

wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 10:22 pm BST

PDB ID : 4B7H

Title: Structure of a highdose liganded bacterial catalase

Authors: Gumiero, A.; Walsh, M.

Deposited on : 2012-08-20

Resolution : 1.39 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 : 2.36.2buster-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)

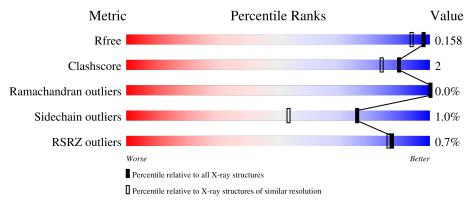
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	95%	•
1	В	515	96%	
1	С	515	94%	6%
1	D	515	96%	



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18897 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.

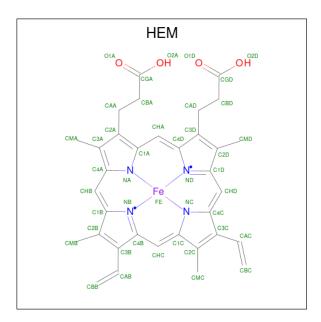
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A 515	Total	С	N	О	S	0	10	0	
1	A	313	4206	2643	737	817	9	0	10	
1	В	514	Total	С	N	О	S	0	6	0
1		514	4176	2624	735	808	9	0	U	0
1	С	514	Total	С	N	О	S	0	9	0
1		314	4196	2636	743	808	9	0	9	
1	D	514	Total	С	N	О	S	0	6	0
1	D	314	4176	2624	738	805	9	0	0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ILE	LEU	$\operatorname{conflict}$	UNP Q6M8A6
В	327	ILE	LEU	conflict	UNP Q6M8A6
С	327	ILE	LEU	conflict	UNP Q6M8A6
D	327	ILE	LEU	conflict	UNP Q6M8A6

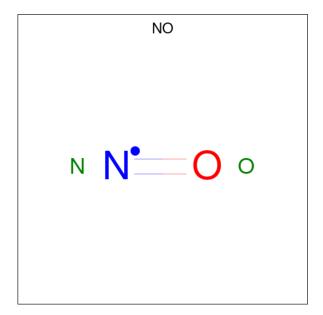
• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
2	٨	٨	1	Total	С	Fe	N	О	0	0
	A	Λ 1	43	34	1	4	4	0		
2	В	1	Total	С	Fe	N	О	0	0	
2	Б	1	43	34	1	4	4	0		
2	С	C 1	Total	С	Fe	N	О	0	0	
2			43	34	1	4	4	0	0	
2	D	D 1	Total	С	Fe	N	О	0	0	
			43	34	1	4	4	U		

• Molecule 3 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



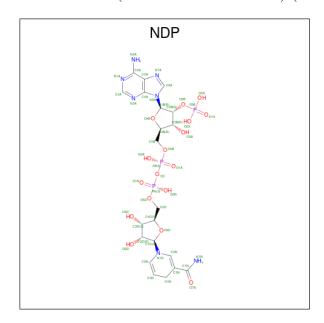


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 2 1 1	0	0
3	В	1	Total N O 2 1 1	0	0
3	С	1	Total N O 2 1 1	0	0
3	D	1	Total N O 2 1 1	0	0

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

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

• Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	Λ	1	Total	С	N	О	Р	0	0
	Λ	1	48	21	7	17	3	U	U
5	B	1	Total	С	N	Ο	Р	0	0
	Б	1	48	21	7	17	3		
5	C	1	Total	С	N	О	Р	0	0
5	C		48	21	7	17	3	0	

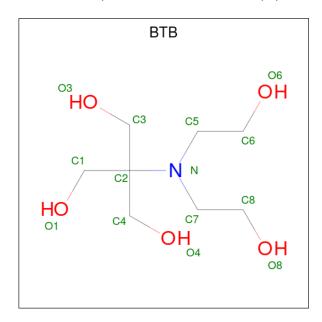
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Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	D	1	Total	С	N	О	Р	0	0
9	D	1	48	21	7	17	3	U	0

• Molecule 6 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
6	В	1	Total C N O 14 8 1 5	0	0
6	В	1	Total C N O 14 8 1 5	0	0
6	С	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

