



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2021 – 06:02 PM EDT

PDB ID : 7KSA  
Title : Crystal structure of human CYP3A4 with the caged inhibitor  
Authors : Sevrioukova, I.S.  
Deposited on : 2020-11-21  
Resolution : 2.50 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.

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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 : 2.18  
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) : 2.18

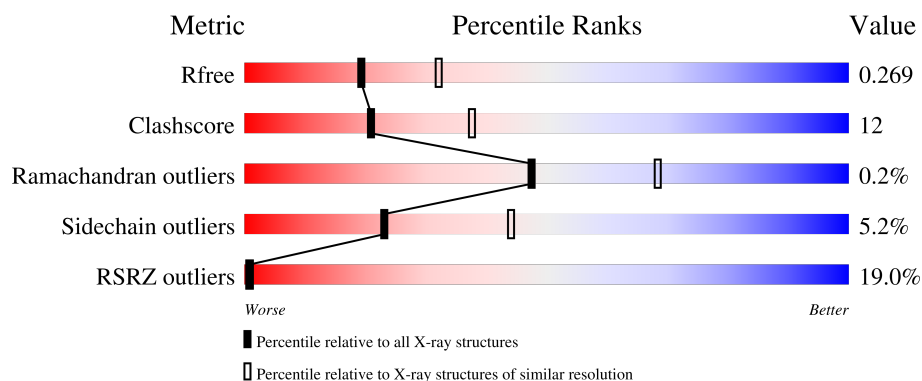
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	<div> <div>17%</div> <div>65%</div> <div>23%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3671 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3548	2313	581	630	24			

There are 24 discrepancies between the modelled and reference sequences:

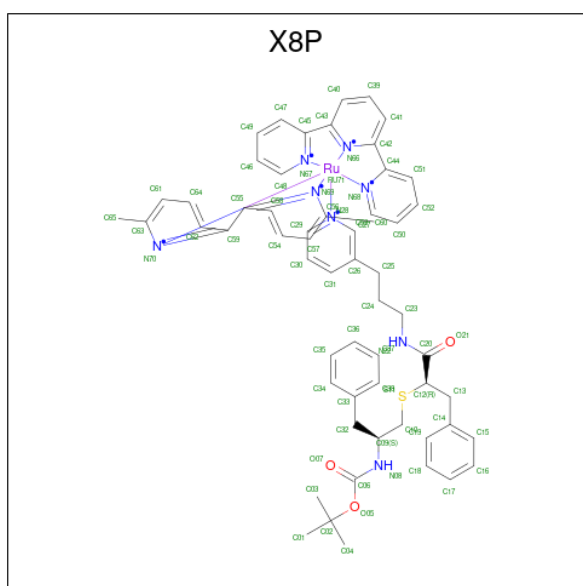
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	UNP P08684
A	?	-	TRP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	SER	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684

- 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
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (tert-butyl {1-[(1-oxo-3-phenyl-1-[[3-(pyridin-3-yl-kappaN)prop-1-en-1-yl]amino}propan-2-yl)sulfanyl]-3-phenylpropan-2-yl}carbamate)(6,6'-dimethyl-2,2'-bipyridine-kappa 2 N 1 ,N 1')(1 2 ,2 2 :2 6 ,3 2 -terpyridine-kappa 3 N 1 ^{1 },N 2 ^{1 },N 3 ^{1 })ruthenium (three-letter code: X8P) (formula: C<sub>58</sub>H<sub>62</sub>N<sub>8</sub>O<sub>3</sub>RuS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	Ru	S	0	0
			71	58	8	3	1	1		

