



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2020 – 06:08 PM EST

PDB ID : 6W0S  
Title : Crystal structure of substrate free cytochrome P450 NasF5053 from Streptomyces sp. NRRL F-5053  
Authors : Luo, Z.; Jia, X.; Sun, C.; Qu, X.; Kobe, B.  
Deposited on : 2020-03-02  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.14.6  
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) : 2.14.6

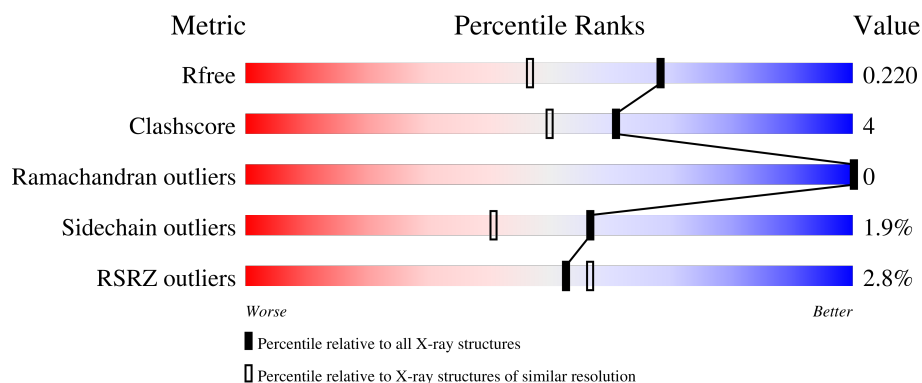
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	398	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12933 atoms, of which 5953 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-F5053.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	H	N	O	S	0	1	0
			6047	1926	2980	558	571	12			
1	B	396	Total	C	H	N	O	S	0	1	0
			6013	1923	2952	557	569	12			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Br	0	0
			2	2		

*Continued on next page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Br 2 2	0	0

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | B     | 2        | Total Cl<br>2 2 | 0       | 0       |
| 4   | A     | 4        | Total Cl<br>4 4 | 0       | 0       |

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | B     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | A     | 1        | Total Na<br>1 1 | 0       | 0       |