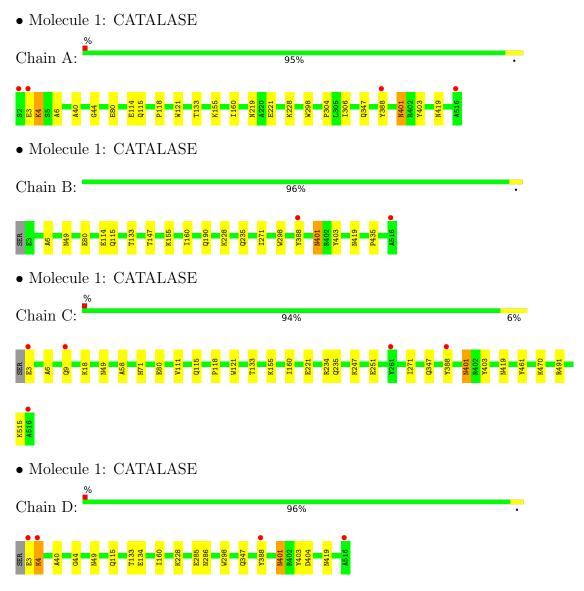
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	552	Total O 552 552	0	0
7	В	433	Total O 433 433	0	0
7	С	389	Total O 389 389	0	0
7	D	339	Total O 339 339	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	151.60Å 151.60Å 156.87Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.33 - 1.39	Depositor
Resolution (A)	78.44 - 1.39	EDS
% Data completeness	99.9 (67.33-1.39)	Depositor
(in resolution range)	99.9 (78.44-1.39)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.61 (at 1.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
D.D.	0.130 , 0.157	Depositor
R, R_{free}	0.131 , 0.158	DCC
R_{free} test set	20518 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 45.6	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	18897	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: NDP, CL, NO, HEM, BTB

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	Во	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.40	2/4346~(0.0%)	0.57	0/5903	
1	В	0.42	3/4304~(0.1%)	0.57	0/5847	
1	С	0.39	$2/4330 \ (0.0\%)$	0.56	1/5881 (0.0%)	
1	D	0.41	3/4304 (0.1%)	0.56	0/5846	
All	All	0.40	$10/17284 \ (0.1\%)$	0.56	$1/23477 \ (0.0\%)$	

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	419	ASN	C-N	-12.09	1.06	1.34
1	D	419	ASN	C-N	-11.25	1.08	1.34
1	A	419	ASN	C-N	-10.78	1.09	1.34
1	С	419	ASN	C-N	-9.53	1.12	1.34
1	В	435	PRO	C-N	6.84	1.49	1.34

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	С	58	ALA	C-N-CA	-5.08	108.99	121.70

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	4206	0	3945	14	0
1	В	4176	0	3914	14	0
1	С	4196	0	3949	23	0
1	D	4176	0	3922	16	0
2	A	43	0	30	0	0
2	В	43	0	30	0	0
2	С	43	0	30	0	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	В	2	0	0	0	0
3	С	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	48	0	26	0	0
5	В	48	0	26	0	0
5	С	48	0	26	0	0
5	D	48	0	26	0	0
6	В	28	0	38	0	0
6	С	14	0	19	0	0
6	D	14	0	19	3	0
7	A	552	0	0	3	0
7	В	433	0	0	5	0
7	С	389	0	0	2	0
7	D	339	0	0	4	0
All	All	18897	0	16030	58	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 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$
1:B:401:ASN:HD22	1:B:403:TYR:H	1.19	0.86
1:A:401:ASN:HD22	1:A:403:TYR:H	1.21	0.86
1:C:401:ASN:HD22	1:C:403:TYR:H	1.21	0.86
1:D:401:ASN:HD22	1:D:403:TYR:H	1.21	0.85
1:B:115[A]:GLN:O	7:B:2097:HOH:O	2.02	0.77

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	Perce	ntiles	
1	A	$523/515 \; (102\%)$	503 (96%)	19 (4%)	1 (0%)	47	21
1	В	518/515 (101%)	501 (97%)	17 (3%)	0	100	100
1	С	521/515 (101%)	504 (97%)	17 (3%)	0	100	100
1	D	518/515 (101%)	499 (96%)	19 (4%)	0	100	100
All	All	2080/2060 (101%)	2007 (96%)	72 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU

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	$445/436 \; (102\%)$	441 (99%)	4 (1%)	78	58	
1	В	440/436 (101%)	437 (99%)	3 (1%)	84	66	
1	С	443/436 (102%)	436 (98%)	7 (2%)	62	33	
1	D	440/436 (101%)	436 (99%)	4 (1%)	78	58	
All	All	1768/1744 (101%)	1750 (99%)	18 (1%)	76	53	