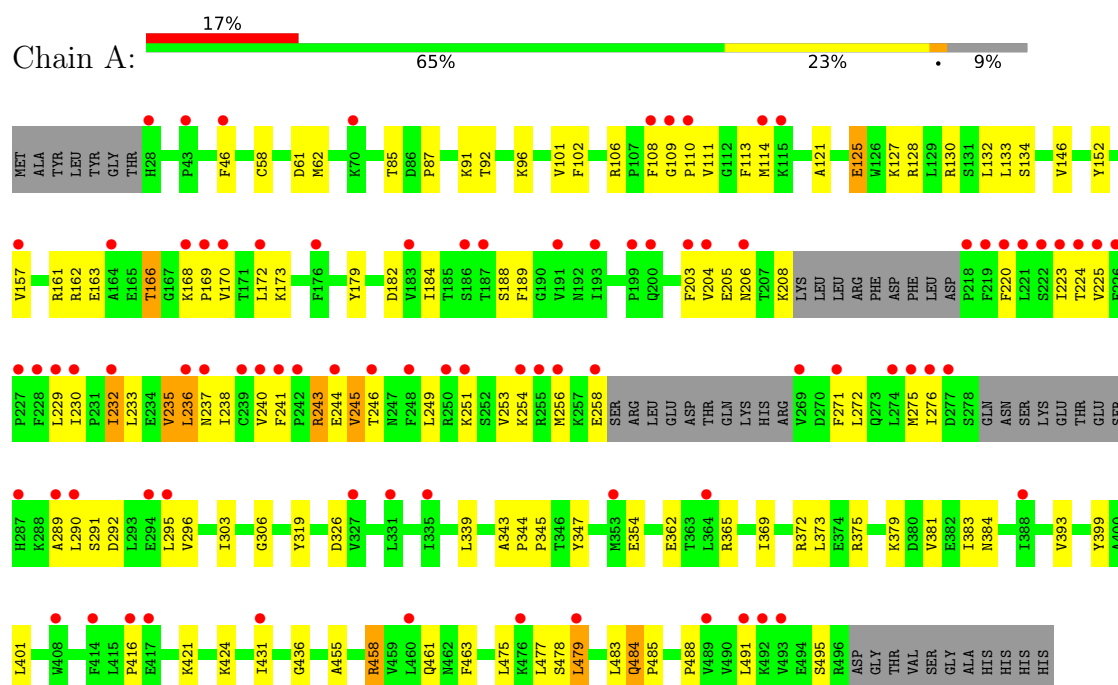
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

### 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 3A4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.57Å 95.00Å 121.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 2.50 47.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.50-2.50) 98.6 (47.50-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.228 , 0.266 0.228 , 0.269	Depositor DCC
$R_{free}$ test set	725 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 98.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: X8P, 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	0.27	0/3635	0.49	0/4916

