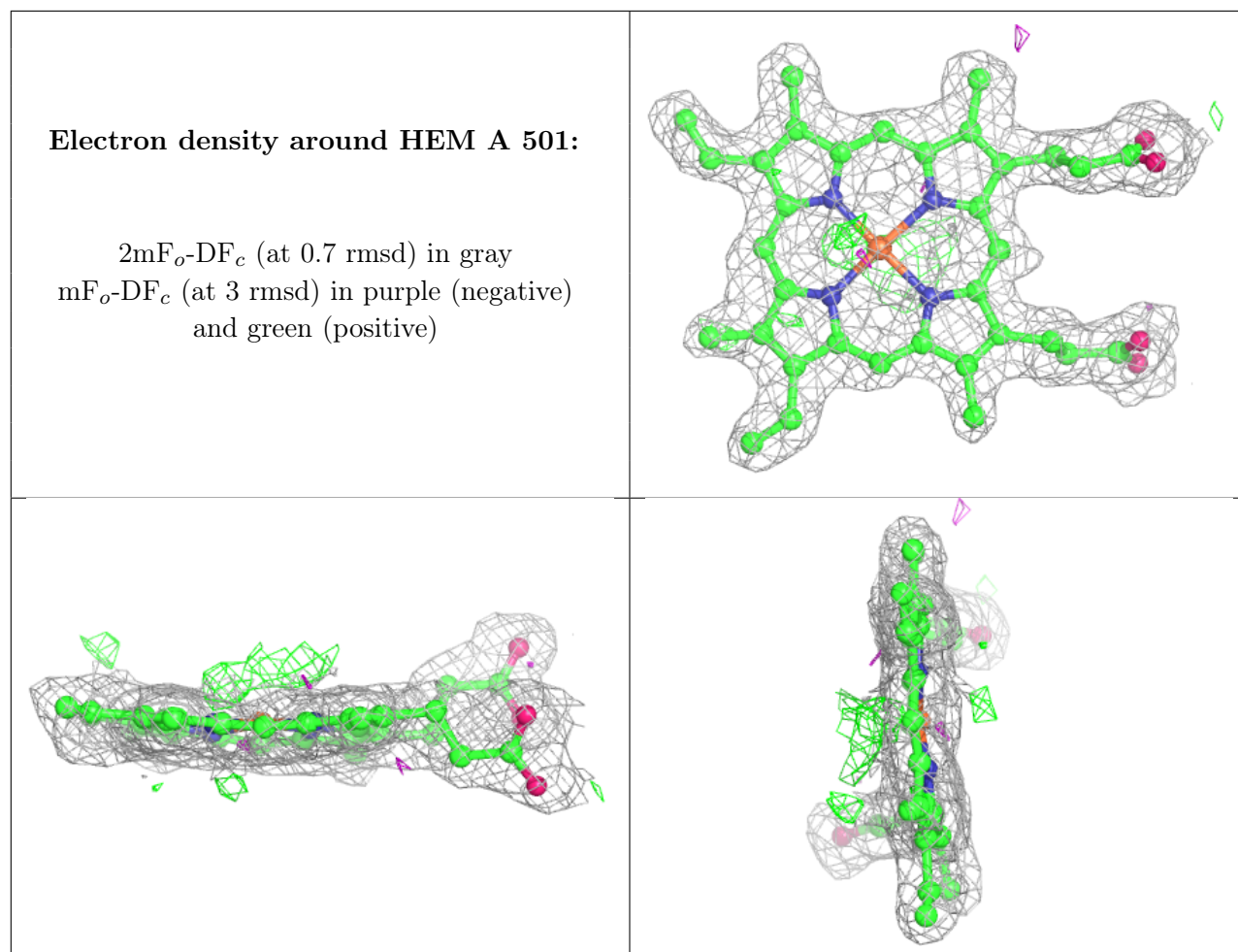
6.4 Ligands [i](#)

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, 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(Å ²)	Q<0.9
4	CL	A	503	1/1	0.53	0.20	61,61,61,61	0
3	4IA	A	502	12/12	0.90	0.13	21,25,28,29	0
2	HEM	A	501	43/43	0.95	0.12	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 [i](#)

There are no such residues in this entry.