- # HEM
- 
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The iron atom is also coordinated by a heme group (O1A, O2A, O1D, O2D) and a proximal histidine residue (CBA). The heme group is shown in red, while the rest of the structure is in green. The side chains are labeled with three-letter codes: CAA, CBA, CAD, CBD, CMA, C3A, C2A, C4A, C3B, C4B, C1B, C2B, CMB, CBB, CAC, C3C, C4C, C1C, C2C, CMC, C1D, C2D, C3D, C4D, C5D, C6D, C7D, C8D, C9D, C10D, C11D, C12D, C13D, C14D, C15D, C16D, C17D, C18D, C19D, C20D, C21D, C22D, C23D, C24D, C25D, C26D, C27D, C28D, C29D, C30D, C31D, C32D, C33D, C34D, C35D, C36D, C37D, C38D, C39D, C40D, C41D, C42D, C43D, C44D, C45D, C46D, C47D, C48D, C49D, C50D, C51D, C52D, C53D, C54D, C55D, C56D, C57D, C58D, C59D, C60D, C61D, C62D, C63D, C64D, C65D, C66D, C67D, C68D, C69D, C70D, C71D, C72D, C73D, C74D, C75D, C76D, C77D, C78D, C79D, C80D, C81D, C82D, C83D, C84D, C85D, C86D, C87D, C88D, C89D, C90D, C91D, C92D, C93D, C94D, C95D, C96D, C97D, C98D, C99D, C100D, C101D, C102D, C103D, C104D, C105D, C106D, C107D, C108D, C109D, C110D, C111D, C112D, C113D, C114D, C115D, C116D, C117D, C118D, C119D, C120D, C121D, C122D, C123D, C124D, C125D, C126D, C127D, C128D, C129D, C130D, C131D, C132D, C133D, C134D, C135D, C136D, C137D, C138D, C139D, C140D, C141D, C142D, C143D, C144D, C145D, C146D, C147D, C148D, C149D, C150D, C151D, C152D, C153D, C154D, C155D, C156D, C157D, C158D, C159D, C160D, C161D, C162D, C163D, C164D, C165D, C166D, C167D, C168D, C169D, C170D, C171D, C172D, C173D, C174D, C175D, C176D, C177D, C178D, C179D, C180D, C181D, C182D, C183D, C184D, C185D, C186D, C187D, C188D, C189D, C190D, C191D, C192D, C193D, C194D, C195D, C196D, C197D, C198D, C199D, C200D, C201D, C202D, C203D, C204D, C205D, C206D, C207D, C208D, C209D, C210D, C211D, C212D, C213D, C214D, C215D, C216D, C217D, C218D, C219D, C220D, C221D, C222D, C223D, C224D, C225D, C226D, C227D, C228D, C229D, C230D, C231D, C232D, C233D, C234D, C235D, C236D, C237D, C238D, C239D, C240D, C241D, C242D, C243D, C244D, C245D, C246D, C247D, C248D, C249D, C250D, C251D, C252D, C253D, C254D, C255D, C256D, C257D, C258D, C259D, C260D, C261D, C262D, C263D, C264D, C265D, C266D, C267D, C268D, C269D, C270D, C271D, C272D, C273D, C274D, C275D, C276D, C277D, C278D, C279D, C280D, C281D, C282D, C283D, C284D, C285D, C286D, C287D, C288D, C289D, C290D, C291D, C292D, C293D, C294D, C295D, C296D, C297D, C298D, C299D, C300D, C301D, C302D, C303D, C304D, C305D, C306D, C307D, C308D, C309D, C310D, C311D, C312D, C313D, C314D, C315D, C316D, C317D, C318D, C319D, C320D, C321D, C322D, C323D, C324D, C325D, C326D, C327D, C328D, C329D, C330D, C331D, C332D, C333D, C334D, C335D, C336D, C337D, C338D, C339D, C340D, C341D, C342D, C343D, C344D, C345D, C346D, C347D, C348D, C349D, C350D, C351D, C352D, C353D, C354D, C355D, C356D, C357D, C358D, C359D, C360D, C361D, C362D, C363D, C364D, C365D, C366D, C367D, C368D, C369D, C370D, C371D, C372D, C373D, C374D, C375D, C376D, C377D, C378D, C379D, C380D, C381D, C382D, C383D, C384D, C385D, C386D, C387D, C388D, C389D, C390D, C391D, C392D, C393D, C394D, C395D, C396D, C397D, C398D, C399D, C400D, C401D, C402D, C403D, C404D, C405D, C406D, C407D, C408D, C409D, C410D, C411D, C412D, C413D, C414D, C415D, C416D, C417D, C418D, C419D, C420D, C421D, C422D, C423D, C424D, C425D, C426D, C427D, C428D, C429D, C430D, C431D, C432D, C433D, C434D, C435D, C436D, C437D, C438D, C439D, C440D, C441D, C442D, C443D, C444D, C445D, C446D, C447D, C448D, C449D, C450D, C451D, C452D, C453D, C454D, C455D, C456D, C457D, C458D, C459D, C460D, C461D, C462D, C463D, C464D, C465D, C466D, C467D, C468D, C469D, C470D, C471D, C472D, C473D, C474D, C475D, C476D, C477D, C478D, C479D, C480D, C481D, C482D, C483D, C484D, C485D, C486D, C487D, C488D, C489D, C490D, C491D, C492D, C493D, C494D, C495D, C496D, C497D, C498D, C499D, C500D, C501D, C502D, C503D, C504D, C505D, C506D, C507D, C508D, C509D, C510D, C511D, C512D, C513D, C514D, C515D, C516D, C517D, C518D, C519D, C520D, C521D, C522D, C523D, C524D, C525D, C526D, C527D, C528D, C529D, C530D, C531D, C532D, C533D, C534D, C535D, C536D, C537D, C538D, C539D, C540D, C541D, C542D, C543D, C544D, C545D, C546D, C547D, C548D, C549D, C550D, C551D, C552D, C553D, C554D, C555D, C556D, C557D, C558D, C559D, C560D, C561D, C562D, C563D, C564D, C565D, C566D, C567D, C568D, C569D, C570D, C571D, C572D, C573D, C574D, C575D, C576D, C577D, C578D, C579D, C580D, C581D, C582D, C583D, C584D, C585D, C586D, C587D, C588D, C589D, C590D, C591D, C592D, C593D, C594D, C595D, C596D, C597D, C598D, C599D, C600D, C601D, C602D, C603D, C604D, C605D, C606D, C607D, C608D, C609D, C610D, C611D, C612D, C613D, C614D, C615D, C616D, C617D, C618D, C619D, C620D, C621D, C622D, C623D, C624D, C625D, C626D, C627D, C628D, C629D, C630D, C631D, C632D, C633D, C634D, C635D, C636D, C637D, C638D, C639D, C640D, C641D, C642D, C643D, C644D, C645D, C646D, C647D, C648D, C649D, C650D, C651D, C652D, C653D, C654D, C655D, C656D, C657D, C658D, C659D, C660D, C661D, C662D, C

