

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 10:46 pm GMT

PDB ID : 4B7F

Title: Structure of a liganded bacterial catalase

Authors: Gumiero, A.; Walsh, M.

Deposited on : 2012-08-20

Resolution : 1.76 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

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)

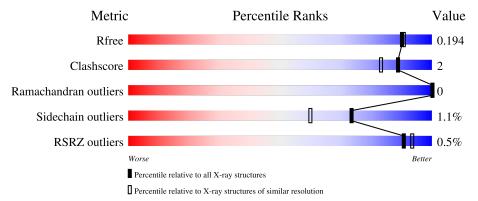
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.76 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 <=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	515	96%	•
1	В	515	95%	5%
1	С	515	95%	5%
1	D	515	95%	5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NO	A	1519	-	-	X	-
4	NO	D	1520	-	-	X	-



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18258 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 Catalase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	515	Total	С	N	О	S	0	9	0
1	A		4197	2638	736	814	9	0	9	
1	В	514	Total	С	N	О	S	0	6	0
1	1 B	314	4170	2619	736	806	9	0		0
1	С	514	Total	С	N	О	S	0	Q	0
1		314	4187	2628	743	807	9	0	8	
1	1 D	D 514	Total	С	N	О	S	0	6	0
1			4173	2623	738	803	9	U	U	U

There are 8 discrepancies between the modelled and reference sequences:

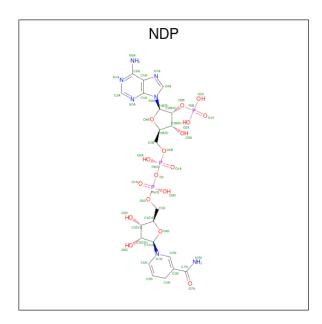
Chain	Residue	Modelled	Actual	Comment	Reference
A	350	ILE	VAL	conflict	UNP A0A0U4WRC5
A	498	ASN	LYS	conflict	UNP A0A0U4WRC5
В	350	ILE	VAL	conflict	UNP A0A0U4WRC5
В	498	ASN	LYS	conflict	UNP A0A0U4WRC5
С	350	ILE	VAL	conflict	UNP A0A0U4WRC5
С	498	ASN	LYS	conflict	UNP A0A0U4WRC5
D	350	ILE	VAL	conflict	UNP A0A0U4WRC5
D	498	ASN	LYS	conflict	UNP A0A0U4WRC5

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	В	1	Total Cl 1 1	0	0

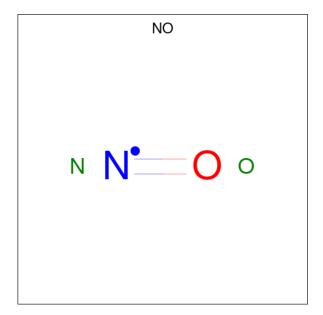
• Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf								
3	Λ	1	Total	С	N	О	Р	0	0							
3	A	1	48	21	7	17	3	U								
2	3 B	D	D	D	D	D	D	D	1	Total	С	N	О	Р	0	0
3		1	48	21	7	17	3	0	U							
3	C	C 1	Total	С	N	О	Р	0	0							
3		1	48	21	7	17	3	U								
2	3 D	1	Total	С	N	О	Р	0	0							
3		1	48	21	7	17	3	U	0							

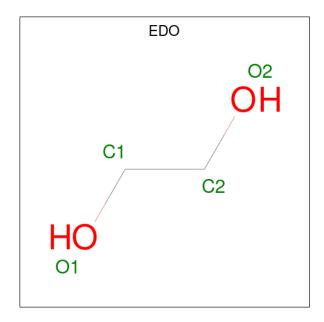
• Molecule 4 is NITRIC OXIDE (three-letter code: NO) (formula: NO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 2 1 1	0	0
4	В	1	Total N O 2 1 1	0	0
4	С	1	Total N O 2 1 1	0	0
4	D	1	Total N O 2 1 1	0	0

 $\bullet$  Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\mathrm{C_2H_6O_2}).$ 

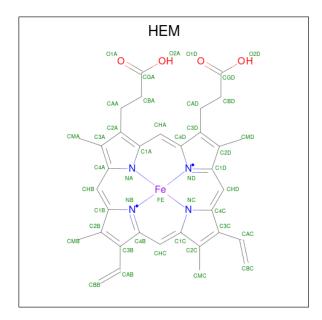


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0
5	С	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

• Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-



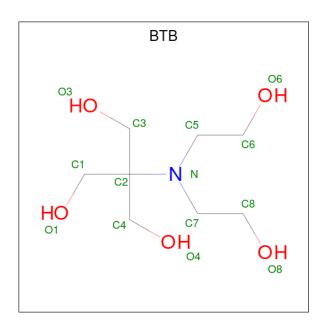
mula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
6	A	1	Total	С	Fe	N	О	0	0
0	Α	1	43	34	1	4	4	0	0
6	В	1	Total	С	Fe	N	О	0	0
0	6 B	1	43	34	1	4	4	0	
6	C	C 1	Total	С	Fe	N	О	0	0
0 0	1	43	34	1	4	4	0	0	
6 D	D	1	Total	С	Fe	N	О	0	0
	1	43	34	1	4	4	U	U	

• Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula:  $C_8H_{19}NO_5$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C N O 14 8 1 5	0	0

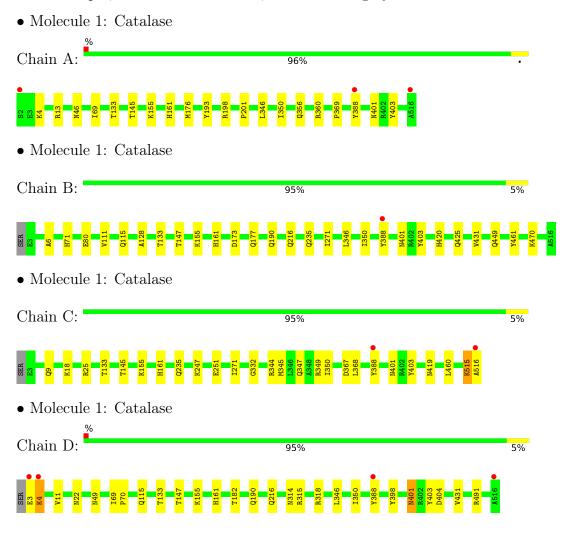
#### • Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	378	Total O 378 378	0	0
8	В	276	Total O 276 276	0	0
8	С	265	Total O 265 265	0	0
8	D	196	Total O 196 196	0	0



# 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.





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 63	Depositor	
Cell constants	151.51Å 151.51Å 156.62Å	Donogitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	100.58 - 1.76	Depositor	
Resolution (A)	100.58 - 1.76	EDS	
% Data completeness	93.0 (100.58-1.76)	Depositor	
(in resolution range)	93.0 (100.58-1.76)	EDS	
$R_{merge}$	0.10	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.35  (at  1.76Å)	Xtriage	
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor	
$R, R_{free}$	0.158 , 0.194	Depositor	
it, it free	0.158 , $0.194$	DCC	
$R_{free}$ test set	9387 reflections $(5.02\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage	
Anisotropy	0.429	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39 , 41.2	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage	
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	18258	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: NO, HEM, BTB, NDP, CL, EDO

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	Bo	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.38	0/4334	0.55	1/5888 (0.0%)	
1	В	0.38	1/4297~(0.0%)	0.55	0/5838	
1	С	0.42	$2/4317 \ (0.0\%)$	0.58	1/5863 (0.0%)	
1	D	0.40	1/4301~(0.0%)	0.57	1/5843 (0.0%)	
All	All	0.39	$4/17249 \ (0.0\%)$	0.56	3/23432 (0.0%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
1	С	419	ASN	C-N	-9.40	1.12	1.34
1	С	161	HIS	C-N	-6.57	1.19	1.34
1	В	161	HIS	C-N	-5.69	1.21	1.34
1	D	161	HIS	C-N	-5.53	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	161	HIS	O-C-N	-7.42	110.83	122.70
1	A	161	HIS	O-C-N	-5.81	113.40	122.70
1	D	161	HIS	O-C-N	-5.72	113.55	122.70

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	4197	0	3937	10	0
1	В	4170	0	3912	18	0
1	С	4187	0	3939	15	0
1	D	4173	0	3919	18	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	48	0	26	1	0
3	В	48	0	26	0	0
3	С	48	0	26	1	0
3	D	48	0	26	0	0
4	A	2	0	0	4	0
4	В	2	0	0	0	0
4	С	2	0	0	0	0
4	D	2	0	0	4	0
5	A	4	0	6	0	0
5	В	12	0	18	0	0
5	С	4	0	6	0	0
5	D	8	0	12	0	0
6	A	43	0	30	4	0
6	В	43	0	30	1	0
6	С	43	0	30	0	0
6	D	43	0	30	4	0
7	D	14	0	19	0	0
8	A	378	0	0	0	0
8	В	276	0	0	2	0
8	С	265	0	0	2	0
8	D	196	0	0	1	0
All	All	18258	0	15992	60	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 2.

