

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

#### Oct 9, 2023 – 03:28 PM EDT

PDB ID : 7UAO

Title : Structure of human endothelial nitric oxide synthase heme domain in complex

with (6-(3-(4,4-difluoropiperidin-1-yl)propyl)-4-methylpyridin-2-amine)

Authors : Li, H.; Poulos, T.L.

Deposited on : 2022-03-13

Resolution : 1.90 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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

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)

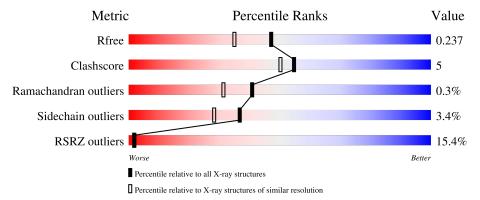
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 1.90 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	6207 (1.90-1.90)		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (1.90-1.90)		

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	
			24%	
1	A	440	78%	11% • 9%
			6%	
1	В	440	82%	9% 9%
			19%	
1	С	440	79%	12% 9%
			7%	
1	D	440	82%	9% 9%

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
6	GOL	A	513	-	X	-	-



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13979 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 Nitric oxide synthase, endothelial.

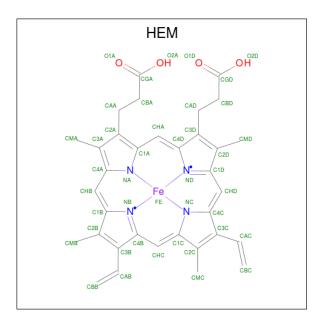
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	401	Total	С	N	О	S	0	1	0
1	1 A	401	3207	2043	564	584	16	0	1	
1	В	401	Total	С	N	О	S	0	3	0
1	Ъ	401	3211	2045	564	586	16	0	3	
1	С	402	Total	С	N	О	S	0	1	0
1		402	3212	2046	565	585	16	0	1	
1	D	402	Total	С	N	О	S	0	1	0
	ע	402	3214	2046	567	585	16	U	1	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
В	298	GLU	ASP	variant	UNP P29474
С	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

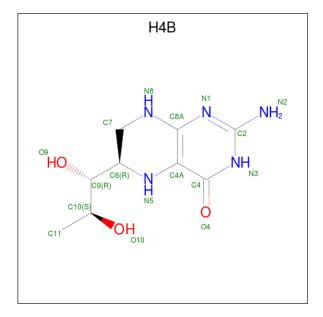
• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





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

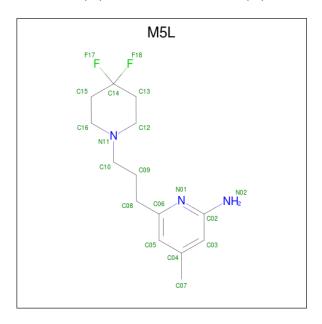
• Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	В	1	Total C N O 17 9 5 3	0	0
3	С	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

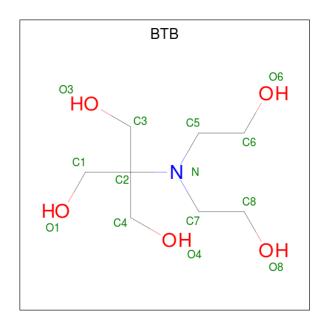
• Molecule 4 is 6-[3-(4,4-difluoropiperidin-1-yl)propyl]-4-methylpyridin-2-amine (three-letter code: M5L) (formula:  $C_{14}H_{21}F_2N_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
1	Λ	1	Total	С	F	N	0	0	
4	А	1	19	14	2	3	U	0	
1	B	1	Total	С	F	N	0	0	
4	Ъ	1	19	14	2	3			
1	$\mathbf{C}$	1	Total	С	F	N	0	0	
4	C	1	19	14	2	3	0	0	
1	D	1	Total	С	F	N	0	0	
4	ש	1	19	14	2	3	0	0	

• Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula:  $C_8H_{19}NO_5$ ).

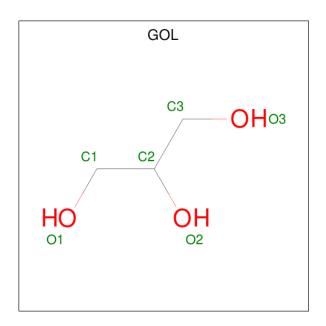




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	В	1	Total C N O 14 8 1 5	0	0
5	В	1	Total C N O 14 8 1 5	0	0
5	С	1	Total C N O 14 8 1 5	0	0
5	С	1	Total C N O 14 8 1 5	0	0
5	С	1	Total C N O 14 8 1 5	0	0
5	D	1	Total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

 $\bullet$  Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0
6	С	1	Total C O 6 3 3	0	0
6	С	1	Total C O 6 3 3	0	0
6	С	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

 $\bullet$  Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total Cl 2 2	0	0

• Molecule 8 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Gd 1 1	0	0
8	В	2	Total Gd 2 2	0	0
8	D	1	Total Gd 1 1	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Zn 1 1	0	0
9	С	1	Total Zn 1 1	0	0

• Molecule 10 is water.