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	3548	0	3633	85	0
2	A	43	0	30	3	0
3	A	71	0	0	4	0
4	A	9	0	0	0	0
All	All	3671	0	3663	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (89) 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:203:PHE:CD2	1:A:204:VAL:HG23	1.85	1.10
1:A:203:PHE:CE2	1:A:204:VAL:HG23	2.06	0.91
1:A:188:SER:HA	1:A:271:PHE:HB2	1.68	0.75
1:A:245:VAL:HG12	1:A:246:THR:H	1.52	0.73
1:A:189:PHE:HE2	1:A:303:ILE:HD11	1.52	0.73
1:A:373:LEU:HD21	1:A:436:GLY:HA2	1.72	0.71
1:A:166:THR:HG23	1:A:168:LYS:HG2	1.72	0.70
1:A:475:LEU:HD11	1:A:485:PRO:HB3	1.73	0.69
1:A:275:MET:CE	1:A:295:LEU:HG	2.22	0.69
1:A:275:MET:HE1	1:A:295:LEU:HG	1.75	0.68
1:A:204:VAL:O	1:A:204:VAL:HG12	1.91	0.68
1:A:188:SER:O	1:A:272:LEU:HG	1.93	0.68
1:A:233:LEU:HB3	1:A:238:ILE:HB	1.75	0.68
1:A:204:VAL:HG11	1:A:303:ILE:HD13	1.78	0.65
1:A:206:ASN:CG	1:A:245:VAL:HG11	2.17	0.65
1:A:203:PHE:CE2	1:A:204:VAL:CG2	2.78	0.64
1:A:121:ALA:HB1	1:A:125:GLU:HG3	1.80	0.63
1:A:189:PHE:CE2	1:A:303:ILE:HD11	2.33	0.61
1:A:146:VAL:HG21	1:A:347:TYR:HB2	1.83	0.60
1:A:132:LEU:HD13	1:A:290:LEU:HG	1.84	0.60
1:A:478:SER:HB2	1:A:484:GLN:HG2	1.83	0.60
1:A:229:LEU:HA	1:A:232:ILE:HG13	1.84	0.59
1:A:109:GLY:HA2	1:A:230:ILE:HG12	1.86	0.58
1:A:106:ARG:HD3	1:A:393:VAL:HG21	1.86	0.57
1:A:108:PHE:HE1	1:A:240:VAL:HG21	1.70	0.57
1:A:292:ASP:O	1:A:296:VAL:HG23	2.05	0.57
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.86	0.57
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.87	0.56
1:A:235:VAL:HG12	1:A:236:LEU:HD23	1.86	0.56
1:A:362:GLU:HG3	1:A:416:PRO:HA	1.88	0.56
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.88	0.56
1:A:113:PHE:CZ	1:A:246:THR:HG21	2.41	0.56
1:A:256:MET:SD	1:A:272:LEU:HD13	2.46	0.55
1:A:458:ARG:NH2	1:A:461:GLN:OE1	2.39	0.55
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.90	0.54
1:A:91:LYS:HG2	1:A:96:LYS:HE3	1.88	0.54
1:A:133:LEU:HD21	1:A:275:MET:HE3	1.89	0.54
1:A:184:ILE:HD13	1:A:303:ILE:HA	1.91	0.53
1:A:46:PHE:O	1:A:225:VAL:HG13	2.09	0.53
1:A:256:MET:SD	1:A:272:LEU:HB3	2.49	0.53
1:A:61:ASP:OD1	1:A:372:ARG:NH2	2.42	0.53
1:A:189:PHE:HD1	1:A:272:LEU:HD11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HB3	1:A:170:VAL:HG22	1.94	0.49
1:A:220:PHE:O	1:A:224:THR:OG1	2.24	0.49
1:A:108:PHE:HB2	3:A:602:X8P:C60	2.43	0.49
3:A:602:X8P:C53	3:A:602:X8P:C27	2.91	0.49
1:A:233:LEU:HA	1:A:236:LEU:HB2	1.94	0.48
1:A:362:GLU:OE2	1:A:365:ARG:NE	2.38	0.48
1:A:339:LEU:HB3	1:A:343:ALA:HB3	1.95	0.48
1:A:110:PRO:HB3	1:A:233:LEU:HB2	1.94	0.48
1:A:243:ARG:NH2	1:A:244:GLU:OE2	2.45	0.48
1:A:256:MET:SD	1:A:276:ILE:HD11	2.53	0.48
1:A:85:THR:HB	1:A:401:LEU:HD21	1.96	0.47
1:A:128:ARG:NH2	1:A:289:ALA:O	2.47	0.47
1:A:246:THR:O	1:A:249:LEU:N	2.47	0.47
1:A:92:THR:HA	1:A:96:LYS:HB2	1.96	0.47
1:A:130:ARG:O	1:A:134:SER:OG	2.29	0.47
1:A:319:TYR:CZ	1:A:475:LEU:HB2	2.50	0.46
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.96	0.46
1:A:205:GLU:O	1:A:205:GLU:CG	2.64	0.46
1:A:369:ILE:HA	1:A:483:LEU:HD23	1.98	0.46
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.29	0.46
1:A:108:PHE:HB2	3:A:602:X8P:C57	2.46	0.46
1:A:157:VAL:HG13	1:A:463:PHE:CE2	2.51	0.46
1:A:111:VAL:HG22	1:A:114:MET:HB2	1.98	0.46
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.51	0.45
1:A:173:LYS:HD3	1:A:488:PRO:HB3	1.98	0.45
1:A:206:ASN:OD1	1:A:245:VAL:HG11	2.16	0.45
1:A:383:ILE:O	1:A:384:ASN:C	2.56	0.44
1:A:152:TYR:CD2	1:A:182:ASP:HB3	2.53	0.44
1:A:172:LEU:HD11	1:A:491:LEU:HD12	2.00	0.44
1:A:421:LYS:HA	1:A:424:LYS:HE3	1.99	0.44
1:A:114:MET:HG3	1:A:241:PHE:CD1	2.53	0.44
1:A:477:LEU:HD13	1:A:483:LEU:HD11	1.99	0.43
1:A:326:ASP:OD1	1:A:326:ASP:N	2.46	0.43
3:A:602:X8P:C20	3:A:602:X8P:C19	2.96	0.43
1:A:245:VAL:HG12	1:A:246:THR:N	2.26	0.42
1:A:168:LYS:HB2	1:A:169:PRO:HD2	2.02	0.42
1:A:229:LEU:O	1:A:233:LEU:HG	2.20	0.42
1:A:184:ILE:HD11	1:A:306:GLY:C	2.40	0.42
1:A:275:MET:HB3	1:A:275:MET:HE2	1.98	0.42
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.55	0.42
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.95	0.41
1:A:127:LYS:HE3	1:A:127:LYS:HB2	1.82	0.41
1:A:479:LEU:H	1:A:479:LEU:HD13	1.86	0.41
1:A:101:VAL:HG21	1:A:381:VAL:HG11	2.02	0.41
1:A:275:MET:HE2	1:A:295:LEU:HG	2.00	0.41
1:A:161:ARG:NH1	1:A:495:SER:OG	2.53	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	434/487 (89%)	402 (93%)	31 (7%)	1 (0%)	47 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	VAL

### 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	403/443 (91%)	382 (95%)	21 (5%)	23 44

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	MET
1	A	125	GLU
1	A	162	ARG
1	A	166	THR
1	A	208	LYS
1	A	223	ILE
1	A	232	ILE
1	A	235	VAL
1	A	236	LEU
1	A	237	ASN
1	A	243	ARG
1	A	251	LYS
1	A	253	VAL
1	A	254	LYS
1	A	258	GLU
1	A	291	SER
1	A	354	GLU
1	A	379	LYS
1	A	458	ARG
1	A	479	LEU
1	A	484	GLN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 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
2	HEM	A	601	3,1	27,50,50	1.82	4 (14%)	17,82,82	1.55	4 (23%)
3	X8P	A	602	2	70,81,81	3.68	37 (52%)	65,125,125	4.18	31 (47%)