5 of 18 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	D	3	GLU
1	D	401	ASN
1	D	133	THR
1	С	9	GLN
1	С	515	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	401	ASN
1	D	316	ASN
1	С	498	ASN
1	D	49	ASN
1	D	498	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
WIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	BTB	В	1521	-	13,13,13	1.29	3 (23%)	7,16,16	0.62	0
5	NDP	С	1519	-	45,52,52	1.52	4 (8%)	53,80,80	1.18	3 (5%)
3	NO	D	1520	2	0,1,1	-	-	-		
2	HEM	С	1517	3,1	41,50,50	1.70	5 (12%)	45,82,82	1.53	8 (17%)
3	NO	В	1522	2	0,1,1	-	-	-		
6	BTB	D	1519	_	13,13,13	1.26	2 (15%)	7,16,16	0.41	0
6	BTB	В	1520	-	13,13,13	1.34	3 (23%)	7,16,16	0.79	0
2	HEM	D	1517	3,1	41,50,50	1.69	4 (9%)	45,82,82	1.66	12 (26%)
3	NO	С	1520	2	0,1,1	-	-	-		
2	HEM	A	1517	3,1	41,50,50	1.72	4 (9%)	45,82,82	1.66	9 (20%)
5	NDP	D	1518	-	45,52,52	1.52	4 (8%)	53,80,80	1.18	3 (5%)
6	ВТВ	С	1518	-	13,13,13	1.26	2 (15%)	7,16,16	0.54	0
2	HEM	В	1517	3,1	41,50,50	1.74	5 (12%)	45,82,82	1.69	10 (22%)
3	NO	A	1518	2	0,1,1	-	-	-		
5	NDP	В	1518	-	45,52,52	1.51	4 (8%)	53,80,80	1.15	2 (3%)
5	NDP	A	1520	-	45,52,52	1.51	4 (8%)	53,80,80	1.13	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BTB	В	1521	-	-	3/21/21/21	-
5	NDP	С	1519	-	-	7/30/77/77	0/5/5/5
2	HEM	С	1517	3,1	-	4/12/54/54	-
6	BTB	D	1519	-	-	1/21/21/21	-
6	BTB	В	1520	-	-	3/21/21/21	-
2	HEM	D	1517	3,1	-	4/12/54/54	-
2	HEM	A	1517	3,1	-	4/12/54/54	-
5	NDP	D	1518	-	-	6/30/77/77	0/5/5/5
6	BTB	С	1518	-	-	4/21/21/21	-
2	HEM	В	1517	3,1	-	4/12/54/54	-
5	NDP	В	1518	-	-	6/30/77/77	0/5/5/5
5	NDP	A	1520	-	-	6/30/77/77	0/5/5/5

The worst 5 of 44 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	В	1517	HEM	C3D-C2D	6.90	1.51	1.36
2	D	1517	HEM	C3D-C2D	6.82	1.51	1.36
5	В	1518	NDP	O7N-C7N	6.66	1.40	1.24
5	A	1520	NDP	O7N-C7N	6.66	1.40	1.24
2	A	1517	HEM	C3D-C2D	6.65	1.50	1.36

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
5	С	1519	NDP	N3A-C2A-N1A	-5.47	120.12	128.68
5	D	1518	NDP	N3A-C2A-N1A	-5.44	120.17	128.68
5	A	1520	NDP	N3A-C2A-N1A	-5.43	120.19	128.68
5	В	1518	NDP	N3A-C2A-N1A	-5.40	120.23	128.68
2	В	1517	HEM	C4D-ND-C1D	5.36	110.61	105.07

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	1518	NDP	C5D-O5D-PN-O3
6	В	1520	BTB	C1-C2-C3-O3
6	В	1520	BTB	C4-C2-C3-O3
6	В	1520	BTB	N-C2-C3-O3
6	В	1521	BTB	C1-C2-C3-O3

