Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 02:42 PM EDT

PDB ID	:	6PN3
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(cyclobutylmethoxy)phenyl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2019-07-02
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

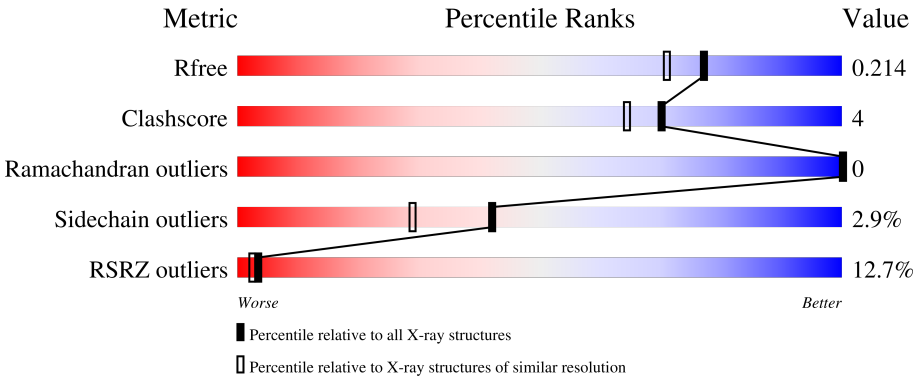
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	422	18% 86% 11%
1	B	422	7% 89% 8%

2 Entry composition

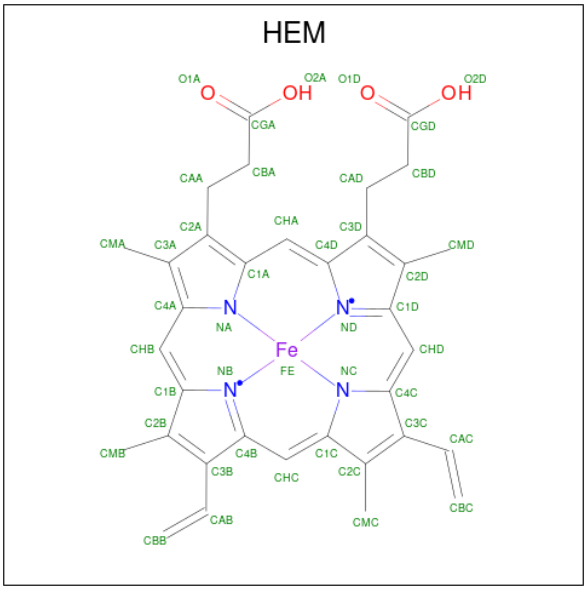
There are 8 unique types of molecules in this entry. The entry contains 7415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, brain.

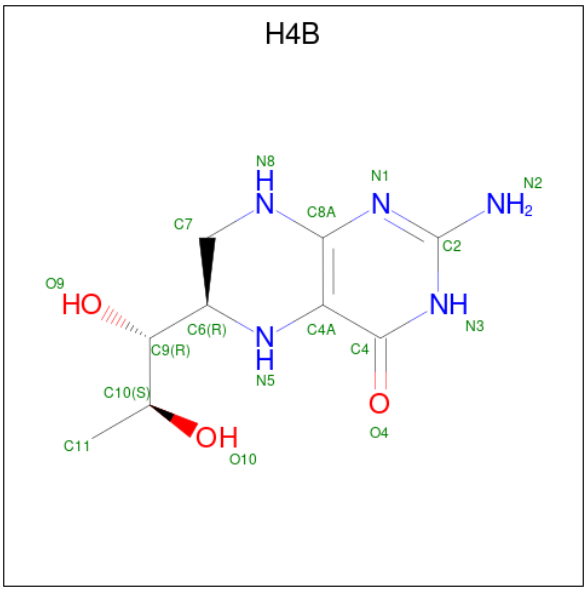
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	2	0
			3342	2138	572	610	22			
1	B	411	Total	C	N	O	S	0	3	0
			3353	2145	574	612	22			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



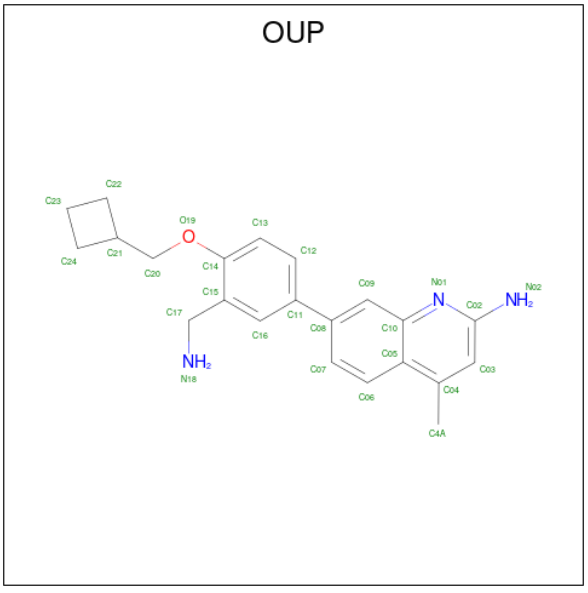
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[3-(aminomethyl)-4-(cyclobutylmethoxy)phenyl]-4-methylquinolin-2-amine (three-letter code: OUP) (formula: $C_{22}H_{25}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	22	3	1		