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	601	3,1	-	0/6/54/54	-
3	X8P	A	602	2	-	18/33/179/179	0/11/11/11

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	X8P	C48-N67	-7.28	1.34	1.49
3	A	602	X8P	C53-N68	-7.16	1.35	1.49
3	A	602	X8P	C29-N28	-6.59	1.35	1.48
3	A	602	X8P	C20-N22	6.39	1.47	1.33
3	A	602	X8P	C51-C44	-6.13	1.40	1.53
3	A	602	X8P	C41-C42	-6.12	1.40	1.53
3	A	602	X8P	C06-N08	6.01	1.49	1.34
3	A	602	X8P	C47-C45	-6.00	1.40	1.53
3	A	602	X8P	C62-C59	-5.97	1.40	1.53
3	A	602	X8P	C58-C55	-5.91	1.40	1.53
3	A	602	X8P	C40-C43	-5.85	1.40	1.53
3	A	602	X8P	C27-C26	-5.46	1.40	1.52
3	A	602	X8P	C64-C62	-5.16	1.39	1.53
3	A	602	X8P	C49-C47	-5.09	1.39	1.53
3	A	602	X8P	C64-C61	-5.08	1.39	1.53
3	A	602	X8P	C52-C51	-5.05	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	X8P	C57-C56	-5.03	1.40	1.53
3	A	602	X8P	C39-C41	-5.01	1.40	1.53
3	A	602	X8P	C54-C58	-5.01	1.40	1.53
3	A	602	X8P	C54-C57	-4.99	1.40	1.53
3	A	602	X8P	C61-C63	-4.96	1.40	1.53
3	A	602	X8P	C30-C31	-4.91	1.40	1.53
3	A	602	X8P	C39-C40	-4.85	1.40	1.53
3	A	602	X8P	C44-C42	-4.67	1.39	1.52
3	A	602	X8P	C45-C43	-4.48	1.39	1.52
3	A	602	X8P	C59-C55	-4.47	1.39	1.52
3	A	602	X8P	C31-C26	-4.44	1.40	1.52
2	A	601	HEM	C3C-CAC	3.91	1.55	1.47
3	A	602	X8P	RU71-N69	-3.82	1.98	2.12
2	A	601	HEM	C3B-CAB	3.78	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.72	1.35	1.40
2	A	601	HEM	C3C-C2C	-3.68	1.35	1.40
3	A	602	X8P	O07-C06	3.52	1.28	1.21
3	A	602	X8P	RU71-N66	-3.09	2.01	2.12
3	A	602	X8P	C53-C50	-2.98	1.40	1.51
3	A	602	X8P	C29-C30	-2.95	1.40	1.51
3	A	602	X8P	C48-C46	-2.94	1.40	1.51
3	A	602	X8P	C52-C50	-2.91	1.40	1.51
3	A	602	X8P	C49-C46	-2.83	1.40	1.51
3	A	602	X8P	C09-N08	2.53	1.51	1.46
3	A	602	X8P	O05-C02	-2.26	1.44	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	X8P	C65-C63-N70	13.04	133.90	113.06
3	A	602	X8P	C61-C63-N70	10.14	121.64	109.71
3	A	602	X8P	C57-C56-N69	9.41	120.78	109.71
3	A	602	X8P	C29-C30-C31	8.58	120.63	111.25
3	A	602	X8P	O05-C06-N08	7.37	122.40	110.02
3	A	602	X8P	C14-C13-C12	7.18	123.61	113.32
3	A	602	X8P	C60-C56-N69	6.99	124.24	113.06
3	A	602	X8P	O07-C06-N08	-6.61	114.01	124.85
3	A	602	X8P	C64-C61-C63	6.55	120.05	112.74
3	A	602	X8P	C27-C26-C31	6.40	117.62	109.71
3	A	602	X8P	C54-C57-C56	6.26	119.73	112.74
3	A	602	X8P	C50-C53-N68	5.98	122.74	113.00
3	A	602	X8P	C46-C48-N67	5.33	121.69	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	X8P	C48-C46-C49	5.19	120.22	111.44
3	A	602	X8P	C53-C50-C52	5.09	120.06	111.44
3	A	602	X8P	C64-C62-C59	4.70	119.68	111.22
3	A	602	X8P	C54-C58-C55	4.61	119.53	111.22
3	A	602	X8P	C39-C40-C43	4.44	119.23	111.22
3	A	602	X8P	C30-C29-N28	4.16	119.60	113.21
3	A	602	X8P	C09-N08-C06	-4.15	115.90	122.30
3	A	602	X8P	C49-C47-C45	4.09	118.59	111.22
3	A	602	X8P	C24-C23-N22	3.87	123.28	112.21
3	A	602	X8P	C65-C63-C61	-3.70	104.46	112.07
3	A	602	X8P	C30-C31-C26	3.63	119.01	112.15
3	A	602	X8P	C25-C26-C31	3.61	120.73	112.11
3	A	602	X8P	C39-C41-C42	3.59	117.69	111.22
3	A	602	X8P	C52-C51-C44	3.37	117.29	111.22
3	A	602	X8P	C50-C52-C51	3.22	117.99	111.42
3	A	602	X8P	C46-C49-C47	3.10	117.74	111.42
3	A	602	X8P	C02-O05-C06	2.67	125.10	120.99
2	A	601	HEM	CMB-C2B-C3B	2.37	129.12	124.68
2	A	601	HEM	CMC-C2C-C3C	2.24	128.87	124.68
2	A	601	HEM	CBD-CAD-C3D	-2.24	108.36	112.48
2	A	601	HEM	CBA-CAA-C2A	-2.19	108.44	112.49
3	A	602	X8P	C41-C39-C40	2.04	118.82	112.87