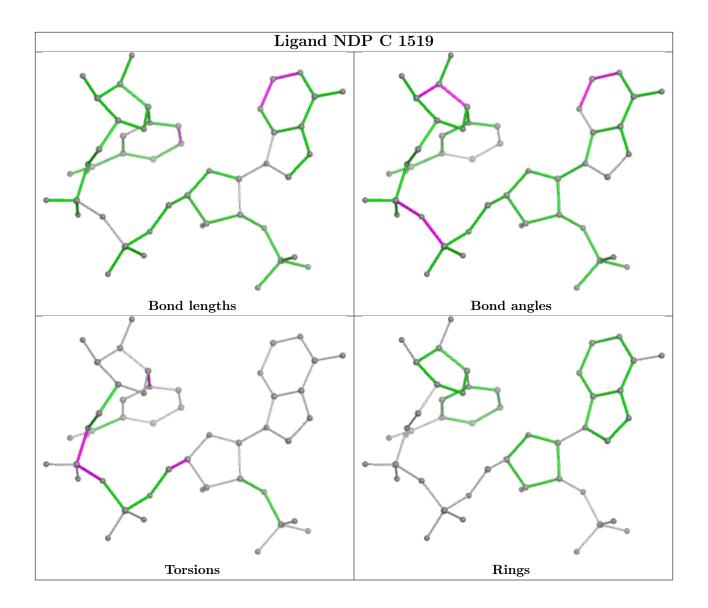
There are no ring outliers.

1 monomer is involved in 3 short contacts:

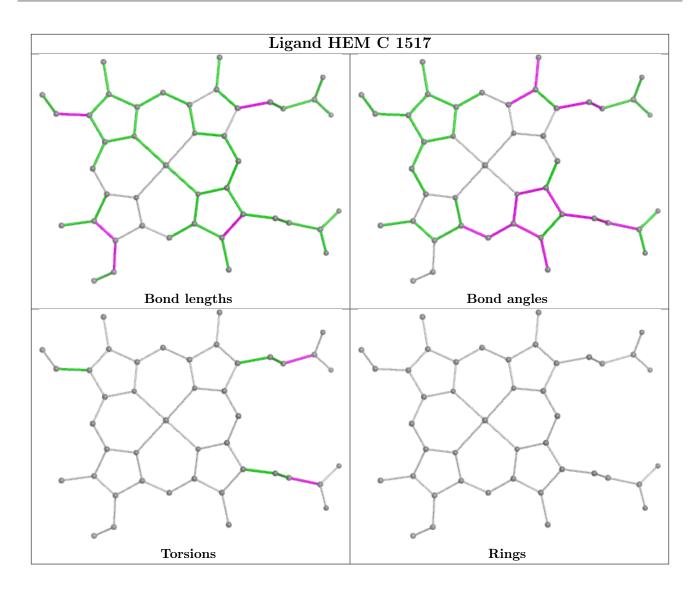
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1519	BTB	3	0

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.