The worst 5 of 60 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:D:216:GLN:HE22	1:D:431:VAL:H	1.09	0.98
1:B:216:GLN:HE22	1:B:431:VAL:H	1.12	0.91
1:A:69:ILE:H	1:A:356:GLN:HE22	1.21	0.89
1:D:401:ASN:HD22	1:D:403:TYR:H	1.20	0.87
1:C:401:ASN:HD22	1:C:403:TYR:H	1.25	0.84



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	Percentile	es
1	A	$522/515 \; (101\%)$	502 (96%)	20 (4%)	0	100 100	0
1	В	518/515 (101%)	494 (95%)	24 (5%)	0	100 100	0
1	C	$520/515 \; (101\%)$	501 (96%)	19 (4%)	0	100 100	0
1	D	518/515 (101%)	496 (96%)	22 (4%)	0	100 100	0
All	All	2078/2060 (101%)	1993 (96%)	85 (4%)	0	100 100	0

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	Perce	$\mathbf{ntiles}$
1	A	$444/436 \; (102\%)$	439 (99%)	5 (1%)	73	60
1	В	440/436 (101%)	436 (99%)	4 (1%)	78	67
1	C	$442/436 \; (101\%)$	437 (99%)	5 (1%)	73	60
1	D	440/436 (101%)	435 (99%)	5 (1%)	73	60
All	All	1766/1744 (101%)	1747 (99%)	19 (1%)	73	60

5 of 19 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	D	4	LYS
1	D	155	LYS
1	D	401	ASN
1	D	133	THR
1	В	449	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	401	ASN
1	D	216	GLN
1	С	498	ASN
1	D	61	ASN
1	D	316	ASN

#### 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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	Во	ond leng	ths	В	ond ang	gles
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	1520	-	3,3,3	0.51	0	2,2,2	0.41	0
5	EDO	D	1519	-	3,3,3	0.58	0	2,2,2	0.33	0
3	NDP	С	1517	_	45,52,52	1.57	4 (8%)	53,80,80	1.21	4 (7%)
4	NO	В	1520	6	0,1,1	-	-	-		
4	NO	D	1520	6	0,1,1	-	-	-		
6	HEM	A	3000	4,1	41,50,50	1.84	6 (14%)	45,82,82	1.75	8 (17%)
6	HEM	С	3002	4,1	41,50,50	1.82	6 (14%)	45,82,82	1.66	8 (17%)
3	NDP	В	1517	-	45,52,52	1.55	4 (8%)	53,80,80	1.21	4 (7%)
3	NDP	D	1518	-	45,52,52	1.58	4 (8%)	53,80,80	1.21	3 (5%)
5	EDO	В	1519	-	3,3,3	0.51	0	2,2,2	0.38	0
3	NDP	A	1518	-	45,52,52	1.56	4 (8%)	53,80,80	1.12	2 (3%)
4	NO	С	1519	6	0,1,1	-	-	-		
5	EDO	С	1518	-	3,3,3	0.54	0	2,2,2	0.29	0
5	EDO	В	1521	-	3,3,3	0.62	0	2,2,2	0.08	0
6	HEM	D	3003	4,1	41,50,50	1.80	6 (14%)	45,82,82	1.77	9 (20%)
4	NO	A	1519	6	0,1,1	-	-	-		
5	EDO	В	1522	-	3,3,3	0.45	0	2,2,2	0.36	0
6	HEM	В	3001	4,1	41,50,50	1.82	6 (14%)	45,82,82	1.72	10 (22%)
5	EDO	D	1521	-	3,3,3	0.56	0	2,2,2	0.26	0
7	BTB	D	1517	-	13,13,13	0.92	0	7,16,16	0.48	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
5	EDO	A	1520	-	-	0/1/1/1	-
5	EDO	D	1519	-	-	0/1/1/1	-
3	NDP	$\mathbf{C}$	1517	_	-	8/30/77/77	0/5/5/5
5	EDO	С	1518	-	-	0/1/1/1	-
5	EDO	В	1522	-	-	0/1/1/1	-
6	HEM	В	3001	4,1	-	4/12/54/54	-
5	EDO	D	1521	-	-	0/1/1/1	-
5	EDO	В	1521	-	-	0/1/1/1	-
7	BTB	D	1517	-	-	3/21/21/21	-
6	HEM	A	3000	4,1	-	2/12/54/54	-
6	HEM	С	3002	4,1	-	4/12/54/54	
3	NDP	В	1517	_	-	9/30/77/77	0/5/5/5