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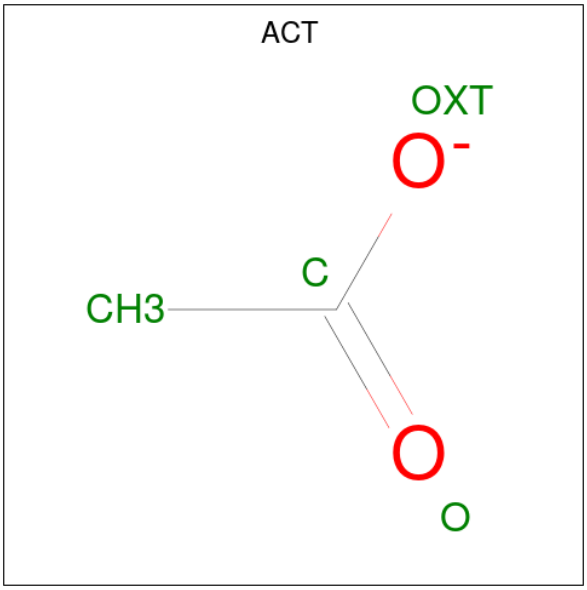
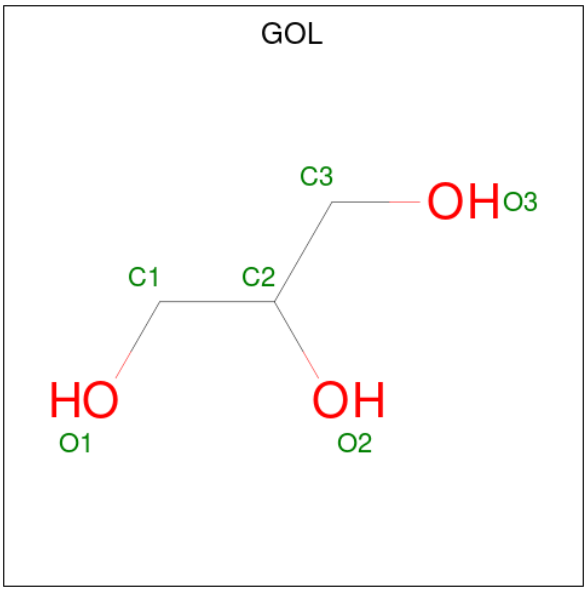
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			26	22	3	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Zn 1 1	0	0

- Molecule 8 is water.

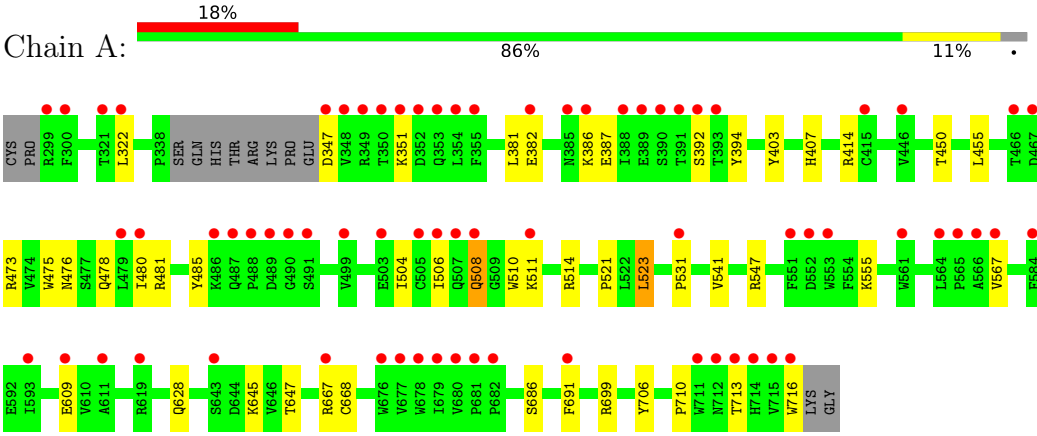
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	207	Total O 207 207	0	0
8	B	320	Total O 320 320	0	0

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.