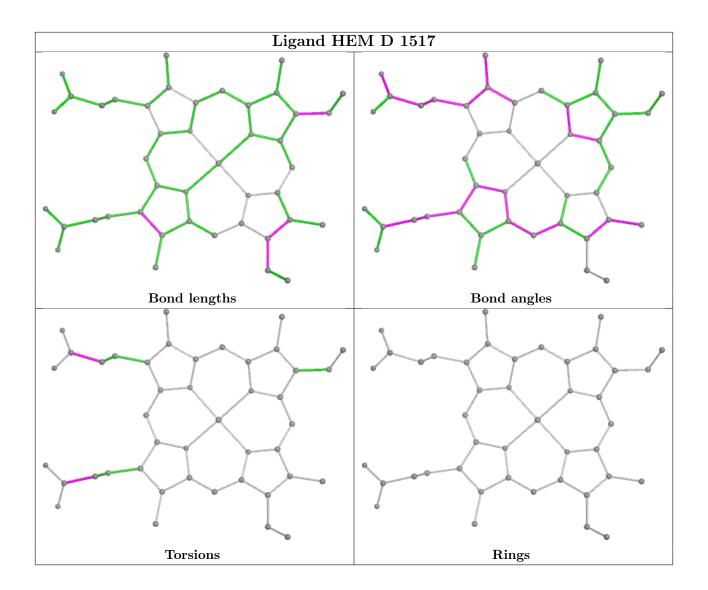




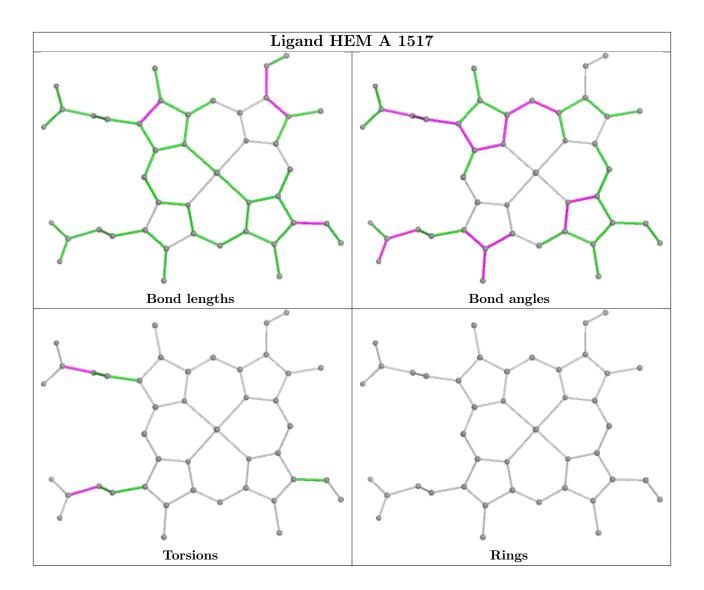




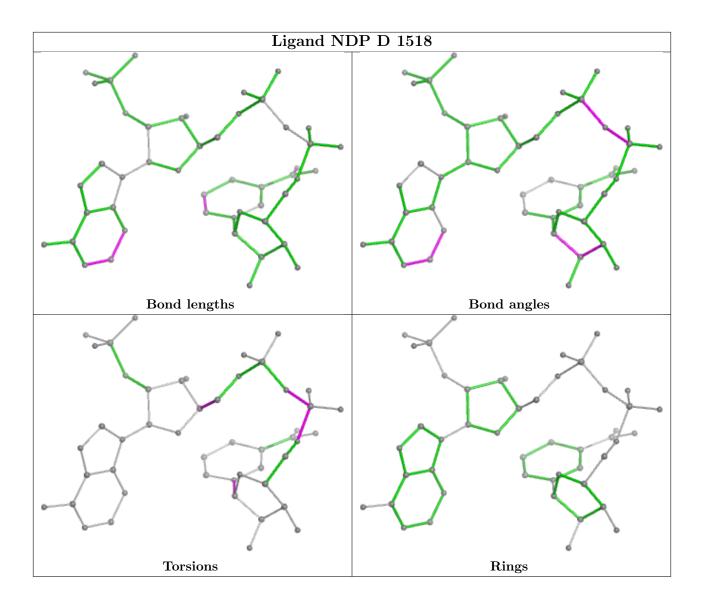




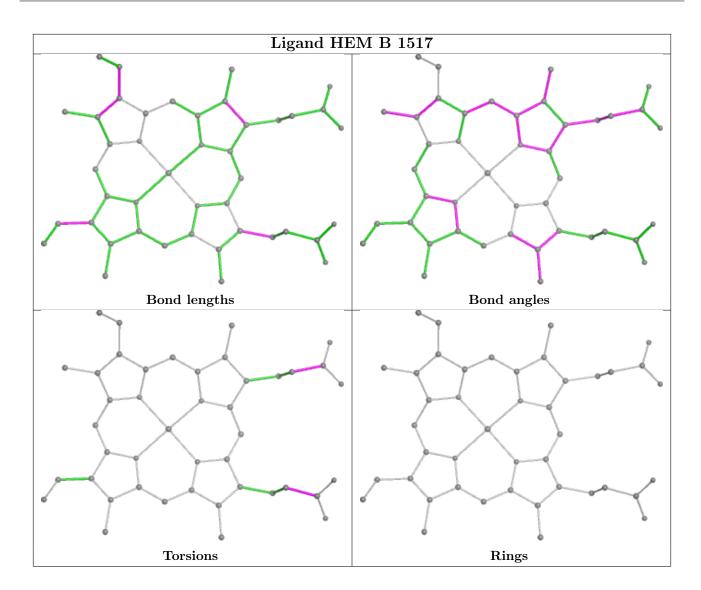




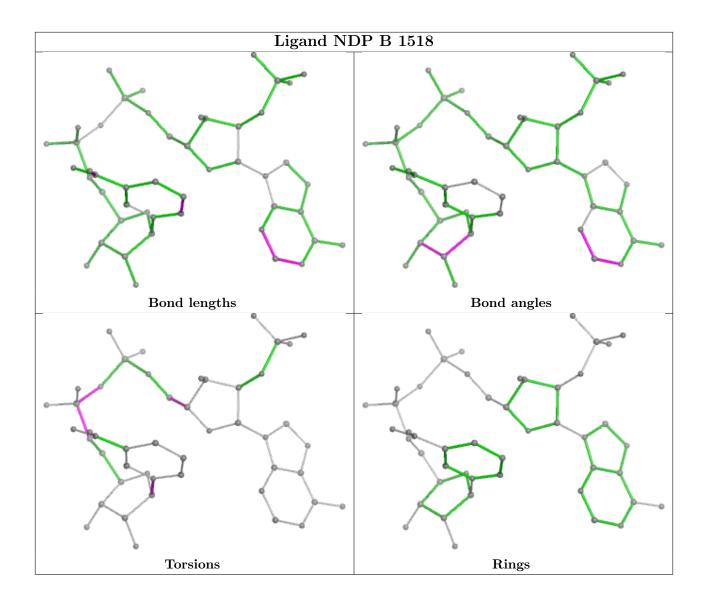




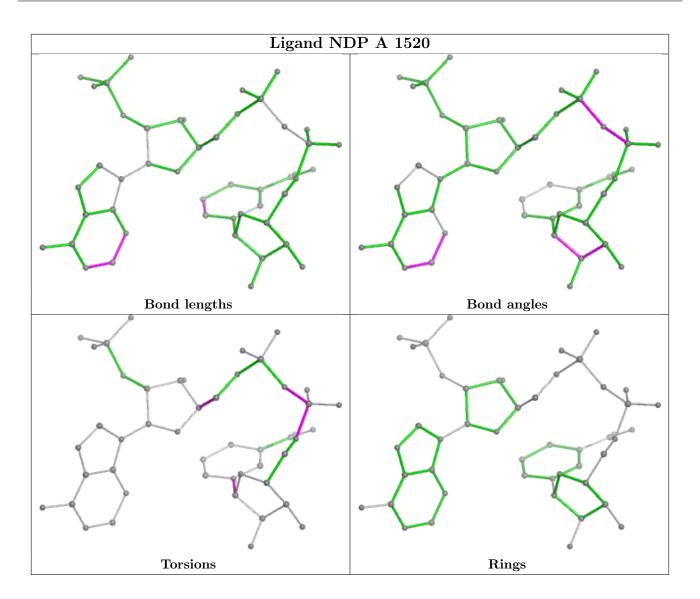












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	С	1
1	A	1
1	D	1
1	В	1

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	419:ASN	С	420:HIS	N	1.12
1	A	419:ASN	С	420:HIS	N	1.09
1	D	419:ASN	С	420:HIS	N	1.08
1	В	419:ASN	С	420:HIS	N	1.06



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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	515/515 (100%)	-0.01	4 (0%) 86 84	7, 11, 20, 83	0
1	В	514/515 (99%)	-0.02	2 (0%) 92 91	7, 12, 22, 76	0
1	С	514/515 (99%)	0.01	5 (0%) 82 80	7, 12, 22, 73	0
1	D	514/515 (99%)	0.01	4 (0%) 86 84	7, 12, 22, 84	0
All	All	2057/2060 (99%)	-0.00	15 (0%) 87 86	7, 12, 22, 84	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	516	ALA	11.8
1	A	2	SER	11.2
1	A	516	ALA	10.9