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Fe	H	N	O	0	0
			49	34	1	6	4	4		



WORLD WIDE  
PDB  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total	C	Fe	H	N	O	0	0
			50	34	1	7	4	4		

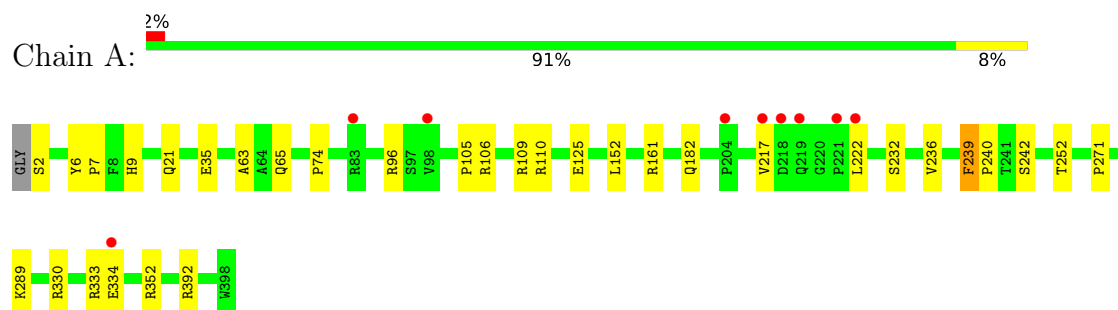
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	378	Total	O	0	0
			378	378		
7	B	370	Total	O	0	0
			370	370		

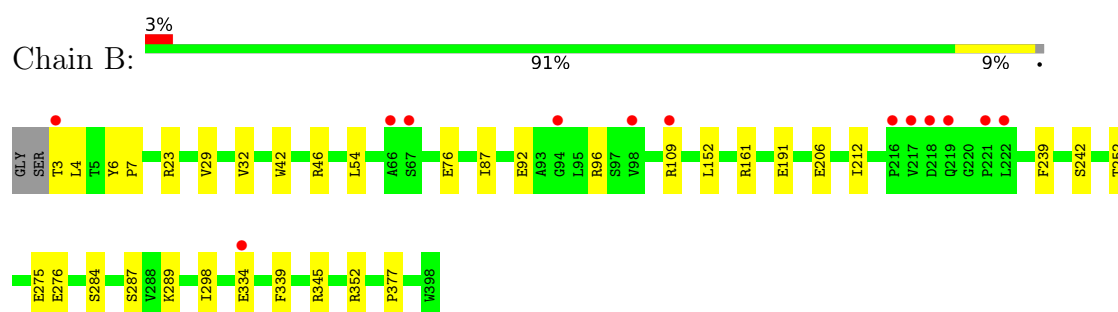
### 3 Residue-property plots [i](#)

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-F5053



- Molecule 1: cytochrome P450-F5053



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.21Å 91.33Å 98.28Å 90.00° 96.41° 90.00°	Depositor
Resolution (Å)	43.06 – 1.70 43.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.06-1.70) 94.5 (43.06-1.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.186 , 0.220 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	4133 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2301e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEM, NA, BR, 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	0.56	1/3140 (0.0%)	0.67	0/4270
1	B	1.02	10/3134 (0.3%)	0.81	0/4262
All	All	0.82	11/6274 (0.2%)	0.74	0/8532