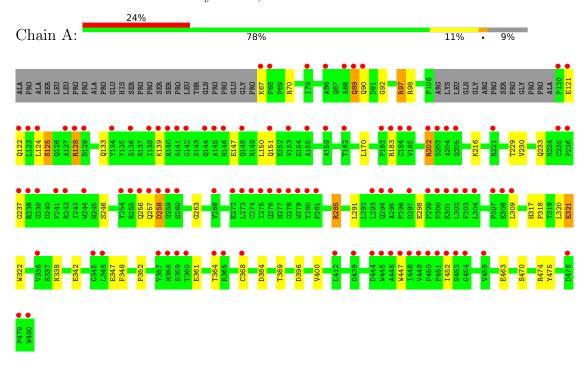
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	120	Total O 120 120	0	0
10	В	191	Total O 191 191	0	0
10	С	124	Total O 124 124	0	0
10	D	179	Total O 179 179	0	0



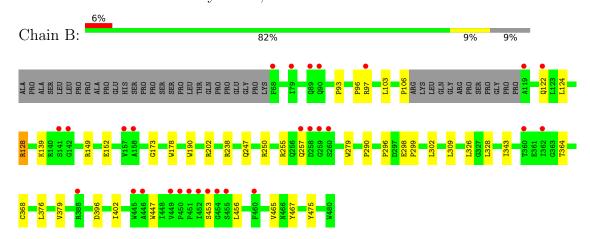
# 3 Residue-property plots (i)

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.

• Molecule 1: Nitric oxide synthase, endothelial

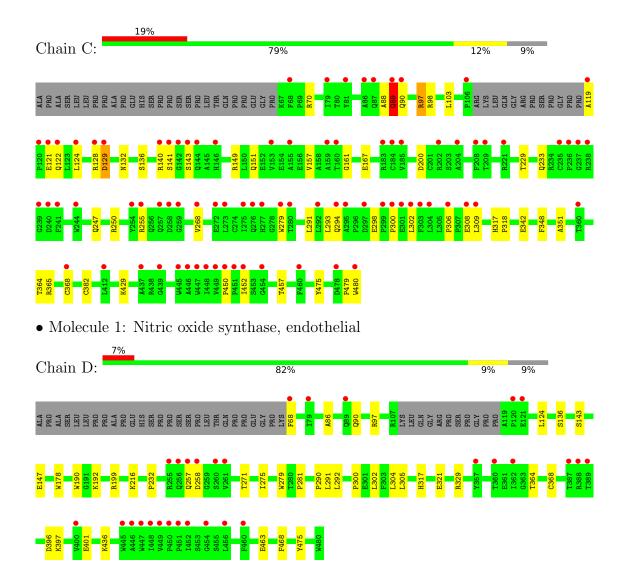


• Molecule 1: Nitric oxide synthase, endothelial



• Molecule 1: Nitric oxide synthase, endothelial







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	59.49Å 152.85Å 108.74Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.75^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	39.06 - 1.90	Depositor
Resolution (A)	39.05 - 1.90	EDS
% Data completeness	84.4 (39.06-1.90)	Depositor
(in resolution range)	87.7 (39.05-1.90)	EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.06 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D.D.	0.201 , $0.245$	Depositor
$R, R_{free}$	0.192 , $0.237$	DCC
$R_{free}$ test set	6712  reflections  (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 57.8	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.094 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13979	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.35% 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: GD, M5L, ZN, HEM, BTB, CL, GOL, H4B

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.35	0/3302	0.52	0/4498
1	В	0.40	0/3312	0.53	0/4514
1	С	0.36	0/3307	0.51	0/4506
1	D	0.43	0/3309	0.56	0/4509
All	All	0.39	0/13230	0.53	0/18027

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	3207	0	3112	38	0
1	В	3211	0	3114	27	0
1	С	3212	0	3116	31	0
1	D	3214	0	3116	21	0
2	A	43	0	30	3	0
2	В	43	0	30	1	0
2	С	43	0	30	3	0
2	D	43	0	30	2	0
3	A	17	0	15	0	0

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Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
3	В	17	0	15	1	0
3	С	17	0	15	1	0
3	D	17	0	15	0	0
4	A	19	0	0	1	0
4	В	19	0	0	0	0
4	С	19	0	0	0	0
4	D	19	0	0	0	0
5	A	42	0	56	9	0
5	В	28	0	35	4	0
5	С	42	0	55	12	0
5	D	28	0	36	4	0
6	A	24	0	32	4	0
6	В	6	0	8	0	0
6	С	18	0	24	1	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	В	1	0	0	0	0
7	С	1	0	0	0	0
7	D	2	0	0	0	0
8	A	1	0	0	0	0
8	В	2	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	С	1	0	0	0	0
10	A	120	0	0	5	0
10	В	191	0	0	1	0
10	С	124	0	0	1	0
10	D	179	0	0	3	1
All	All	13979	0	12892	137	1

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 5.