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	X8P	S11-C12-C13-C14
3	A	602	X8P	C13-C12-S11-C10
3	A	602	X8P	C24-C25-C26-C27
3	A	602	X8P	O05-C06-N08-C09
3	A	602	X8P	O07-C06-N08-C09
3	A	602	X8P	C03-C02-O05-C06
3	A	602	X8P	C01-C02-O05-C06
3	A	602	X8P	C04-C02-O05-C06
3	A	602	X8P	C24-C23-N22-C20
3	A	602	X8P	O07-C06-O05-C02
3	A	602	X8P	C12-C13-C14-C15
3	A	602	X8P	C12-C13-C14-C19
3	A	602	X8P	C20-C12-C13-C14
3	A	602	X8P	N08-C06-O05-C02
3	A	602	X8P	C10-C09-N08-C06

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Mol	Chain	Res	Type	Atoms
3	A	602	X8P	C20-C12-S11-C10
3	A	602	X8P	C13-C12-C20-O21
3	A	602	X8P	C09-C10-S11-C12

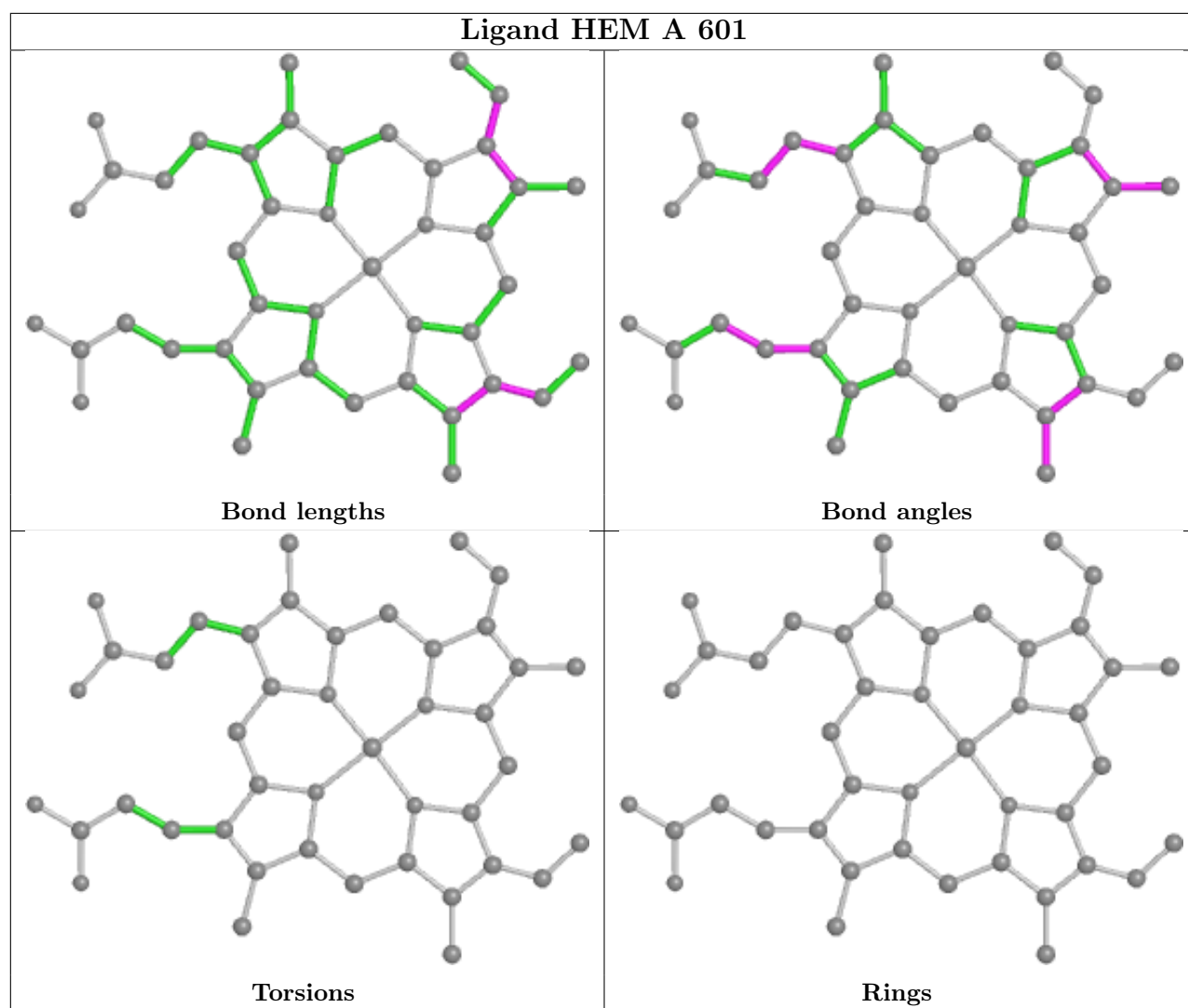
There are no ring outliers.