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	GLU	CD-OE2	-6.96	1.18	1.25
1	B	191	GLU	CD-OE1	-6.37	1.18	1.25
1	B	76	GLU	CD-OE1	-6.01	1.19	1.25
1	B	276	GLU	CD-OE1	-6.01	1.19	1.25
1	B	284	SER	CA-CB	-5.92	1.44	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ALA	Mainchain



## 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	3067	2980	3004	25	0
1	B	3061	2952	2999	18	0
2	A	6	8	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	2	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	43	6	30	12	0
6	B	43	7	30	8	0
7	A	378	0	0	10	4
7	B	370	0	0	5	2
All	All	6980	5953	6071	55	6

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 4.

The worst 5 of 55 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:271:PRO:HB3	7:A:851:HOH:O	1.78	0.84
1:A:152:LEU:HD21	6:A:409:HEM:HBC1	1.69	0.75
1:B:242:SER:HA	6:B:406:HEM:HBB1	1.69	0.74
1:A:96:ARG:NH1	7:A:501:HOH:O	2.22	0.71
6:A:409:HEM:HHC	6:A:409:HEM:HBB2	1.73	0.70

The worst 5 of 6 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)
7:B:791:HOH:O	7:B:796:HOH:O[1_455]	2.01	0.19
7:B:828:HOH:O	7:B:842:HOH:O[2_646]	2.04	0.16
7:A:759:HOH:O	7:A:851:HOH:O[1_655]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:711:HOH:O	7:A:851:HOH:O[1_655]	2.11	0.09
7:A:834:HOH:O	7:A:845:HOH:O[2_545]	2.12	0.08

## 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	395/398 (99%)	388 (98%)	7 (2%)	0	100	100
1	B	394/398 (99%)	388 (98%)	6 (2%)	0	100	100
All	All	789/796 (99%)	776 (98%)	13 (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	319/318 (100%)	314 (98%)	5 (2%)	62	48
1	B	318/318 (100%)	311 (98%)	7 (2%)	52	34
All	All	637/636 (100%)	625 (98%)	12 (2%)	57	41

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	GLU

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Mol	Chain	Res	Type
1	B	109	ARG
1	B	289	LYS
1	A	352	ARG
1	B	239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	179	HIS
1	A	182	GLN
1	B	182	GLN
1	B	184	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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
6	HEM	B	406	1,7	27,50,50	2.06	7 (25%)	17,82,82	2.16	7 (41%)
6	HEM	A	409	1,7	27,50,50	2.16	6 (22%)	17,82,82	2.09	6 (35%)
2	GOL	A	401	-	5,5,5	0.53	0	5,5,5	0.97	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
6	HEM	B	406	1,7	-	0/6/54/54	-
6	HEM	A	409	1,7	-	0/6/54/54	-
2	GOL	A	401	-	-	2/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	406	HEM	C3B-C2B	-6.30	1.31	1.40
6	A	409	HEM	C3B-C2B	-5.69	1.32	1.40
6	A	409	HEM	C3C-C2C	-4.91	1.33	1.40
6	B	406	HEM	C3C-C2C	-4.53	1.34	1.40
6	A	409	HEM	CAA-C2A	3.89	1.57	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	406	HEM	C4C-C3C-C2C	4.81	110.26	106.90
6	A	409	HEM	C4C-C3C-C2C	4.63	110.13	106.90
6	A	409	HEM	CMD-C2D-C1D	-3.66	122.84	128.46
6	B	406	HEM	CMD-C2D-C1D	-3.32	123.37	128.46
6	A	409	HEM	C4A-C3A-C2A	3.26	109.26	107.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