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:C:233:GLN:NE2	10:C:601:HOH:O	2.17	0.75
5:C:505:BTB:HO1	5:C:505:BTB:HO6	1.34	0.75
5:A:505:BTB:O4	5:A:505:BTB:O3	2.03	0.74
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.69	0.72
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.73	0.70



All (1) 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	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
10:D:778:HOH:O	10:D:779:HOH:O[1_655]	2.15	0.05	

#### 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	398/440 (90%)	377 (95%)	19 (5%)	2 (0%)	29	18
1	В	400/440 (91%)	391 (98%)	9 (2%)	0	100	100
1	$\mathbf{C}$	399/440 (91%)	386 (97%)	11 (3%)	2 (0%)	29	18
1	D	399/440 (91%)	391 (98%)	8 (2%)	0	100	100
All	All	1596/1760 (91%)	1545 (97%)	47 (3%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASP
1	A	257	GLN
1	С	89	GLN
1	С	143	SER

#### 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	342/373~(92%)	325 (95%)	17 (5%)	24 15
1	В	343/373~(92%)	336 (98%)	7 (2%)	55 51
1	С	342/373~(92%)	327 (96%)	15 (4%)	28 19
1	D	342/373 (92%)	334 (98%)	8 (2%)	50 45
All	All	$1369/1492 \ (92\%)$	1322 (97%)	47 (3%)	37 28

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	98	ARG
1	С	200	ASP
1	С	121	GLU
1	С	140	ARG
1	С	342	GLU

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

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 11 are monoatomic - leaving 31 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	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	gles
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ВТВ	В	504	8	13,13,13	0.48	0	7,16,16	0.96	0
4	M5L	D	503	-	20,20,20	1.47	4 (20%)	26,28,28	1.81	6 (23%)
5	BTB	D	505	-	13,13,13	0.58	0	7,16,16	0.89	0
6	GOL	A	508	-	5,5,5	0.45	0	5,5,5	0.46	0
6	GOL	A	509	_	5,5,5	0.44	0	5,5,5	0.30	0
2	HEM	В	501	1	41,50,50	1.44	5 (12%)	45,82,82	1.87	11 (24%)
5	BTB	A	504	8	13,13,13	0.63	0	7,16,16	1.48	1 (14%)
6	GOL	С	508	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	A	513	-	5,5,5	0.73	0	5,5,5	1.92	2 (40%)
4	M5L	В	503	-	20,20,20	1.52	4 (20%)	26,28,28	1.94	4 (15%)
5	BTB	A	505	-	13,13,13	0.54	0	7,16,16	0.66	0
3	H4B	В	502	-	16,18,18	0.76	0	11,26,26	2.79	5 (45%)
3	H4B	С	502	-	16,18,18	0.80	0	11,26,26	2.71	6 (54%)
5	BTB	С	506	-	13,13,13	0.41	0	7,16,16	0.34	0
5	BTB	С	504	8	13,13,13	0.37	0	7,16,16	1.71	1 (14%)
5	ВТВ	С	505	-	13,13,13	0.60	0	7,16,16	0.90	0
5	BTB	A	506	-	13,13,13	0.37	0	7,16,16	0.38	0
5	BTB	В	505	-	13,13,13	0.48	0	7,16,16	0.93	0
2	HEM	A	501	1	41,50,50	1.49	5 (12%)	45,82,82	1.68	11 (24%)
6	GOL	С	507	-	5,5,5	0.43	0	5,5,5	0.33	0
6	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.36	0
5	BTB	D	504	8	13,13,13	0.44	0	7,16,16	0.49	0
4	M5L	С	503	-	20,20,20	1.34	4 (20%)	26,28,28	1.87	2 (7%)
2	HEM	С	501	1	41,50,50	1.50	6 (14%)	45,82,82	2.01	11 (24%)
3	H4B	A	502	-	16,18,18	0.84	0	11,26,26	2.64	5 (45%)
6	GOL	С	509	-	5,5,5	0.32	0	5,5,5	0.31	0
6	GOL	D	506		5,5,5	0.37	0	5,5,5	0.26	0
3	H4B	D	502	-	16,18,18	0.84	0	11,26,26	2.67	5 (45%)
2	HEM	D	501	1	41,50,50	1.44	3 (7%)	45,82,82	1.97	10 (22%)
6	GOL	В	506		5,5,5	0.37	0	5,5,5	0.30	0
4	M5L	A	503	-	20,20,20	1.36	4 (20%)	26,28,28	1.93	2 (7%)