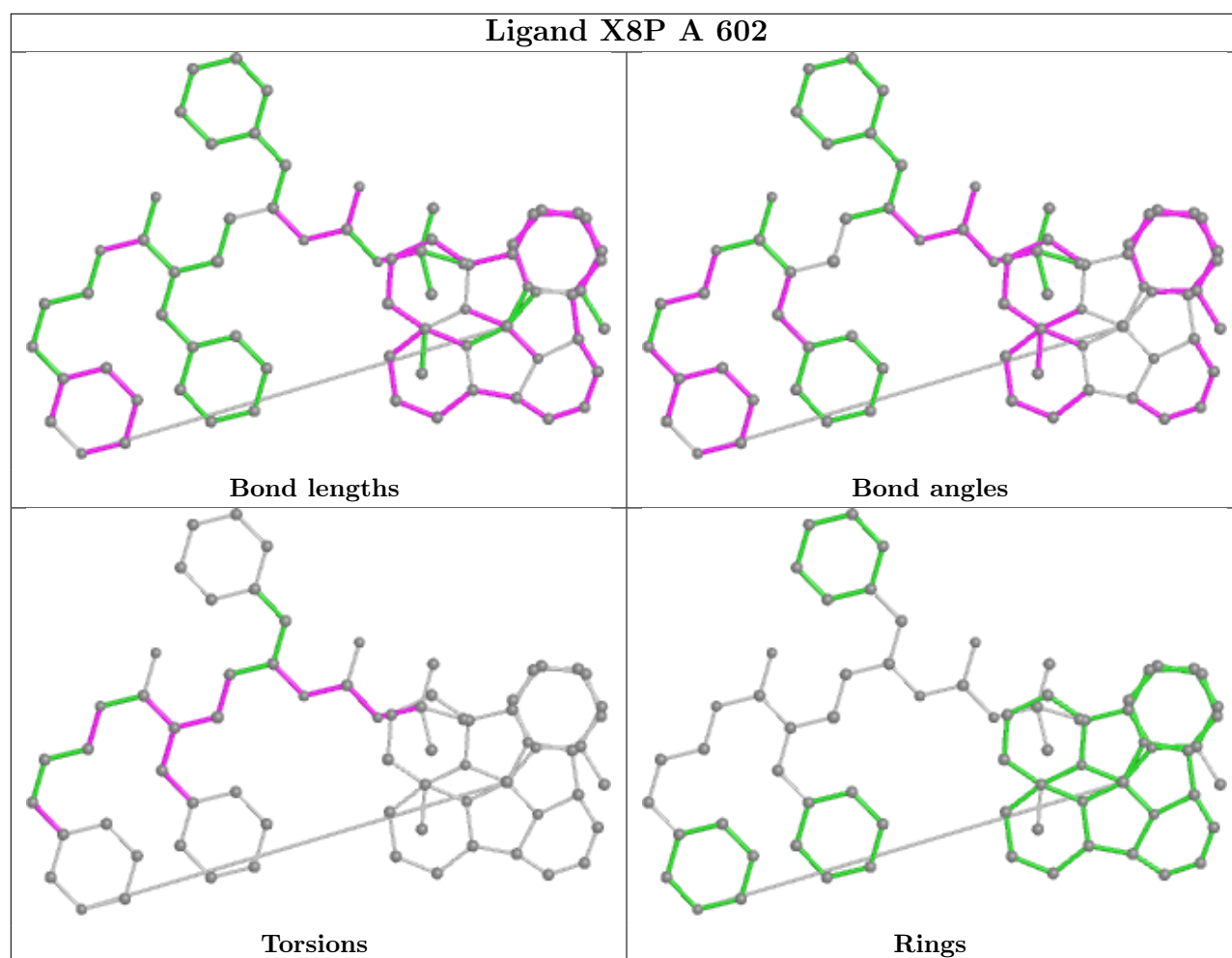
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	3	0
3	A	602	X8P	4	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	442/487 (90%)	1.24	84 (19%) <b>1</b> <b>1</b>	62, 114, 213, 286	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	16.1
1	A	240	VAL	11.2
1	A	239	CYS	11.0
1	A	229	LEU	9.7
1	A	109	GLY	9.0
1	A	203	PHE	8.6
1	A	226	PHE	7.6
1	A	219	PHE	7.5
1	A	218	PRO	7.5
1	A	491	LEU	7.3
1	A	110	PRO	7.1
1	A	221	LEU	6.6
1	A	230	ILE	6.6
1	A	275	MET	6.6
1	A	225	VAL	6.3
1	A	108	PHE	6.3
1	A	493	VAL	6.2
1	A	227	PRO	6.2
1	A	269	VAL	6.1
1	A	170	VAL	6.0
1	A	274	LEU	5.7
1	A	276	ILE	5.6
1	A	460	LEU	5.5
1	A	250	ARG	5.2
1	A	256	MET	5.1
1	A	206	ASN	4.9
1	A	255	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	236	LEU	4.5
1	A	169	PRO	4.5
1	A	489	VAL	4.5
1	A	222	SER	4.4
1	A	223	ILE	4.3
1	A	251	LYS	4.3
1	A	492	LYS	4.2
1	A	277	ASP	4.2
1	A	115	LYS	4.1
1	A	204	VAL	3.8
1	A	242	PRO	3.8
1	A	220	PHE	3.8
1	A	228	PHE	3.6
1	A	331	LEU	3.6
1	A	168	LYS	3.6
1	A	289	ALA	3.3
1	A	193	ILE	3.2
1	A	408	TRP	3.1
1	A	246	THR	3.1
1	A	258	GLU	3.1
1	A	114	MET	3.0
1	A	157	VAL	3.0
1	A	431	ILE	3.0
1	A	237	ASN	3.0
1	A	327	VAL	2.9
1	A	200	GLN	2.9
1	A	248	PHE	2.9
1	A	290	LEU	2.9
1	A	191	VAL	2.9
1	A	172	LEU	2.7
1	A	353	MET	2.6
1	A	416	PRO	2.6
1	A	46	PHE	2.5
1	A	28	HIS	2.5
1	A	199	PRO	2.5
1	A	232	ILE	2.5
1	A	295	LEU	2.4
1	A	335	ILE	2.3
1	A	417	GLU	2.3
1	A	186	SER	2.3
1	A	388	ILE	2.3
1	A	164	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	2.3
1	A	287	HIS	2.3
1	A	414	PHE	2.3
1	A	271	PHE	2.2
1	A	254	LYS	2.2
1	A	244	GLU	2.1
1	A	479	LEU	2.1
1	A	43	PRO	2.1
1	A	176	PHE	2.1
1	A	476	LYS	2.1
1	A	187	THR	2.1
1	A	70	LYS	2.0
1	A	224	THR	2.0
1	A	364	LEU	2.0
1	A	294	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