1	В	516	ALA	9.1
1	D	516	ALA	7.7

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)

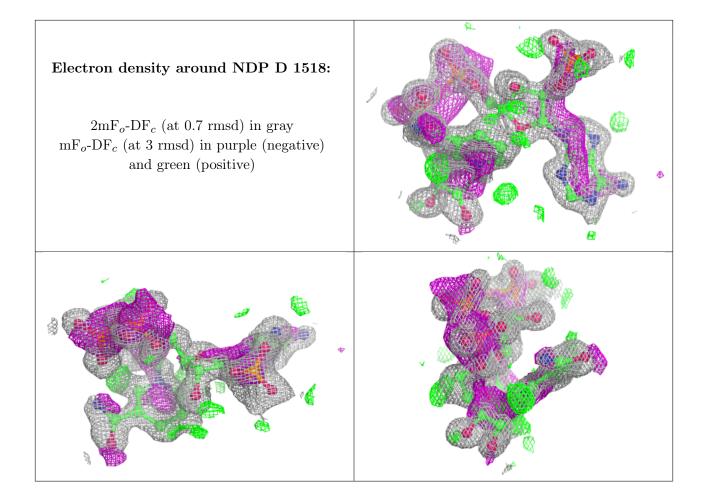
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	NDP	D	1518	48/48	0.80	0.27	22,26,31,33	0
5	NDP	С	1519	48/48	0.81	0.26	19,25,33,34	0
6	BTB	D	1519	14/14	0.84	0.20	23,29,39,48	0
6	BTB	С	1518	14/14	0.88	0.20	22,29,40,41	0
6	BTB	В	1520	14/14	0.88	0.16	22,24,39,43	0
5	NDP	В	1518	48/48	0.91	0.19	19,21,24,26	0
6	BTB	В	1521	14/14	0.91	0.14	20,24,31,35	0
5	NDP	A	1520	48/48	0.92	0.15	15,17,21,21	0
3	NO	D	1520	2/2	0.96	0.13	20,20,20,20	0
3	NO	С	1520	2/2	0.97	0.11	20,20,20,20	0
3	NO	A	1518	2/2	0.98	0.12	20,20,20,20	0
3	NO	В	1522	2/2	0.98	0.12	20,20,20,20	0
2	HEM	В	1517	43/43	0.98	0.08	7,9,11,12	0
2	HEM	D	1517	43/43	0.98	0.08	7,8,11,13	0
2	HEM	С	1517	43/43	0.99	0.08	7,8,10,12	0
2	HEM	A	1517	43/43	0.99	0.08	7,8,10,13	0
4	CL	A	1519	1/1	1.00	0.06	14,14,14,14	0
4	CL	В	1519	1/1	1.00	0.05	14,14,14,14	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.