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	BTB	В	504	8	-	3/21/21/21	-
4	M5L	D	503	-	-	2/6/18/18	0/2/2/2
5	ВТВ	D	505	-	-	7/21/21/21	-
6	GOL	A	508	-	-	3/4/4/4	-
6	GOL	A	509	-	-	4/4/4/4	-
2	HEM	В	501	1	-	0/12/54/54	-
5	BTB	A	504	8	-	5/21/21/21	-
6	GOL	С	508	_	-	2/4/4/4	-
6	GOL	A	513	-	-	4/4/4/4	-
4	M5L	В	503	-	-	2/6/18/18	0/2/2/2
5	BTB	A	505	-	-	11/21/21/21	-
3	H4B	В	502	-	-	0/8/17/17	0/2/2/2
3	H4B	С	502	-	-	0/8/17/17	0/2/2/2
5	BTB	С	506	_	-	5/21/21/21	-
5	ВТВ	С	504	8	-	3/21/21/21	-
5	BTB	С	505	-	-	17/21/21/21	-
5	BTB	A	506	-	-	4/21/21/21	-
5	BTB	В	505	-	-	14/21/21/21	-
2	HEM	A	501	1	-	2/12/54/54	-
6	GOL	С	507	-	-	2/4/4/4	-
6	GOL	A	507	-	-	0/4/4/4	-
5	BTB	D	504	8	-	6/21/21/21	-
4	M5L	С	503	-	-	2/6/18/18	0/2/2/2
2	HEM	С	501	1	-	1/12/54/54	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
6	GOL	С	509	-	-	2/4/4/4	-
6	GOL	D	506	_	-	2/4/4/4	
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
2	HEM	D	501	1	-	2/12/54/54	_
6	GOL	В	506	_	-	2/4/4/4	
4	M5L	A	503	-	-	2/6/18/18	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	D	501	HEM	C3C-C2C	-3.95	1.34	1.40
2	A	501	HEM	C3C-CAC	3.81	1.55	1.47
2	D	501	HEM	C3C-CAC	3.75	1.55	1.47

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(A)
2	С	501	HEM	C3C-CAC	3.70	1.55	1.47
4	В	503	M5L	C13-C14	3.69	1.53	1.50

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	503	M5L	C02-N01-C06	7.46	123.75	118.10
4	С	503	M5L	C02-N01-C06	7.09	123.47	118.10
4	В	503	M5L	C02-N01-C06	6.60	123.11	118.10
2	D	501	HEM	CBA-CAA-C2A	-6.48	101.57	112.62
4	D	503	M5L	C02-N01-C06	5.96	122.61	118.10

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4

There are no ring outliers.

20 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	BTB	2	0
6	A	509	GOL	2	0
2	В	501	HEM	1	0
5	A	504	BTB	3	0
6	A	513	GOL	1	0
5	A	505	BTB	2	0
3	В	502	H4B	1	0
3	С	502	H4B	1	0
5	С	506	BTB	3	0
5	С	504	BTB	4	0
5	С	505	BTB	5	0
5	A	506	BTB	4	0
5	В	505	BTB	4	0
2	A	501	HEM	3	0
6	С	507	GOL	1	0

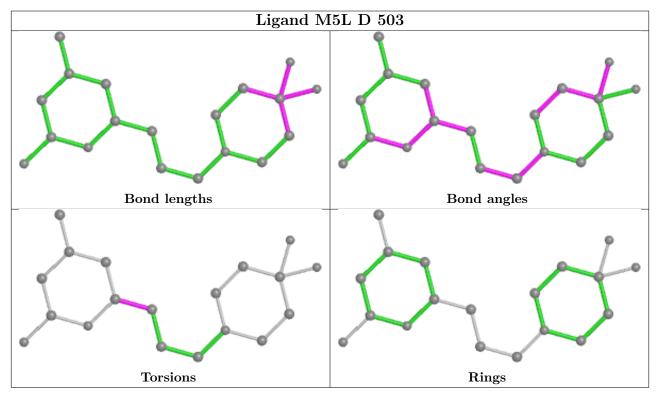
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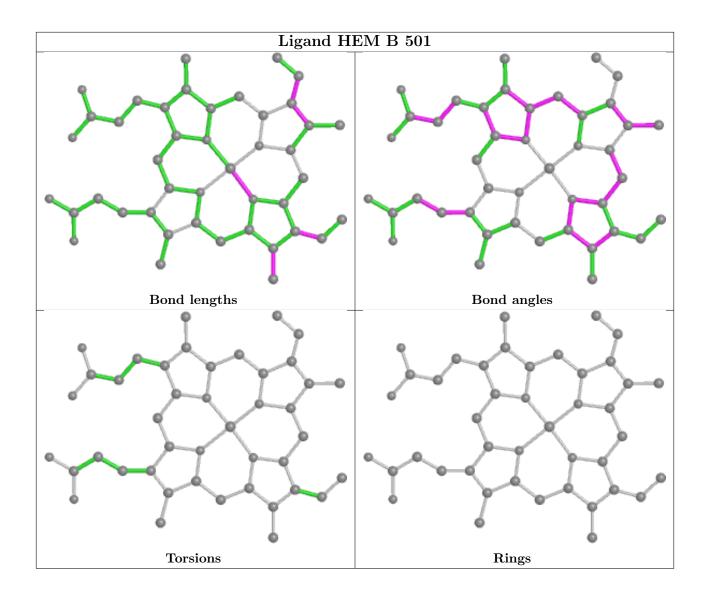
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	GOL	1	0
5	D	504	BTB	2	0
2	С	501	HEM	3	0
2	D	501	HEM	2	0
4	A	503	M5L	1	0