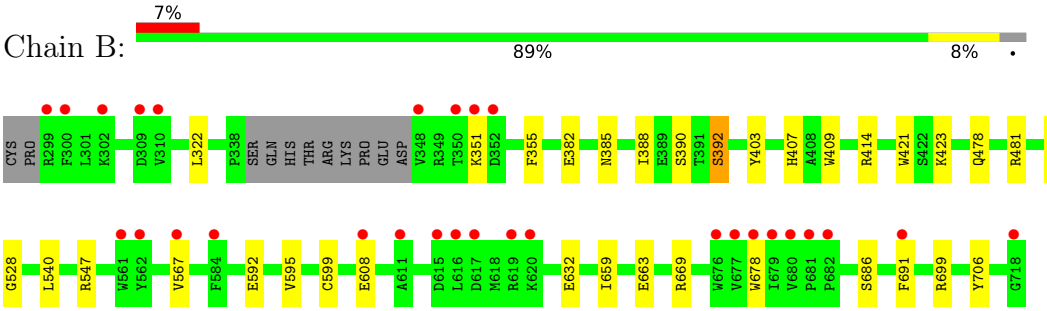
- Molecule 1: Nitric oxide synthase, brain

Chain A:



- Molecule 1: Nitric oxide synthase, brain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.12Å 111.08Å 164.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.05 – 1.80 39.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.05-1.80) 96.9 (39.05-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.67 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.181 , 0.217 0.180 , 0.214	Depositor DCC
R_{free} test set	4304 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7415	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OUP, GOL, ZN, HEM, H4B, ACT

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	0.35	0/3438	0.51	0/4664
1	B	0.38	0/3456	0.52	0/4685
All	All	0.37	0/6894	0.51	0/9349

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

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	3342	0	3252	25	0
1	B	3353	0	3271	20	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	26	0	0	3	0
4	B	26	0	0	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	207	0	0	0	0
8	B	320	0	0	1	0
All	All	7415	0	6635	48	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 4.

All (48) 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:B:669:ARG:HH21	6:B:806:GOL:H32	1.43	0.84
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.64	0.78
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.66	0.77
1:A:414:ARG:HB2	2:A:801:HEM:HBD2	1.64	0.76
1:B:706:TYR:OH	4:B:803:OUP:N18	2.23	0.71
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.71	0.71
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.72	0.71
1:B:414:ARG:HB2	2:B:801:HEM:HBD2	1.75	0.67
1:A:567:VAL:HG21	4:A:803:OUP:C07	2.30	0.62
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.81	0.60
1:B:567:VAL:HG21	4:B:803:OUP:C07	2.33	0.58
2:A:801:HEM:HAD2	4:A:803:OUP:N18	2.19	0.58
1:A:414:ARG:HB2	2:A:801:HEM:CBD	2.34	0.57
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.87	0.57
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.86	0.57
1:A:504:ILE:O	1:A:508:GLN:HB2	2.07	0.54
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.88	0.54
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.91	0.52
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.42	0.52
1:B:414:ARG:HB2	2:B:801:HEM:CBD	2.40	0.52
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.84	0.51
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.47	0.49
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.78	0.49
1:B:608:GLU:HG2	8:B:912:HOH:O	2.12	0.49
1:A:455:LEU:HD12	1:A:647:THR:HB	1.94	0.48
1:B:525:GLN:HE21	1:B:528:GLY:HA2	1.78	0.48
1:B:595:VAL:O	1:B:599:CYS:HB2	2.16	0.46
1:B:388:ILE:O	1:B:392:SER:N	2.39	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.51	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:TRP:HH2	1:A:716:TRP:HZ3	1.66	0.44
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.33	0.44
1:A:387:GLU:OE1	1:A:394:TYR:HA	2.18	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.44
1:A:475:TRP:CH2	1:A:716:TRP:HZ3	2.35	0.44
1:A:382:GLU:OE2	1:A:386:LYS:HE3	2.18	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.54	0.42
1:B:686:SER:HA	1:B:691:PHE:CG	2.54	0.42
1:A:450:THR:HA	1:A:455:LEU:HD23	2.01	0.42
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.56	0.41
1:A:706:TYR:OH	4:A:803:OUP:N18	2.54	0.41
1:B:592:GLU:OE2	4:B:803:OUP:N02	2.54	0.41
1:B:659:ILE:O	1:B:663:GLU:HG3	2.20	0.41
1:B:669:ARG:NH2	6:B:806:GOL:H32	2.22	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:506:ILE:C	1:A:508:GLN:H	2.25	0.40
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/422 (96%)	395 (97%)	12 (3%)	0	100	100
1	B	410/422 (97%)	407 (99%)	3 (1%)	0	100	100
All	All	817/844 (97%)	802 (98%)	15 (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	367/377 (97%)	354 (96%)	13 (4%)	36 21
1	B	369/377 (98%)	361 (98%)	8 (2%)	52 39
All	All	736/754 (98%)	715 (97%)	21 (3%)	42 29

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

Mol	Chain	Res	Type
1	A	347	ASP
1	A	381	LEU
1	A	469	LYS
1	A	470	HIS
1	A	476	ASN
1	A	508	GLN
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	609	GLU
1	A	645	LYS
1	A	713	THR
1	B	351	LYS
1	B	382	GLU
1	B	390	SER
1	B	392	SER
1	B	423	LYS
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	ACT	B	804	-	3,3,3	0.88	0	3,3,3	0.45	0
6	GOL	B	806	-	5,5,5	0.37	0	5,5,5	0.42	0
4	OUP	B	803	-	29,29,29	0.90	0	40,41,41	1.91	10 (25%)
6	GOL	B	805	-	5,5,5	0.33	0	5,5,5	0.32	0
3	H4B	A	802	-	16,18,18	0.90	0	11,26,26	2.67	5 (45%)
2	HEM	A	801	1	41,50,50	1.47	6 (14%)	45,82,82	2.06	13 (28%)
3	H4B	B	802	-	16,18,18	1.08	2 (12%)	11,26,26	2.50	5 (45%)
2	HEM	B	801	1	41,50,50	1.52	6 (14%)	45,82,82	1.77	11 (24%)
5	ACT	A	804	-	3,3,3	0.78	0	3,3,3	0.77	0
4	OUP	A	803	-	29,29,29	0.93	1 (3%)	40,41,41	1.62	9 (22%)