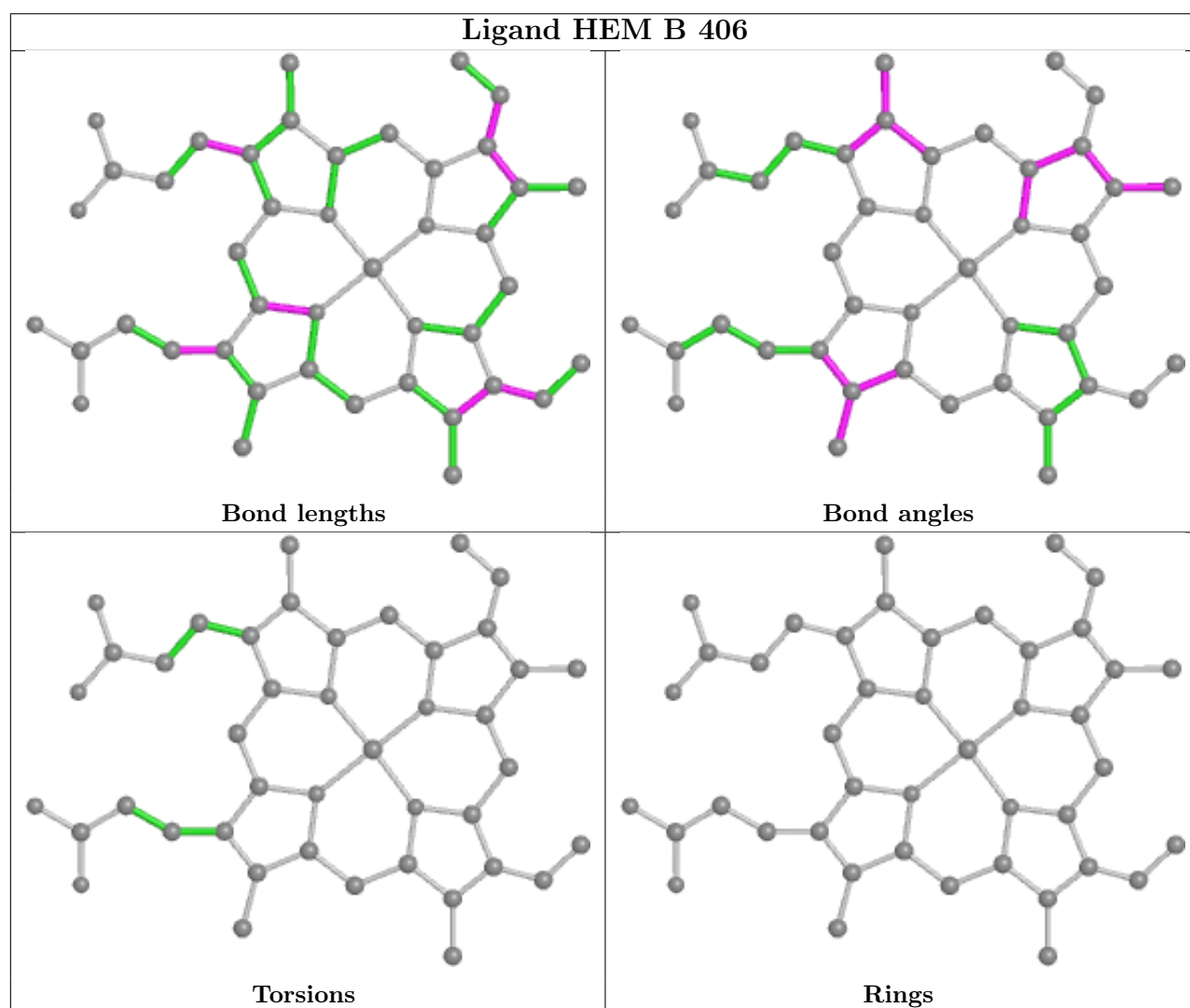
Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3