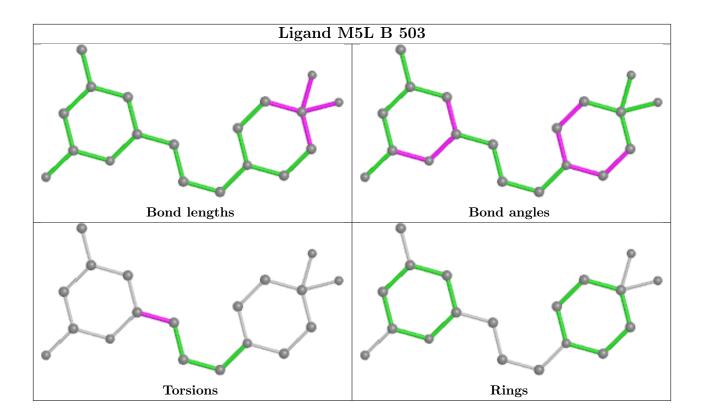
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



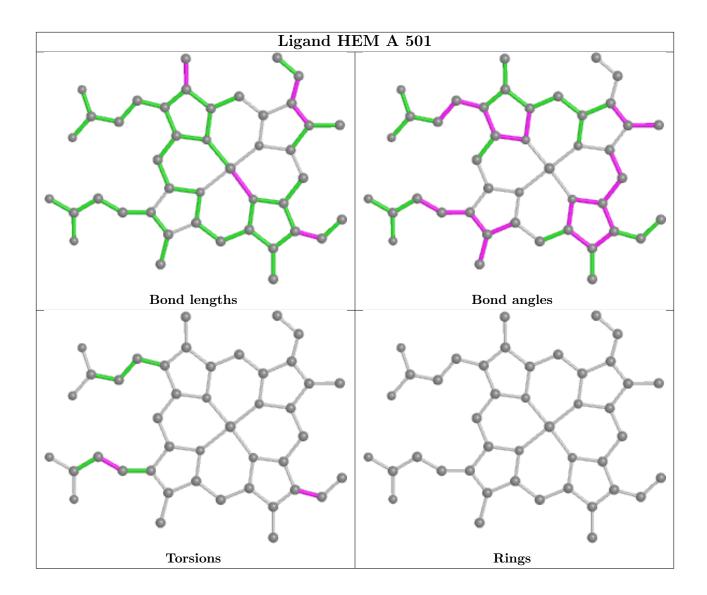




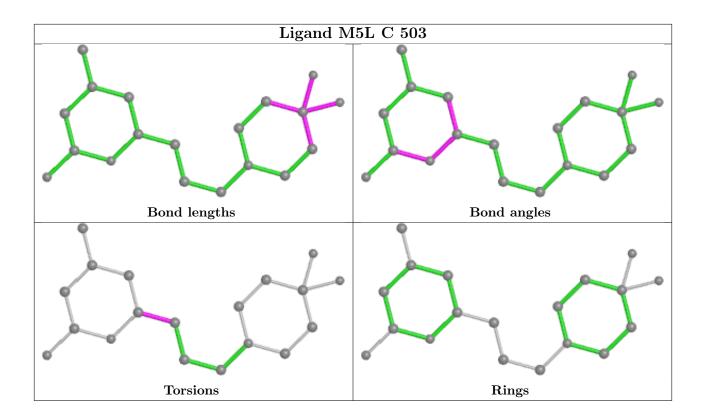




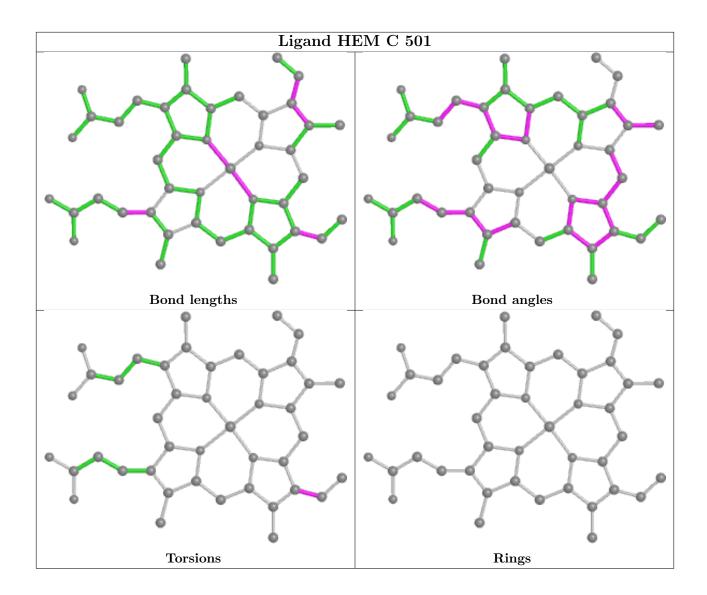




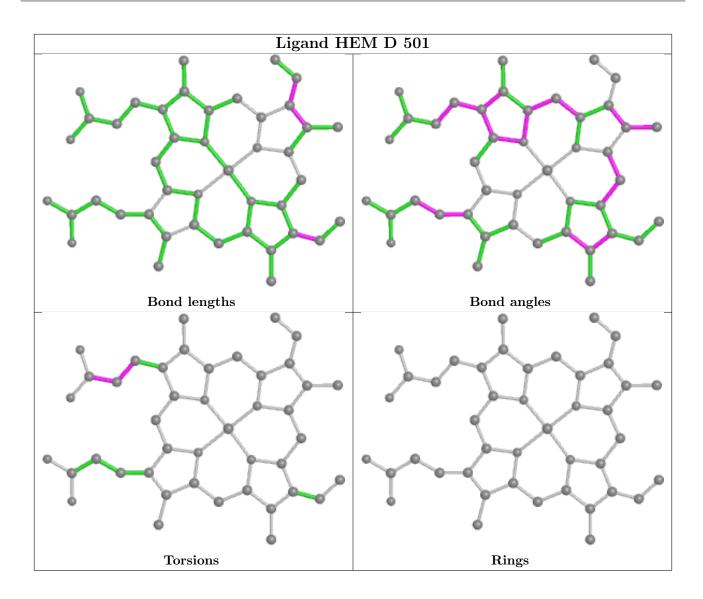




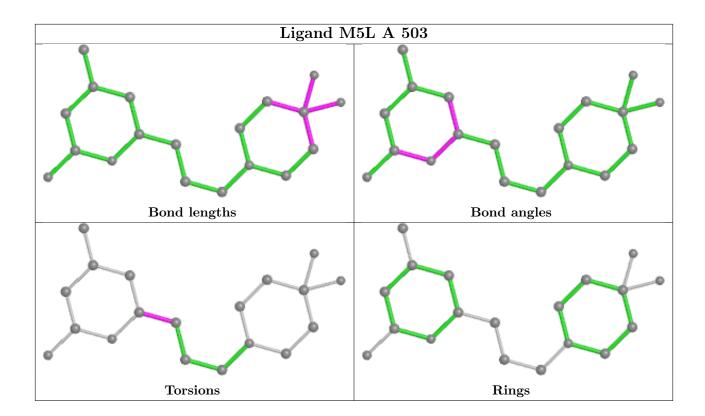












## 5.7 Other polymers $\bigcirc$

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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	401/440 (91%)	1.33	106 (26%) 0 0	29, 58, 112, 144	0
1	В	401/440 (91%)	0.43	28 (6%) 16 18	26, 40, 77, 121	0
1	С	402/440 (91%)	1.08	84 (20%) 1 1	28, 54, 103, 140	0
1	D	402/440 (91%)	0.31	29 (7%) 15 17	24, 39, 68, 133	0
All	All	1606/1760 (91%)	0.79	247 (15%) 2 2	24, 47, 99, 144	0

The worst 5 of 247 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	8.7
1	A	480	TRP	8.4
1	A	259	GLY	7.1
1	A	153	VAL	6.6
1	A	295	ALA	6.3