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	GOL	B	806	-	-	2/4/4/4	-
4	OUP	B	803	-	-	4/11/17/17	0/4/4/4
6	GOL	B	805	-	-	2/4/4/4	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	2/12/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	B	801	1	-	2/12/54/54	-
4	OUP	A	803	-	-	7/11/17/17	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-4.12	1.34	1.40
2	A	801	HEM	C3C-CAC	3.50	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.47	1.35	1.40
2	B	801	HEM	C3C-CAC	3.34	1.54	1.47
2	A	801	HEM	CAB-C3B	3.01	1.55	1.47
2	B	801	HEM	CMD-C2D	2.87	1.56	1.50
4	A	803	OUP	C02-N01	2.71	1.36	1.33
2	B	801	HEM	CAB-C3B	2.57	1.54	1.47
2	A	801	HEM	CMB-C2B	2.44	1.56	1.50
3	B	802	H4B	C7-C6	2.28	1.54	1.52
2	B	801	HEM	CMB-C2B	2.16	1.55	1.50
2	A	801	HEM	CMD-C2D	2.15	1.55	1.50
3	B	802	H4B	C4A-C4	-2.14	1.38	1.41
2	B	801	HEM	C2C-C1C	2.04	1.47	1.42
2	A	801	HEM	CMC-C2C	2.00	1.56	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	CBA-CAA-C2A	-7.99	98.98	112.62
3	A	802	H4B	C8A-C4A-C4	5.26	119.24	114.57
4	B	803	OUP	C12-C11-C08	-4.82	113.01	121.36
3	B	802	H4B	C8A-C4A-C4	4.73	118.78	114.57
2	B	801	HEM	CBA-CAA-C2A	-4.49	104.96	112.62
4	B	803	OUP	O19-C14-C15	4.31	121.41	115.78
4	B	803	OUP	C20-O19-C14	4.27	127.77	118.27
4	A	803	OUP	O19-C14-C15	4.15	121.20	115.78
4	B	803	OUP	C16-C11-C08	3.81	127.17	120.86
2	B	801	HEM	C4B-CHC-C1C	3.79	127.56	122.56
2	B	801	HEM	CBD-CAD-C3D	-3.73	102.25	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	OUP	C04-C05-C10	3.58	119.95	118.01
4	B	803	OUP	C16-C15-C14	3.48	121.91	118.26
2	A	801	HEM	CBD-CAD-C3D	-3.47	102.98	112.63
3	A	802	H4B	C2-N3-C4	3.46	121.43	115.93
2	B	801	HEM	CAD-CBD-CGD	3.41	120.95	113.60
3	A	802	H4B	N1-C2-N3	-3.36	120.15	125.42
2	A	801	HEM	C4B-CHC-C1C	3.29	126.89	122.56
3	B	802	H4B	C2-N3-C4	3.22	121.05	115.93
3	B	802	H4B	N1-C2-N3	-3.15	120.48	125.42
4	A	803	OUP	C16-C15-C14	3.12	121.54	118.26
2	A	801	HEM	CHD-C1D-ND	3.10	127.80	124.43
4	B	803	OUP	C04-C05-C10	3.09	119.69	118.01
2	B	801	HEM	C3D-C4D-ND	-3.08	106.73	110.17
3	B	802	H4B	C4-C4A-N5	3.01	121.65	119.12
2	A	801	HEM	CAD-CBD-CGD	2.99	120.03	113.60
4	A	803	OUP	C12-C11-C08	-2.91	116.32	121.36
2	A	801	HEM	C4D-ND-C1D	2.86	108.02	105.07
4	A	803	OUP	C05-C10-N01	-2.84	119.80	122.81
2	A	801	HEM	C4C-CHD-C1D	2.82	126.28	122.56
2	A	801	HEM	O1D-CGD-CBD	-2.74	114.29	123.08
3	A	802	H4B	C4-C4A-N5	2.72	121.40	119.12
4	B	803	OUP	C11-C16-C15	-2.69	117.87	121.90
4	B	803	OUP	C05-C10-N01	-2.66	119.99	122.81
3	A	802	H4B	C2-N1-C8A	2.65	120.47	114.54
2	B	801	HEM	CHD-C1D-ND	2.64	127.30	124.43
3	B	802	H4B	C2-N1-C8A	2.62	120.40	114.54
4	B	803	OUP	C17-C15-C14	-2.61	115.01	120.12
2	B	801	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
2	B	801	HEM	CAD-C3D-C2D	-2.52	123.19	127.88
2	B	801	HEM	C4D-ND-C1D	2.45	107.61	105.07
2	A	801	HEM	C3D-C4D-ND	-2.44	107.45	110.17
2	A	801	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
2	A	801	HEM	CMC-C2C-C3C	2.31	128.99	124.68
2	B	801	HEM	C1B-NB-C4B	2.30	107.45	105.07
4	B	803	OUP	O19-C14-C13	-2.29	119.02	123.97
4	A	803	OUP	N02-C02-N01	2.27	120.14	118.26
2	A	801	HEM	O2D-CGD-CBD	2.22	121.17	114.03
4	A	803	OUP	O19-C14-C13	-2.15	119.32	123.97
4	A	803	OUP	C16-C11-C08	2.08	124.30	120.86
4	A	803	OUP	C03-C04-C05	2.07	119.82	117.78
2	B	801	HEM	C4D-C3D-C2D	2.02	109.84	106.90
2	A	801	HEM	CHC-C4B-C3B	2.01	127.65	124.57