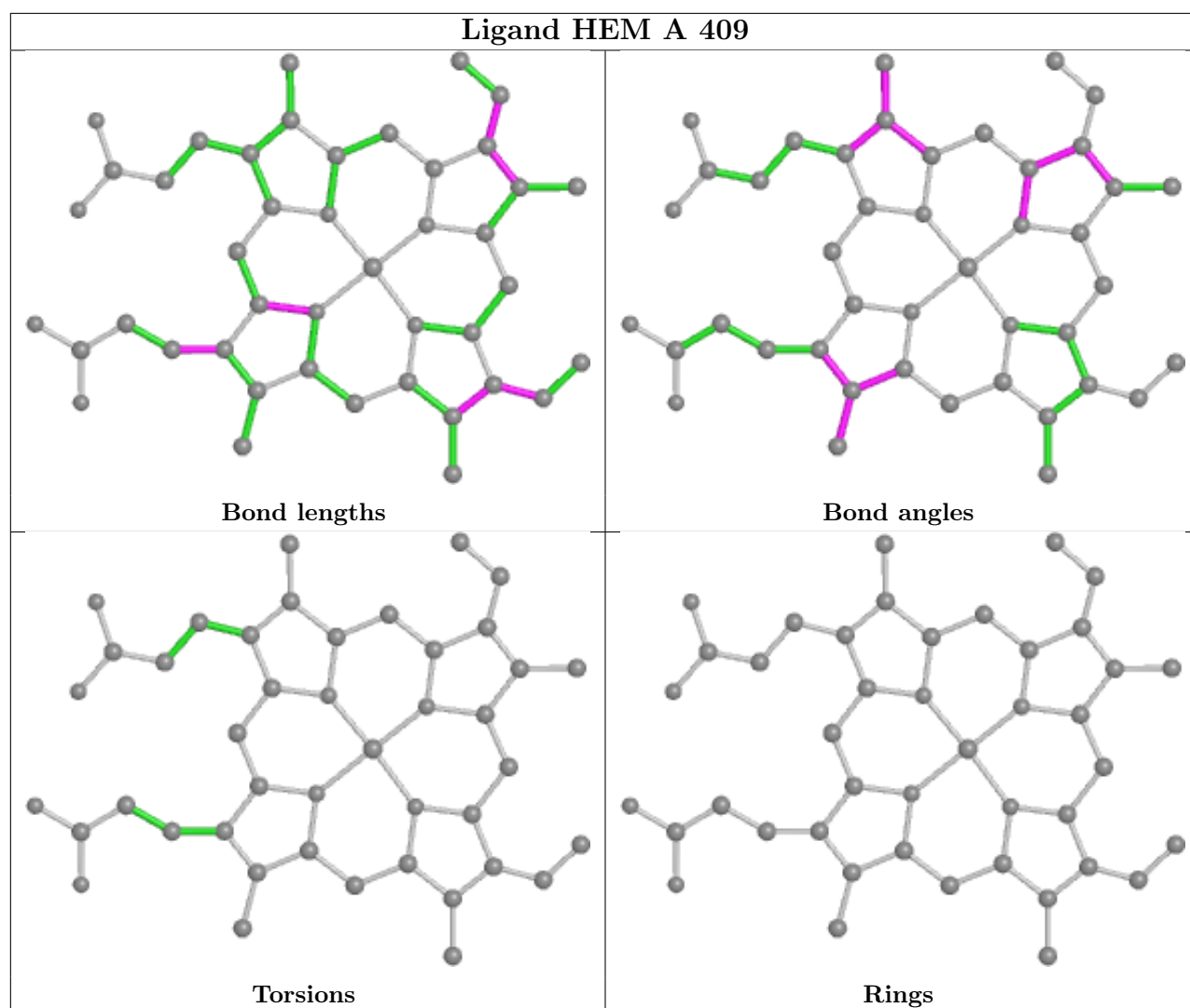
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	406	HEM	8	0
6	A	409	HEM	12	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 [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, 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	397/398 (99%)	0.01	9 (2%) 60 65	11, 20, 42, 67	0
1	B	396/398 (99%)	0.03	13 (3%) 46 51	12, 20, 44, 68	0
All	All	793/796 (99%)	0.02	22 (2%) 53 57	11, 20, 43, 68	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	VAL	5.8
1	A	221	PRO	5.3
1	B	218	ASP	4.6
1	B	3	THR	4.2
1	A	219	GLN	4.1