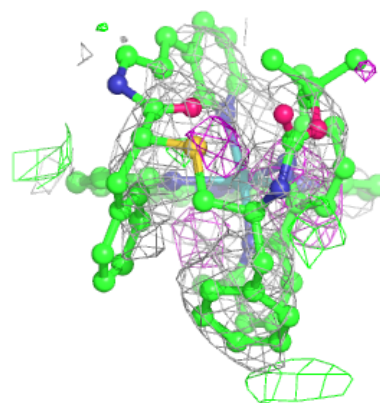
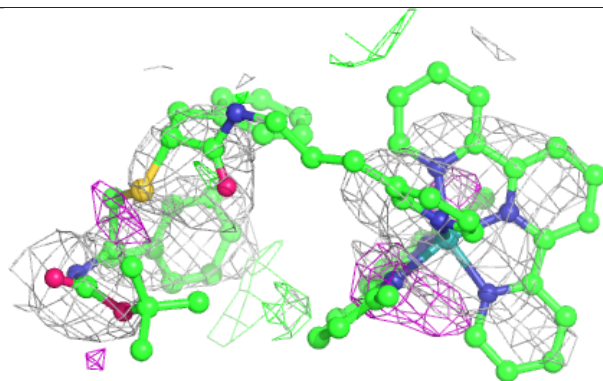
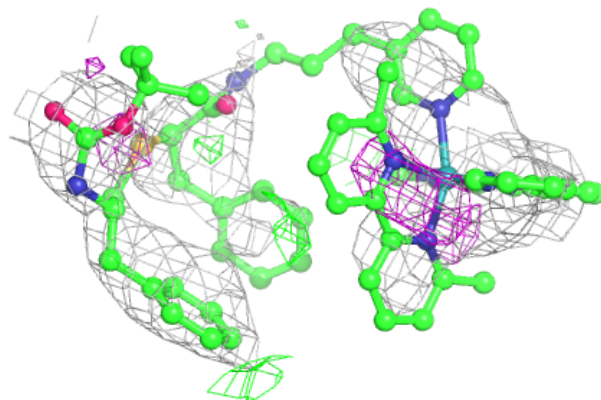
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