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Mol	Type	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
3	NDP	D	1518	-	-	10/30/77/77	0/5/5/5
5	EDO	В	1519	-	-	0/1/1/1	-
3	NDP	A	1518	-	-	6/30/77/77	0/5/5/5
6	HEM	D	3003	4,1	-	4/12/54/54	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
6	В	3001	HEM	C3D-C2D	7.44	1.52	1.36
6	A	3000	HEM	C3D-C2D	7.36	1.52	1.36
6	С	3002	HEM	C3D-C2D	7.14	1.51	1.36
6	D	3003	HEM	C3D-C2D	6.99	1.51	1.36
3	D	1518	NDP	O7N-C7N	6.95	1.41	1.24

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
6	A	3000	HEM	C4D-ND-C1D	5.94	111.21	105.07
6	В	3001	HEM	C4D-ND-C1D	5.83	111.10	105.07
6	D	3003	HEM	C4D-ND-C1D	5.71	110.97	105.07
6	С	3002	HEM	C4D-ND-C1D	5.61	110.87	105.07
3	D	1518	NDP	N3A-C2A-N1A	-5.54	120.02	128.68

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1518	NDP	C5D-O5D-PN-O3
3	В	1517	NDP	C2B-O2B-P2B-O3X
3	В	1517	NDP	C5D-O5D-PN-O3
3	С	1517	NDP	C5D-O5D-PN-O1N
3	С	1517	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1517	NDP	1	0
4	D	1520	NO	4	0
6	A	3000	HEM	4	0

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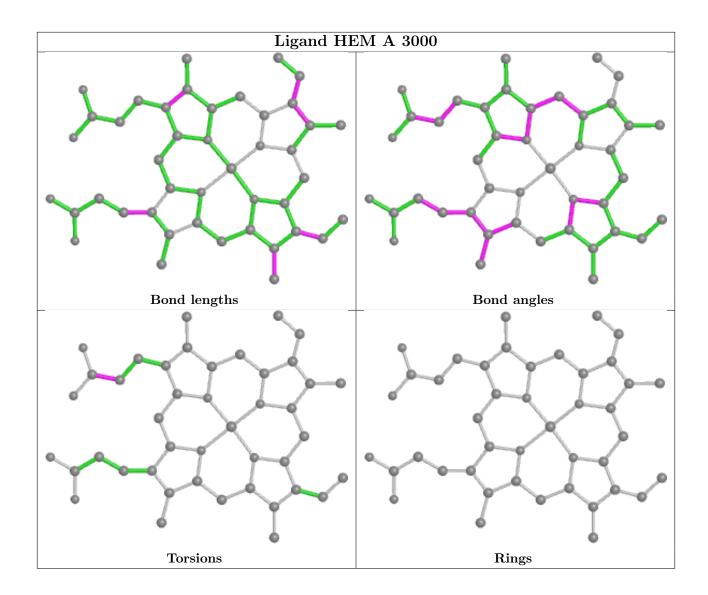


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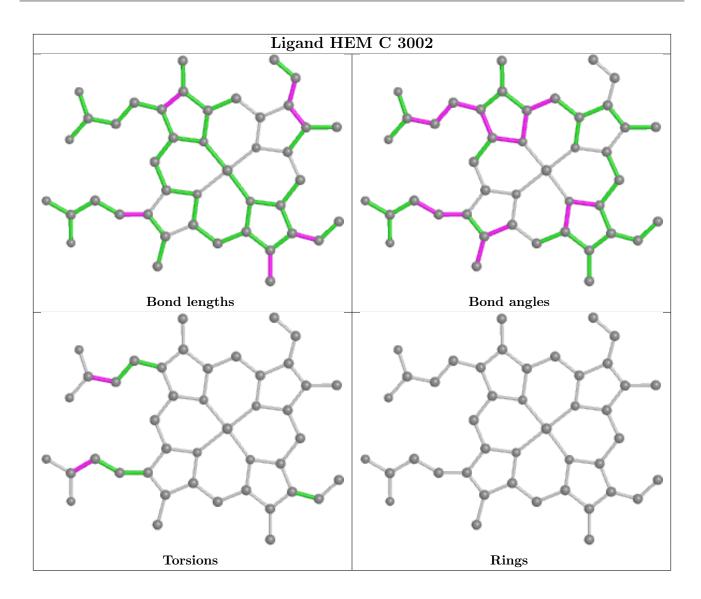
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1518	NDP	1	0
6	D	3003	HEM	4	0
4	A	1519	NO	4	0
6	В	3001	HEM	1	0

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 then 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.