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	OUP	C14-C15-C17-N18
6	B	805	GOL	O1-C1-C2-C3
6	B	806	GOL	C1-C2-C3-O3
4	A	803	OUP	C14-C15-C17-N18
2	B	801	HEM	C2A-CAA-CBA-CGA
6	B	805	GOL	O1-C1-C2-O2
6	B	806	GOL	O2-C2-C3-O3
4	A	803	OUP	C07-C08-C11-C12
2	A	801	HEM	C4B-C3B-CAB-CBB
4	A	803	OUP	C09-C08-C11-C12
4	A	803	OUP	C13-C14-O19-C20
4	A	803	OUP	C15-C14-O19-C20
4	A	803	OUP	C07-C08-C11-C16
4	B	803	OUP	C15-C14-O19-C20
4	B	803	OUP	C13-C14-O19-C20
2	B	801	HEM	C4B-C3B-CAB-CBB
4	A	803	OUP	C09-C08-C11-C16
4	B	803	OUP	O19-C20-C21-C22
2	A	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

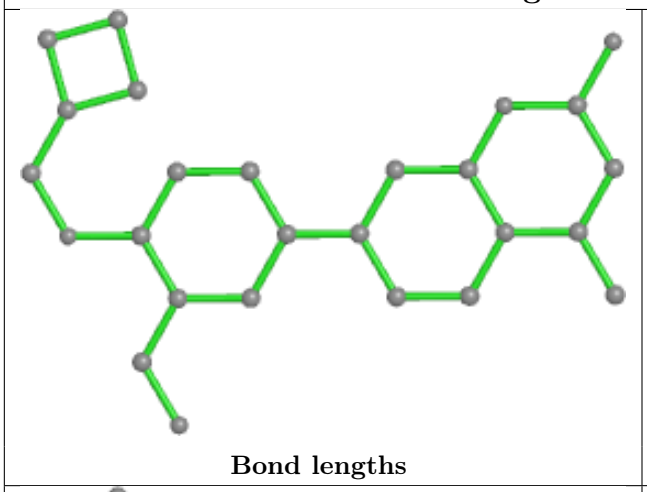
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	806	GOL	2	0
4	B	803	OUP	3	0
2	A	801	HEM	5	0
2	B	801	HEM	3	0
4	A	803	OUP	3	0

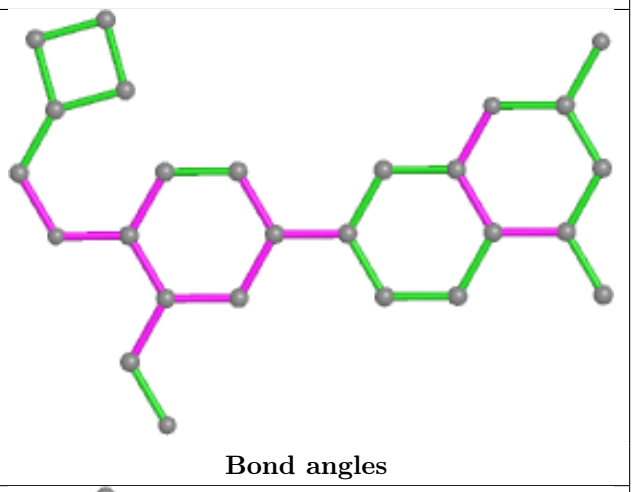
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