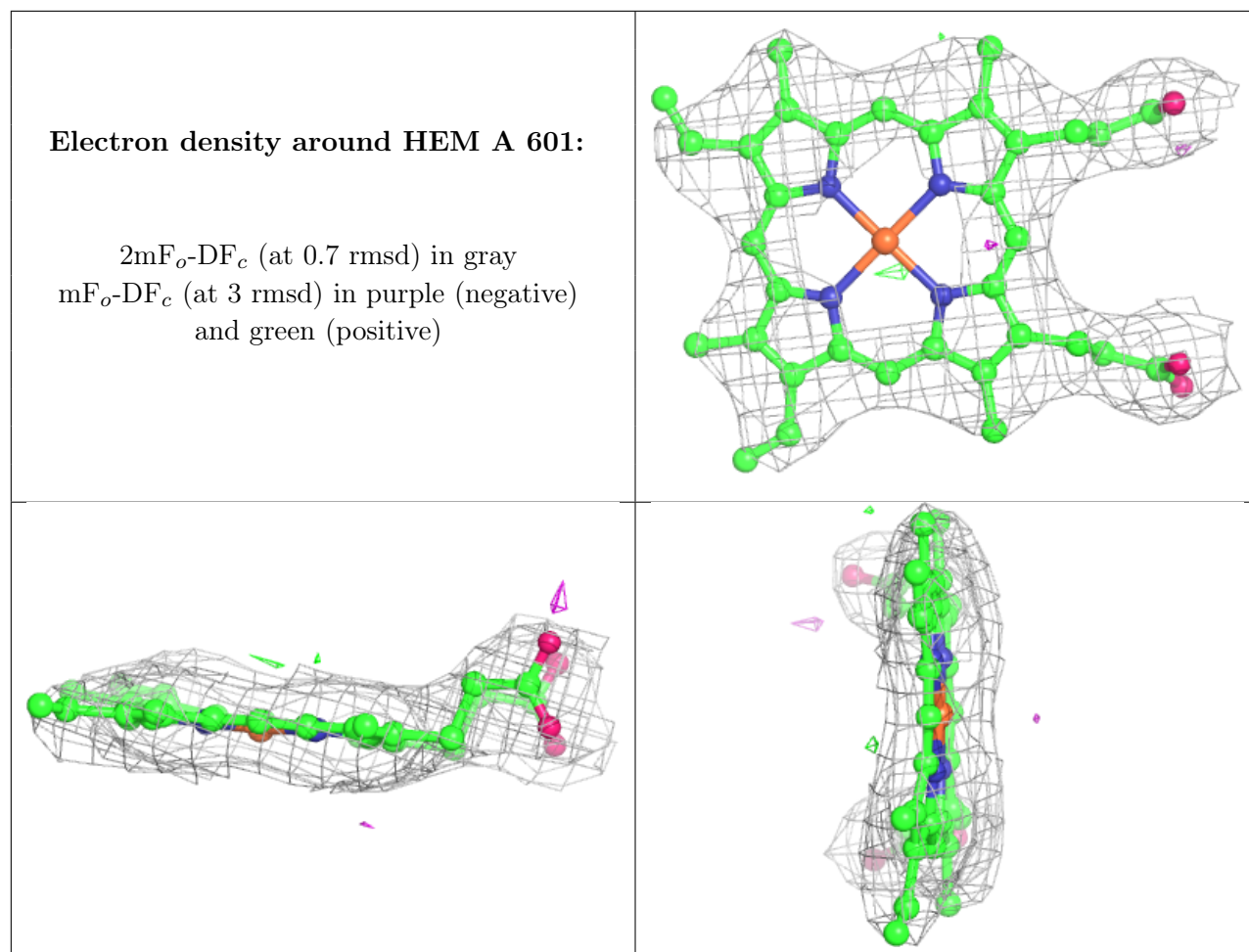
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	X8P	A	602	71/71	0.81	0.40	94,188,257,286	0
2	HEM	A	601	43/43	0.97	0.18	44,71,82,84	0

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 X8P A 602:**

$2mF_o-DF_c$  (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.