#### 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.

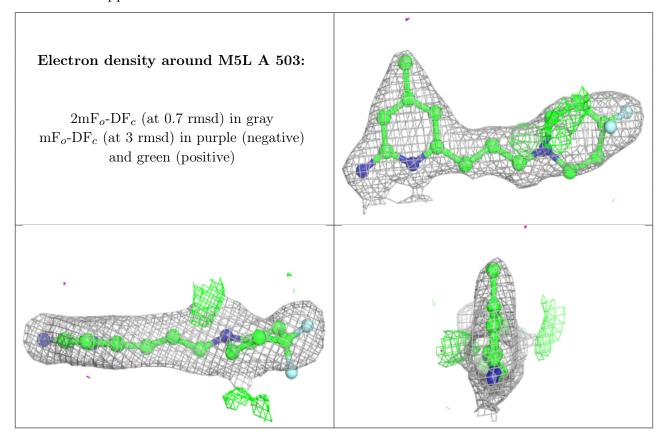


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}( \mathring{\mathbf{A}}^2 )$	Q<0.9
6	GOL	A	509	6/6	0.64	0.16	71,81,84,85	0
6	GOL	С	508	6/6	0.71	0.16	60,71,75,80	0
5	BTB	D	504	14/14	0.74	0.22	35,66,85,89	0
6	GOL	С	509	6/6	0.75	0.13	69,79,81,85	0
5	BTB	A	506	14/14	0.77	0.22	85,97,102,103	0
5	BTB	В	504	14/14	0.80	0.19	39,50,81,86	0
5	BTB	С	506	14/14	0.80	0.16	76,89,105,108	0
6	GOL	D	506	6/6	0.82	0.31	60,71,78,80	0
5	BTB	A	505	14/14	0.85	0.16	59,79,86,90	0
5	BTB	В	505	14/14	0.86	0.18	54,67,76,78	0
6	GOL	A	508	6/6	0.86	0.19	60,71,77,78	0
4	M5L	A	503	19/19	0.89	0.34	37,59,107,108	0
6	GOL	A	513	6/6	0.90	0.14	26,37,55,57	0
4	M5L	В	503	19/19	0.90	0.17	24,37,73,74	0
3	H4B	С	502	17/17	0.91	0.23	37,43,47,51	0
4	M5L	С	503	19/19	0.91	0.26	40,53,91,92	0
5	BTB	A	504	14/14	0.91	0.27	27,74,83,93	0
5	BTB	С	505	14/14	0.92	0.15	25,61,76,80	0
3	H4B	A	502	17/17	0.92	0.25	37,46,55,63	0
6	GOL	В	506	6/6	0.92	0.26	68,76,77,81	0
5	BTB	D	505	14/14	0.93	0.17	57,70,84,94	0
6	GOL	С	507	6/6	0.94	0.22	48,56,60,60	0
2	HEM	A	501	43/43	0.94	0.23	26,53,62,67	0
4	M5L	D	503	19/19	0.94	0.16	24,35,88,91	0
2	HEM	С	501	43/43	0.94	0.22	28,45,64,78	0
3	H4B	В	502	17/17	0.95	0.17	26,39,45,46	0
2	HEM	В	501	43/43	0.95	0.13	18,30,49,56	0
3	H4B	D	502	17/17	0.95	0.19	31,41,48,52	0
5	BTB	С	504	14/14	0.95	0.20	16,63,74,81	0
2	HEM	D	501	43/43	0.96	0.14	20,29,53,73	0
6	GOL	A	507	6/6	0.96	0.24	48,58,68,72	0
7	CL	A	510	1/1	0.97	0.20	60,60,60,60	0
7	CL	D	508	1/1	0.97	0.25	38,38,38,38	0
8	GD	A	511	1/1	0.98	0.07	73,73,73,73	1
8	GD	D	509	1/1	0.98	0.12	47,47,47,47	0
9	ZN	A	512	1/1	0.98	0.09	44,44,44,44	0
7	CL	С	510	1/1	0.99	0.20	48,48,48,48	0
8	GD	В	508	1/1	0.99	0.10	42,42,42,42	0
7	CL	D	507	1/1	0.99	0.07	42,42,42,42	0
7	CL	В	507	1/1	0.99	0.12	48,48,48,48	0
8	GD	В	509	1/1	1.00	0.07	56,56,56,56	1
9	ZN	С	511	1/1	1.00	0.10	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all



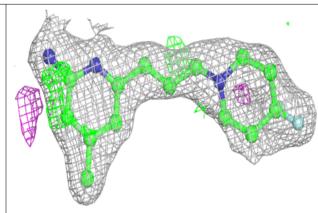
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

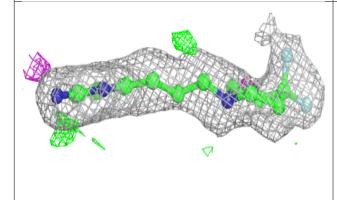


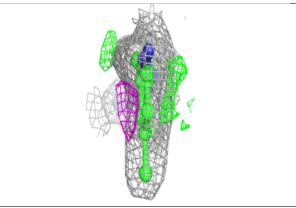


#### Electron density around M5L B 503:

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

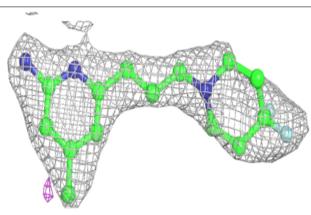


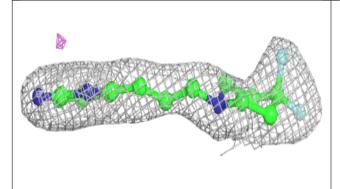


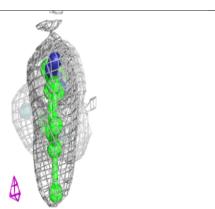


#### Electron density around M5L C 503:

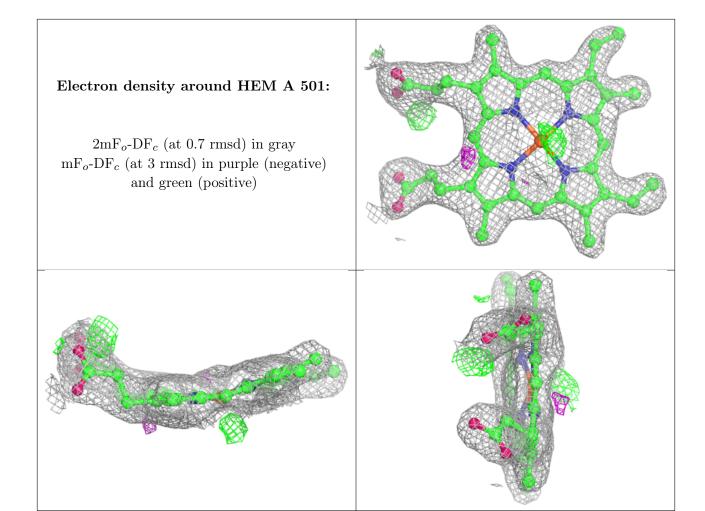
 $2 \mathrm{mF}_o\text{-DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