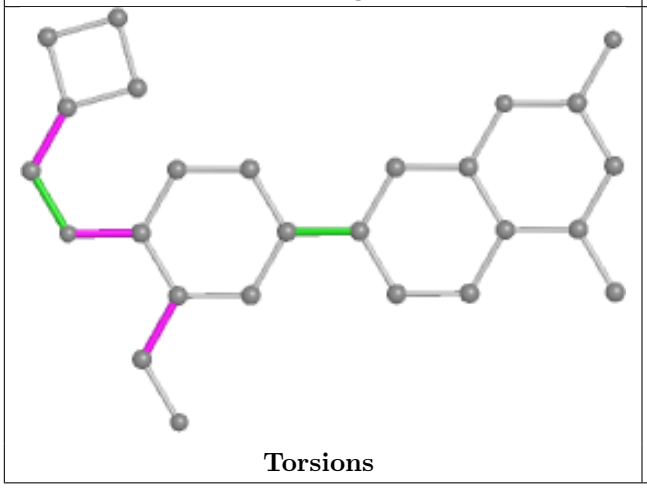
Ligand OUP B 803



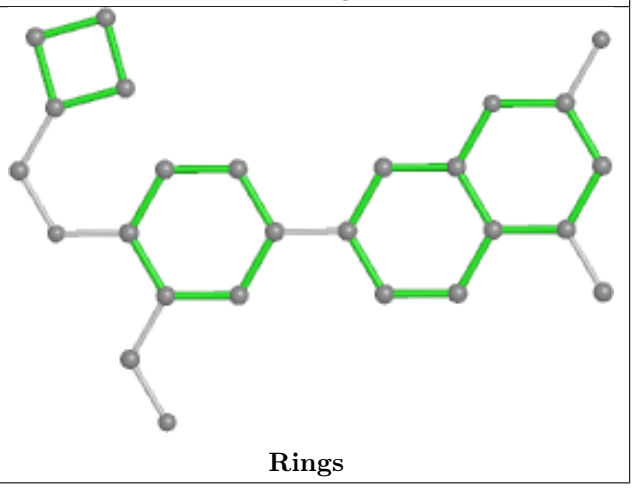
Bond lengths



Bond angles

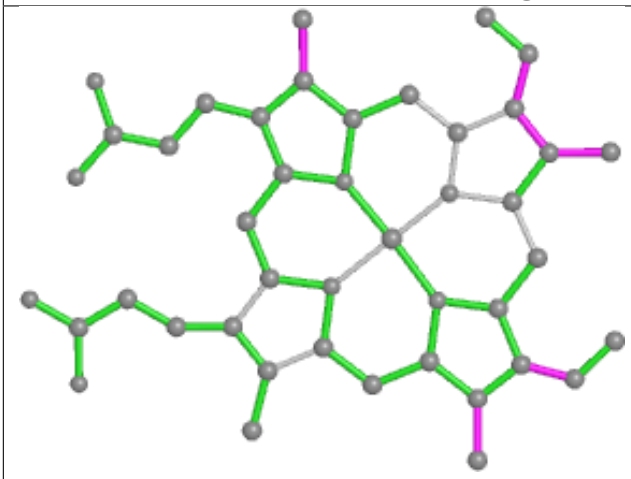


Torsions

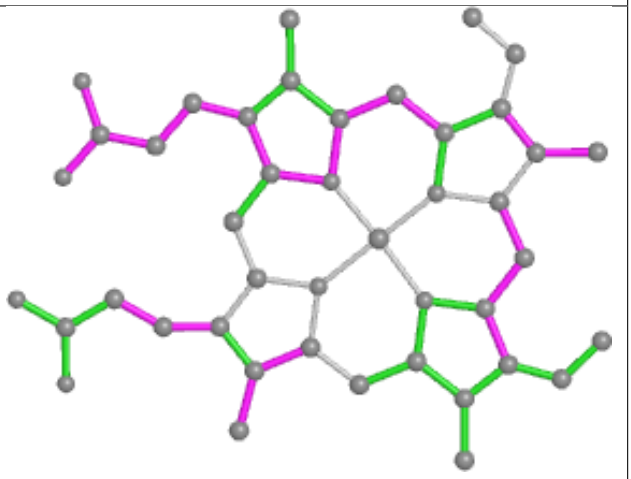


Rings

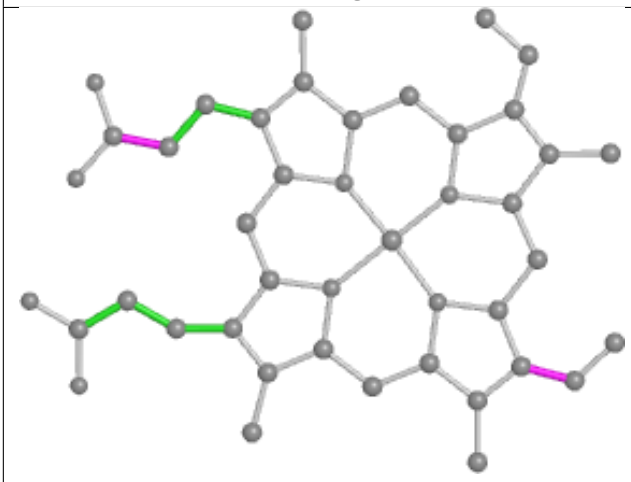
Ligand HEM A 801



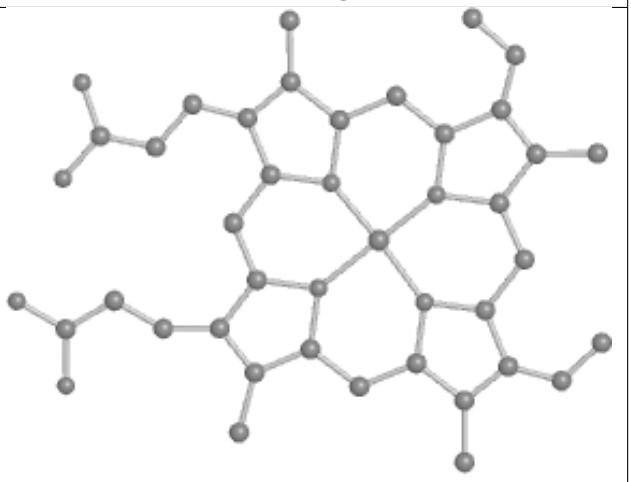
Bond lengths



Bond angles

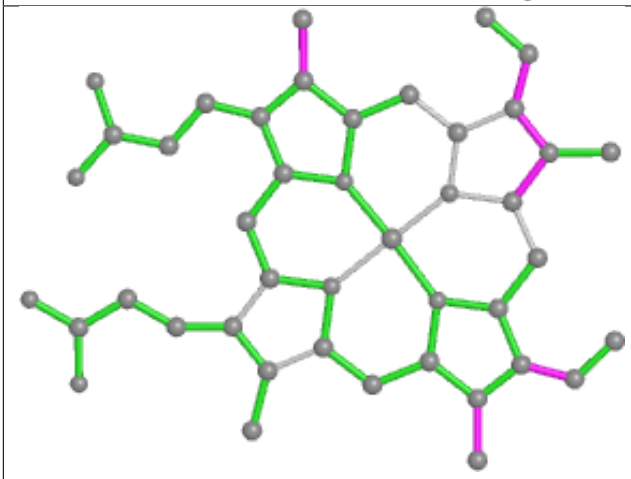


Torsions

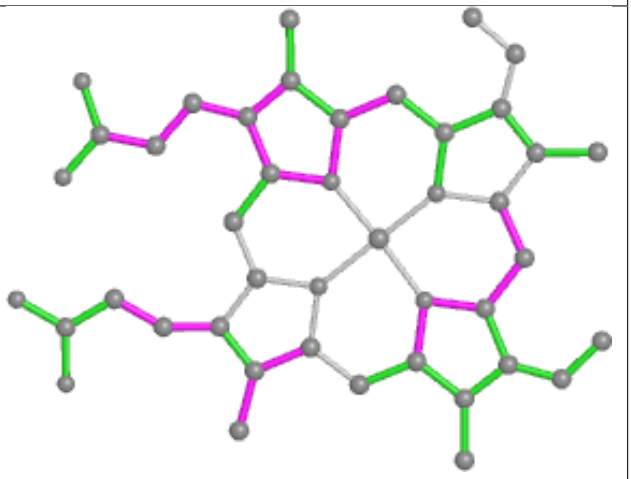