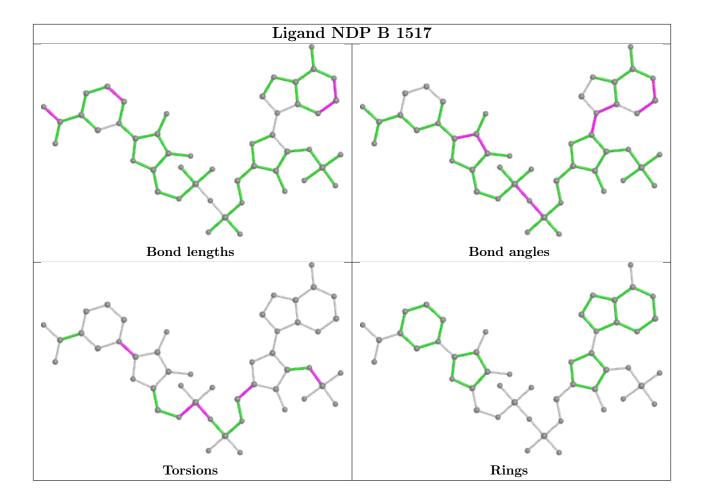




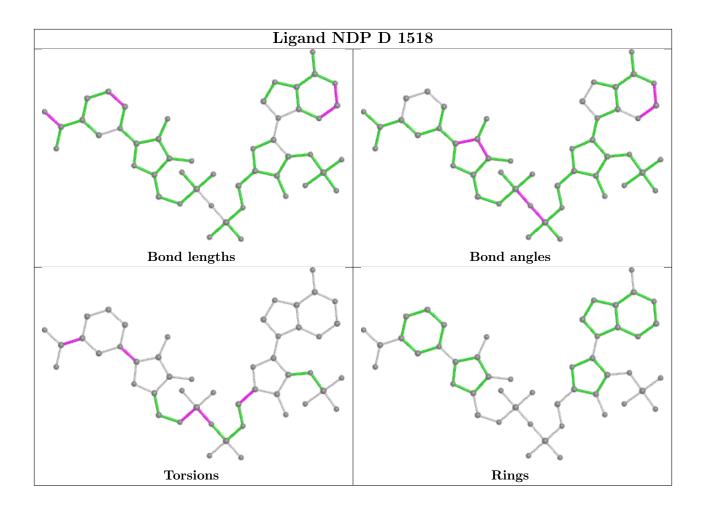




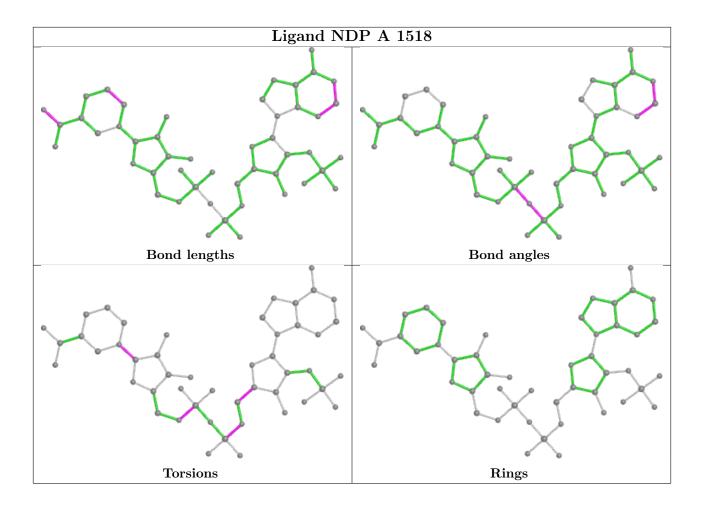




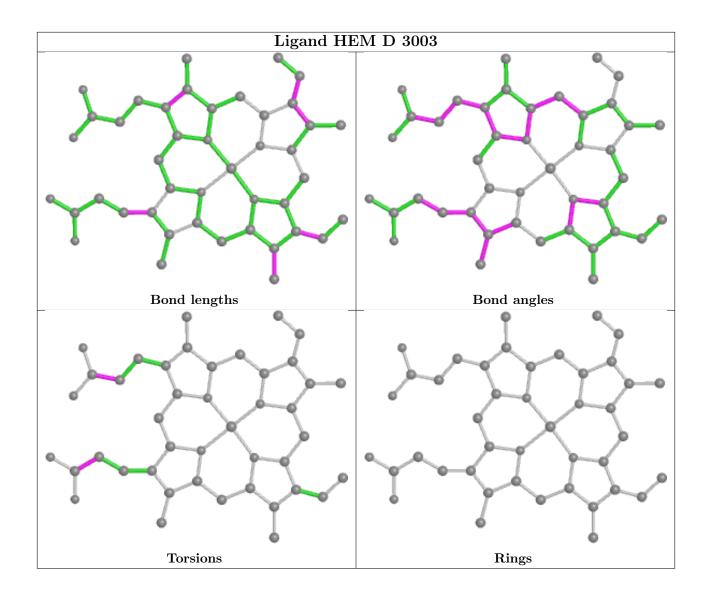




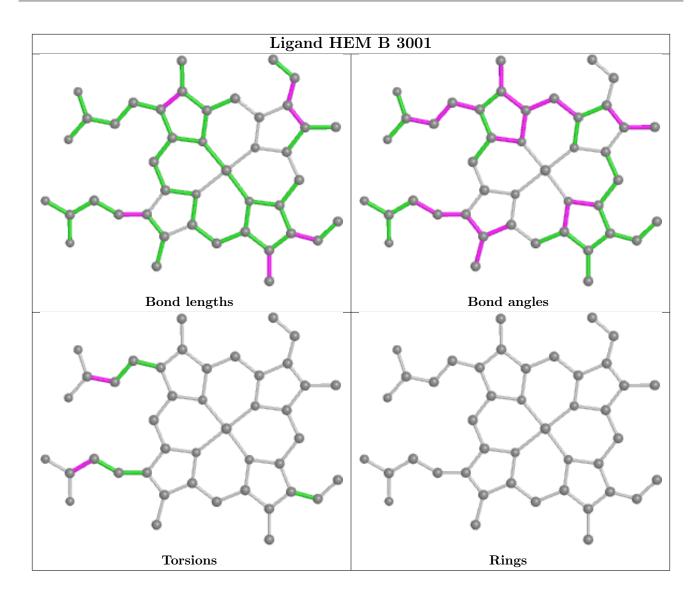












## 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

M	[ol	Chain	Number of breaks
	1	С	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	161:HIS	С	162:SER	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	419:ASN	С	420:HIS	N	1.12



### 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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	515/515 (100%)	-0.43	3 (0%) 89 92	9, 14, 24, 65	0
1	В	514/515 (99%)	-0.39	1 (0%) 95 96	9, 16, 26, 55	0
1	С	514/515 (99%)	-0.40	2 (0%) 92 94	9, 14, 24, 52	0
1	D	514/515 (99%)	-0.32	4 (0%) 86 90	9, 15, 26, 56	0
All	All	2057/2060 (99%)	-0.39	10 (0%) 91 93	9, 15, 25, 65	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	516	ALA	4.6
1	A	2	SER	4.0
1	D	3	GLU	3.5
1	D	4	LYS	3.3
1	D	516	ALA	3.1