### 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](#)

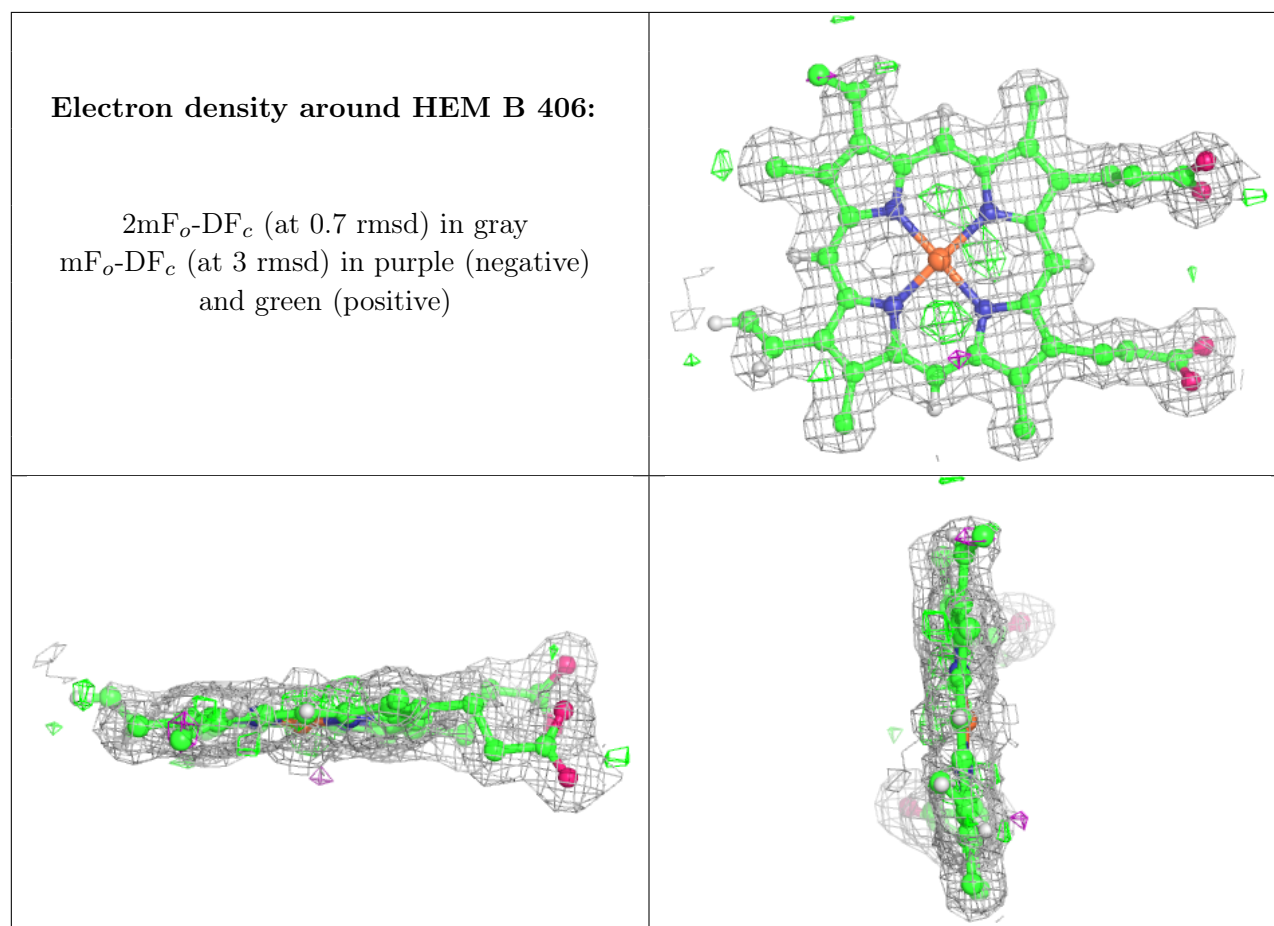
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