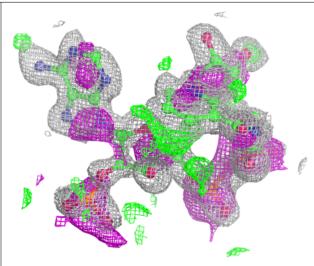


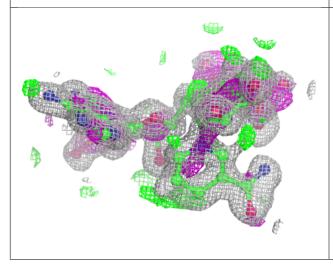


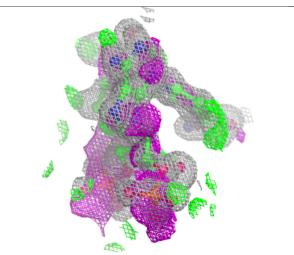


Electron density around NDP C 1519:

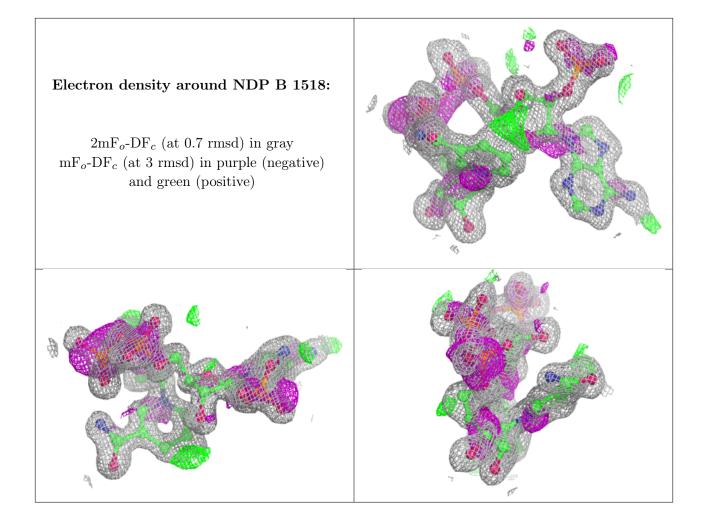
 $2mF_o$ -DF_c (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)