#### 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,  $95^{th}$  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	${f B ext{-}factors}({f \AA}^2)$	Q<0.9
7	BTB	D	1517	14/14	0.74	0.32	30,51,64,71	0
3	NDP	С	1517	48/48	0.83	0.23	21,36,52,57	0
3	NDP	D	1518	48/48	0.86	0.20	25,35,49,58	0
3	NDP	A	1518	48/48	0.92	0.13	20,26,32,37	0
3	NDP	В	1517	48/48	0.94	0.14	20,29,37,40	0
5	EDO	В	1521	4/4	0.95	0.08	16,17,17,18	0
5	EDO	В	1522	4/4	0.96	0.10	14,15,17,18	0
5	EDO	D	1521	4/4	0.97	0.07	15,17,21,22	0
5	EDO	D	1519	4/4	0.97	0.08	12,12,15,16	0
5	EDO	В	1519	4/4	0.98	0.08	12,13,16,17	0
6	HEM	A	3000	43/43	0.98	0.08	7,10,13,14	0
6	HEM	В	3001	43/43	0.98	0.08	8,12,15,17	0
6	HEM	D	3003	43/43	0.98	0.08	7,11,13,16	0
4	NO	В	1520	2/2	0.98	0.12	20,20,20,20	0
4	NO	A	1519	2/2	0.99	0.10	20,20,20,20	0
4	NO	С	1519	2/2	0.99	0.11	20,20,20,20	0
4	NO	D	1520	2/2	0.99	0.10	20,20,20,20	0
6	HEM	С	3002	43/43	0.99	0.08	8,10,13,15	0
5	EDO	С	1518	4/4	0.99	0.06	11,13,13,13	0
5	EDO	A	1520	4/4	0.99	0.07	11,11,12,13	0
2	CL	A	1517	1/1	1.00	0.05	15,15,15,15	0
2	CL	В	1518	1/1	1.00	0.07	16,16,16,16	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.