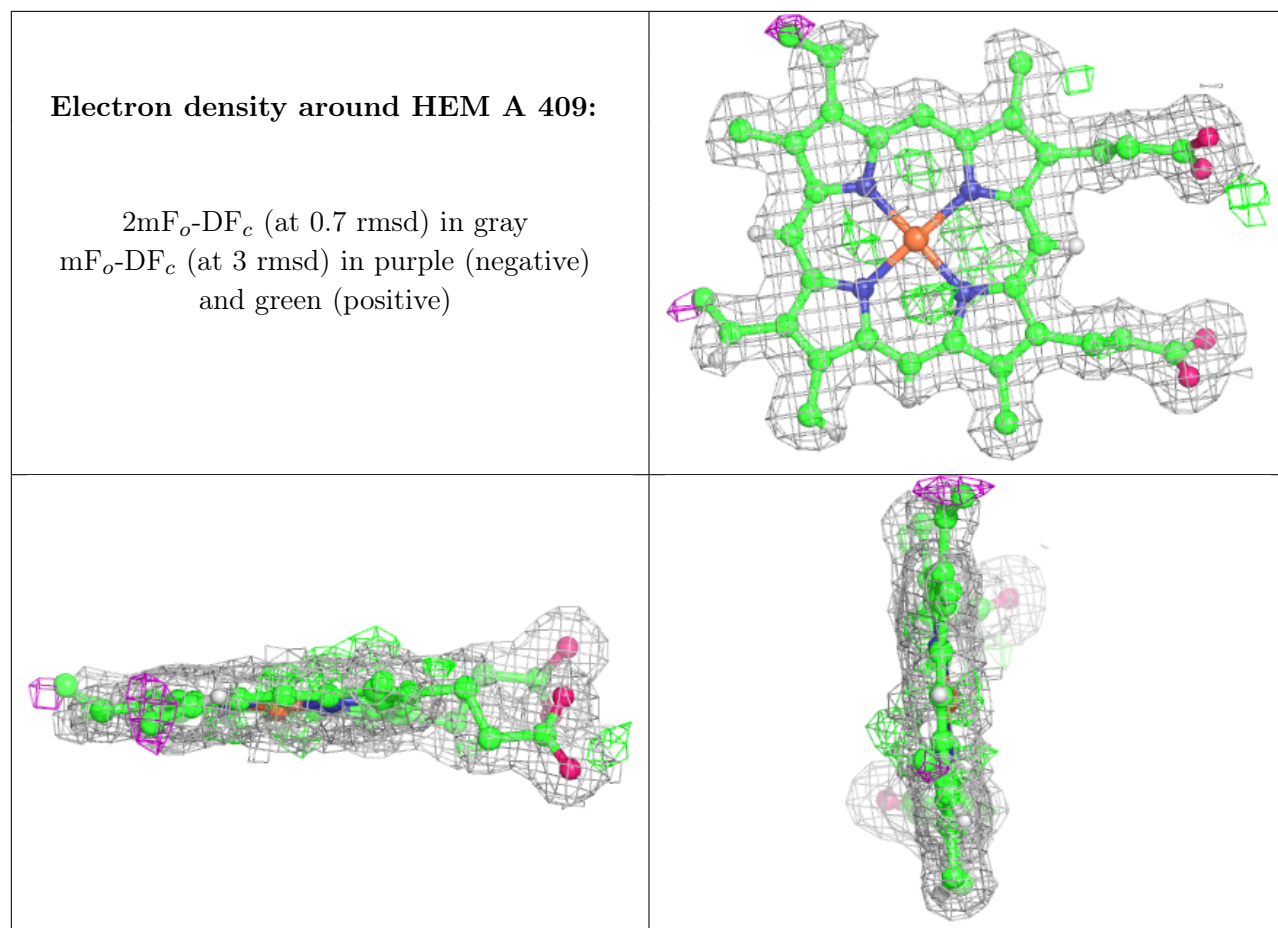
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
2	GOL	A	401	6/6	0.90	0.14	25,35,48,57	0
4	CL	A	405	1/1	0.94	0.07	48,48,48,48	0
5	NA	B	405	1/1	0.95	0.27	23,23,23,23	0
5	NA	A	408	1/1	0.95	0.17	27,27,27,27	0
4	CL	A	404	1/1	0.96	0.06	30,30,30,30	0
4	CL	B	403	1/1	0.97	0.06	27,27,27,27	0
4	CL	A	407	1/1	0.97	0.06	41,41,41,41	0
6	HEM	B	406	43/43	0.98	0.14	6,13,23,45	0
6	HEM	A	409	43/43	0.98	0.14	9,14,22,39	0
4	CL	B	404	1/1	0.98	0.04	34,34,34,34	0
3	BR	B	402	1/1	0.98	0.04	26,26,26,26	1
3	BR	A	403	1/1	0.99	0.05	27,27,27,27	1
3	BR	B	401	1/1	0.99	0.04	27,27,27,27	1
4	CL	A	406	1/1	0.99	0.05	20,20,20,20	0
3	BR	A	402	1/1	0.99	0.03	23,23,23,23	1

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.