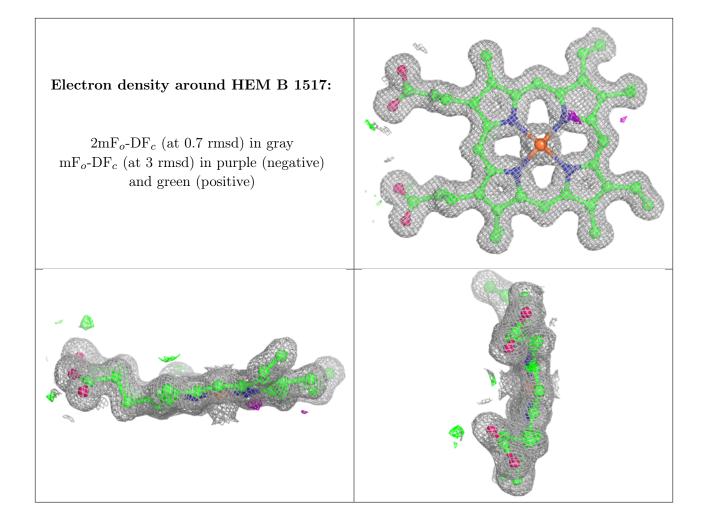




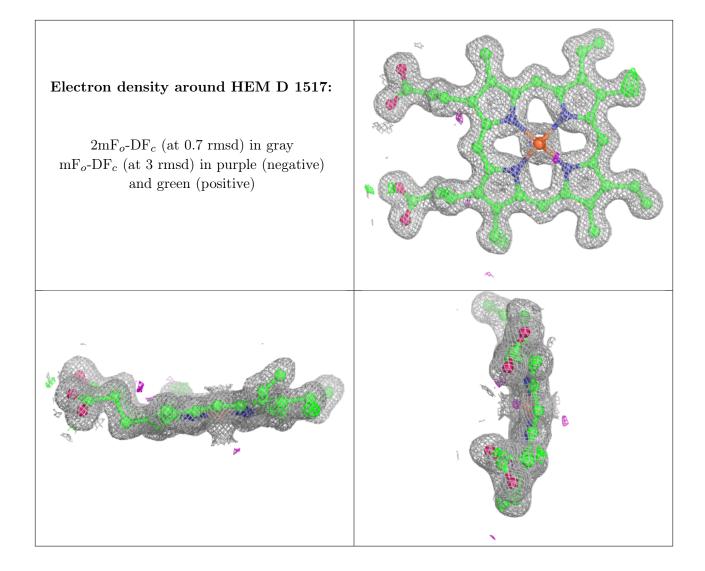


Electron density around NDP A 1520: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

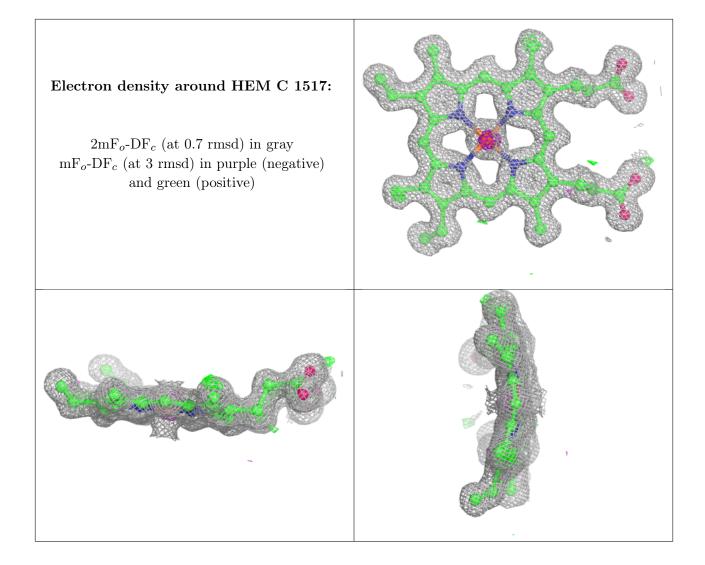




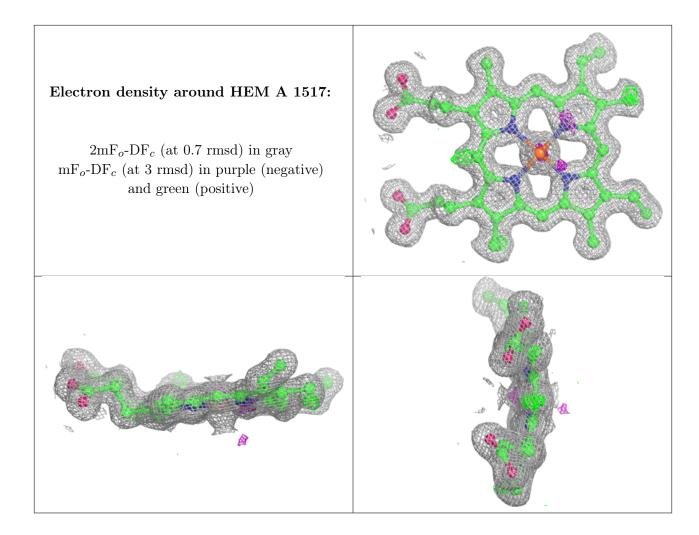












6.5 Other polymers (i)

There are no such residues in this entry.