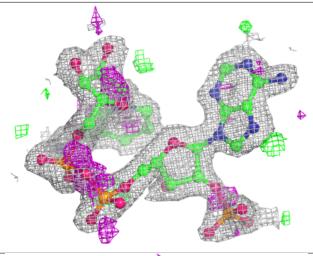


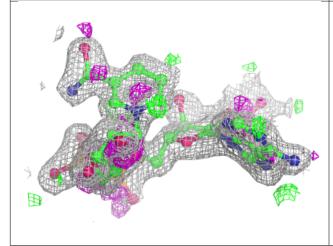
# 

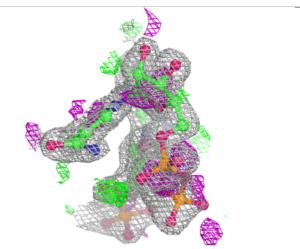


# Electron density around NDP D 1518:

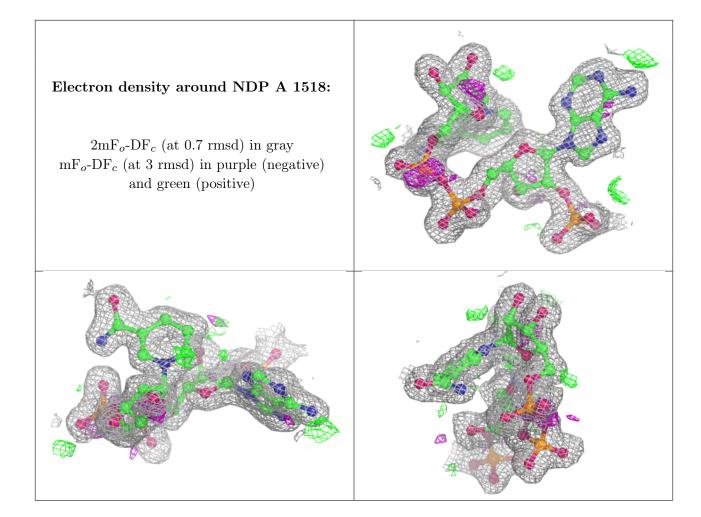
 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