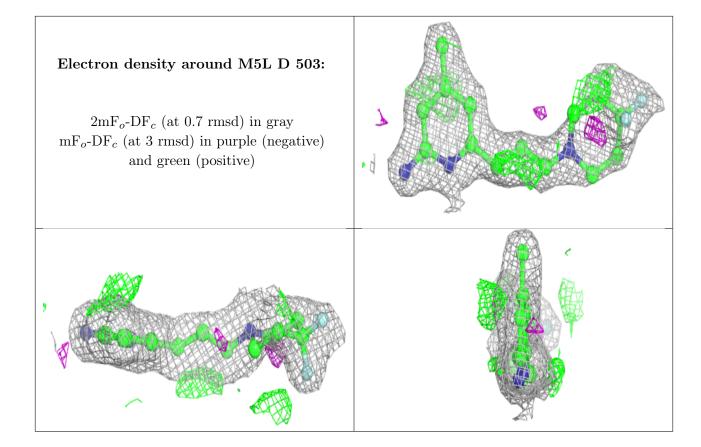




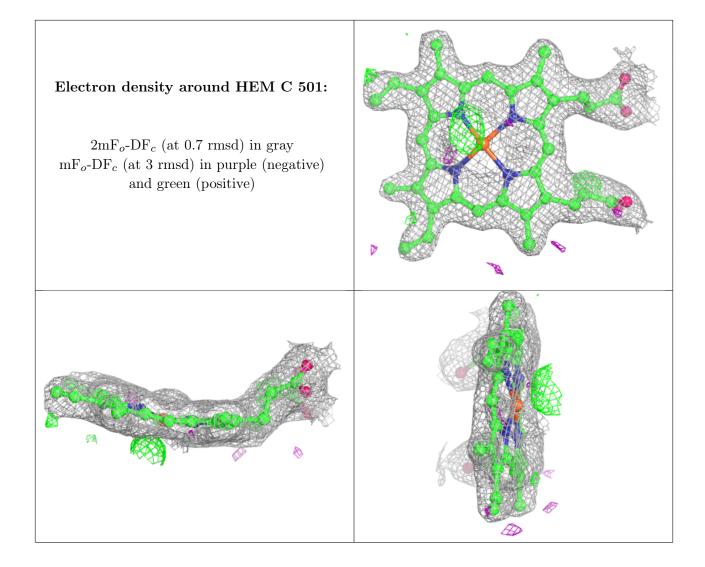




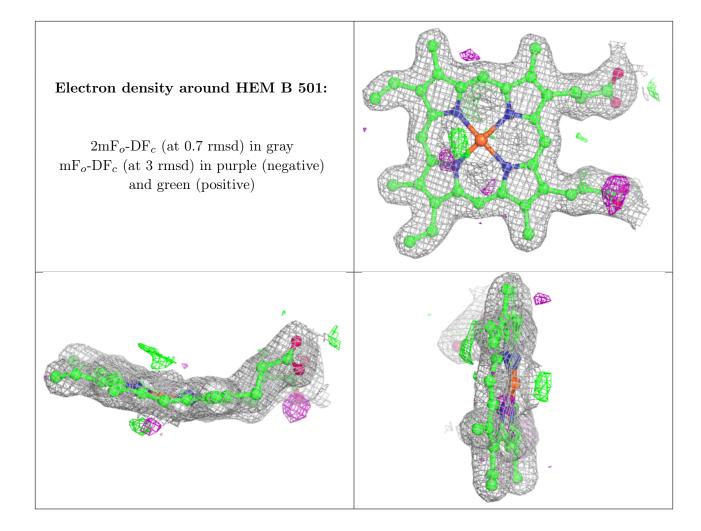




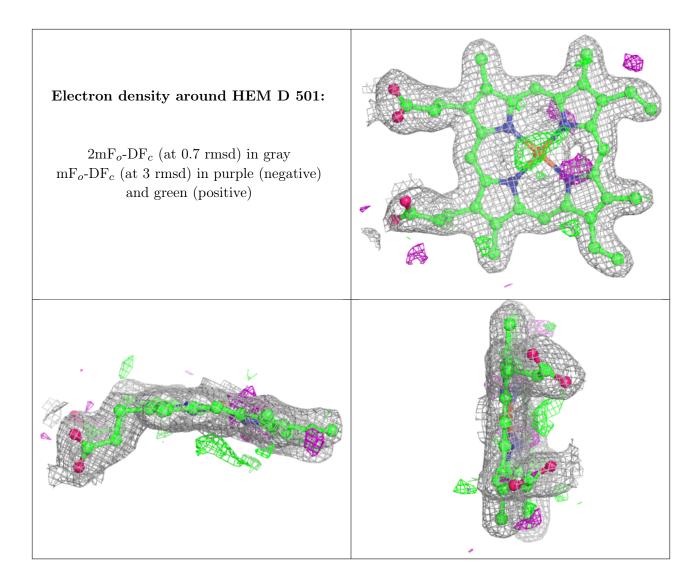












# 6.5 Other polymers (i)

There are no such residues in this entry.