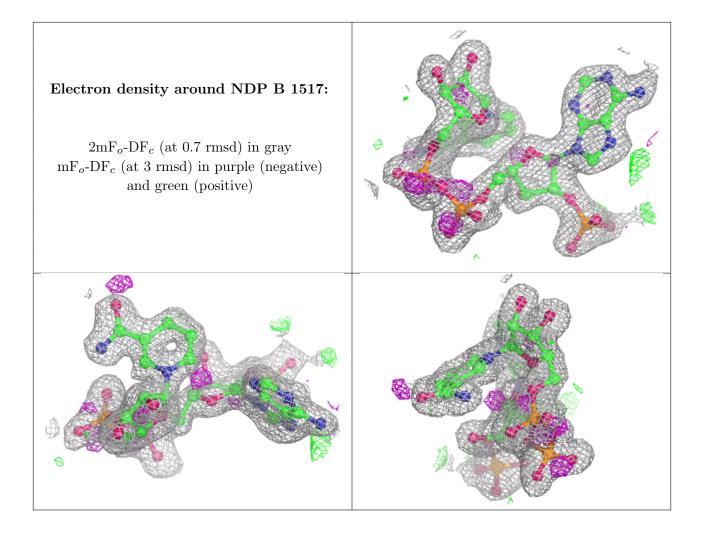




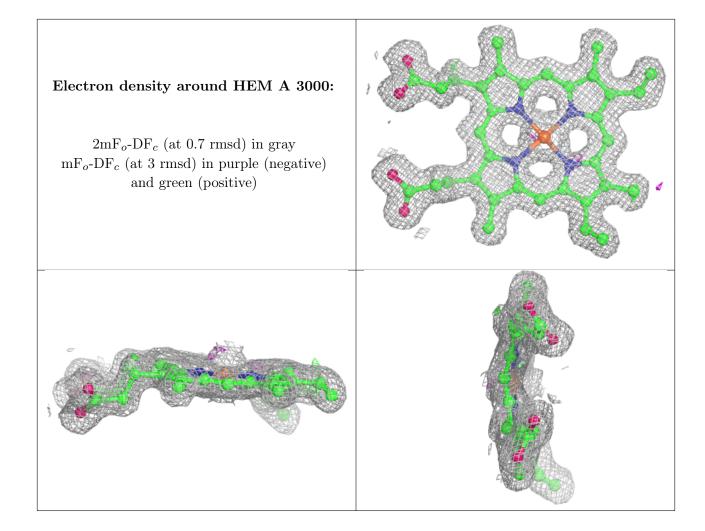




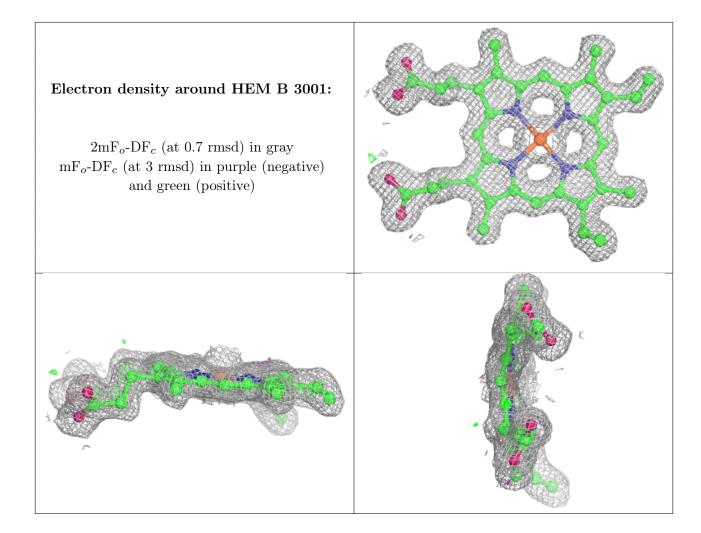




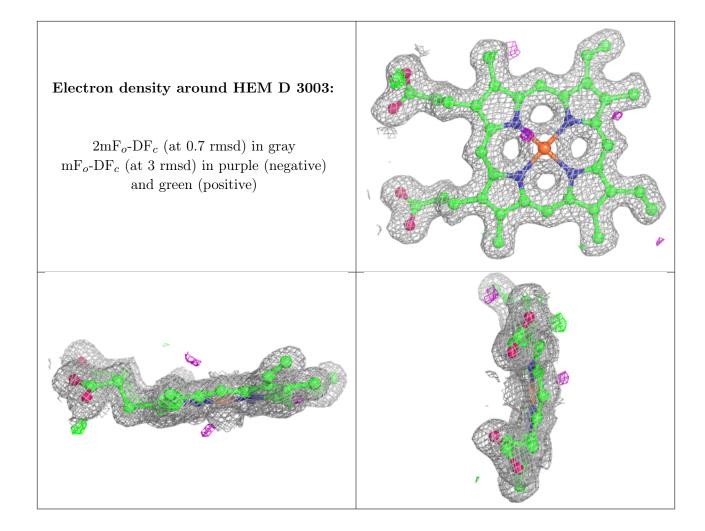




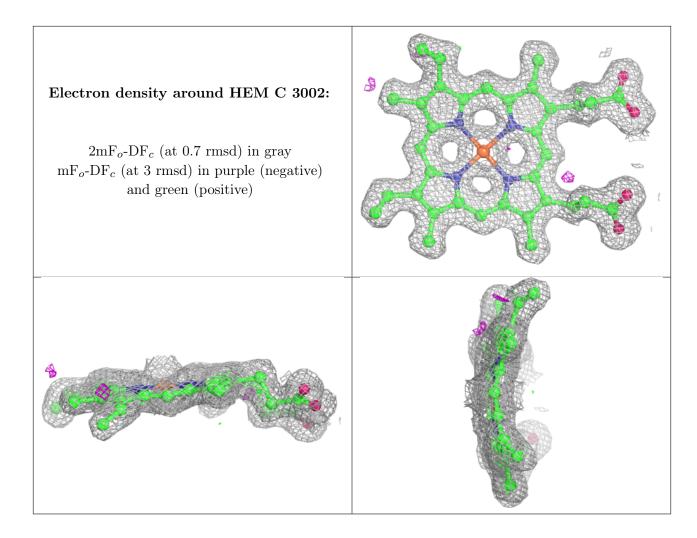












# 6.5 Other polymers (i)

There are no such residues in this entry.