Rings

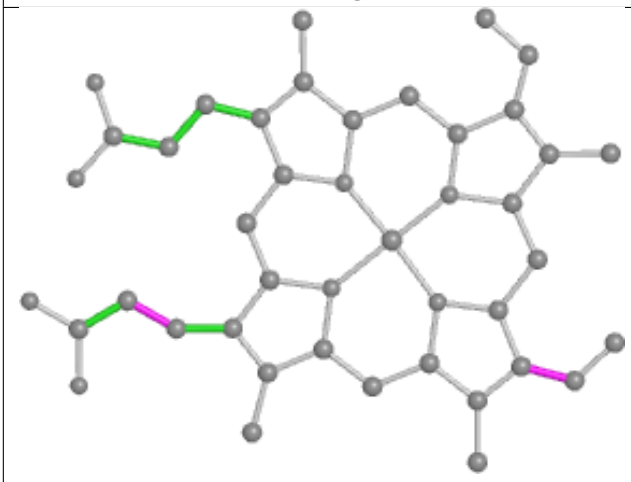
Ligand HEM B 801



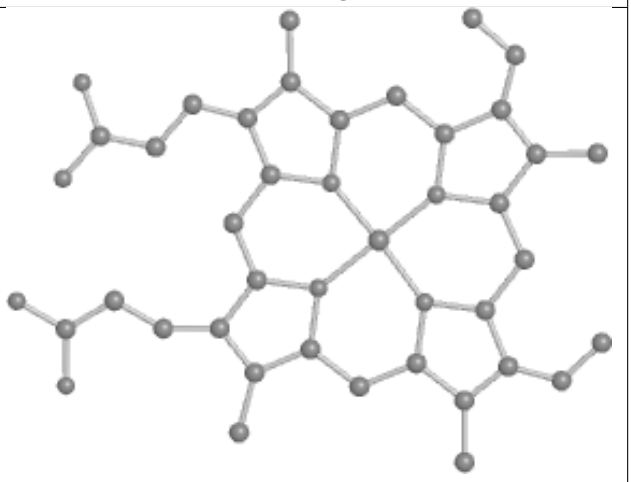
Bond lengths



Bond angles

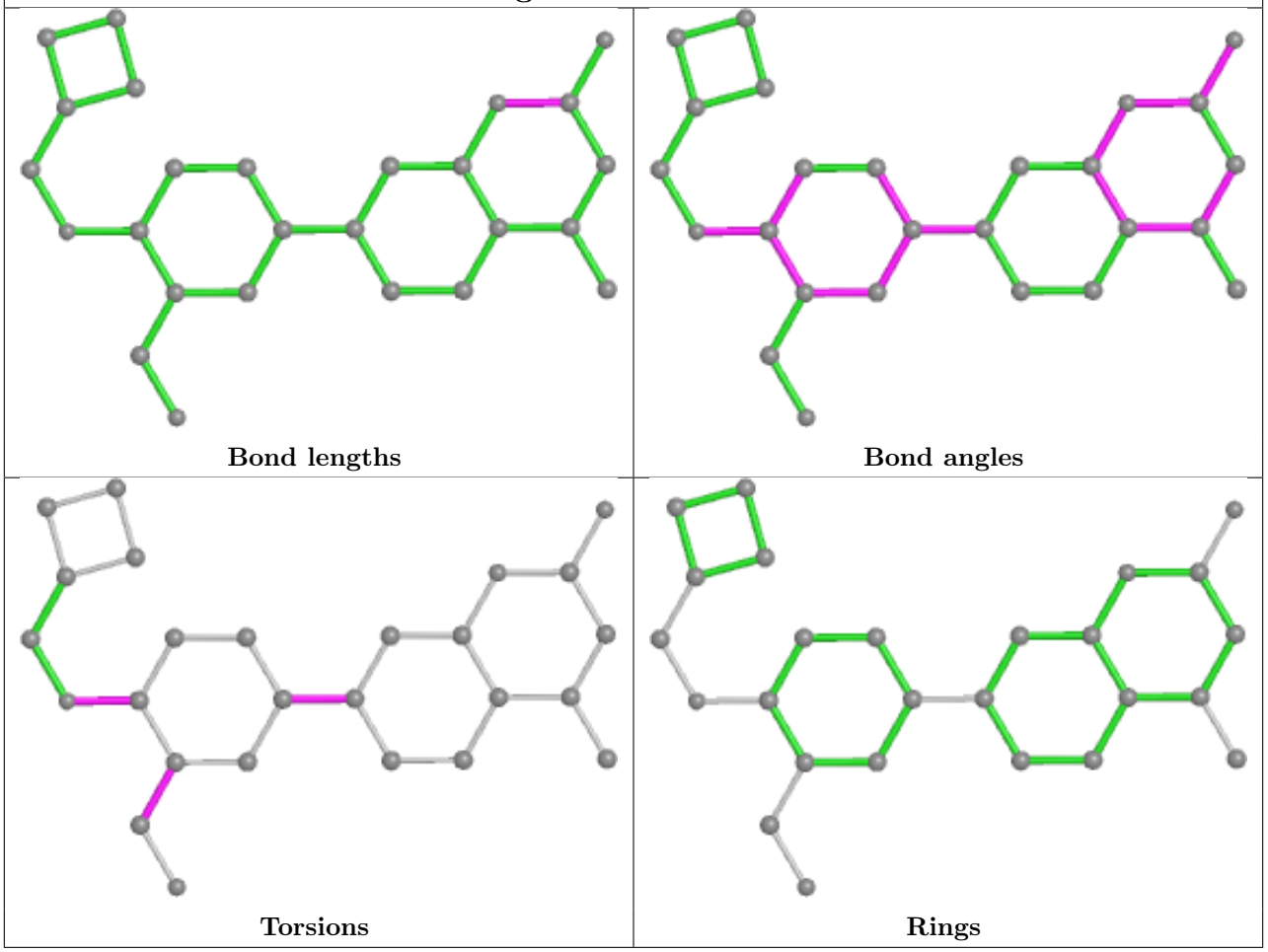


Torsions



Rings

Ligand OUP A 803



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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>2	OWAB(Å^2)	Q<0.9
1	A	410/422 (97%)	0.92	75 (18%) 1 0	30, 58, 107, 144	0
1	B	411/422 (97%)	0.27	29 (7%) 16 12	28, 45, 80, 123	1 (0%)
All	All	821/844 (97%)	0.60	104 (12%) 3 2	28, 50, 100, 144	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	10.5
1	A	348	VAL	8.2
1	B	300	PHE	7.6
1	A	488	PRO	7.5
1	B	348	VAL	7.4
1	A	388	ILE	6.2
1	A	347	ASP	5.8
1	A	355	PHE	5.7
1	A	507	GLN	5.6
1	B	350	THR	5.5
1	A	716	TRP	5.4
1	A	489	ASP	5.2
1	A	713	THR	5.1
1	A	351	LYS	4.9
1	A	506	ILE	4.9
1	A	391	THR	4.8
1	A	491	SER	4.8
1	A	299	ARG	4.7
1	A	350	THR	4.6
1	A	352	ASP	4.5
1	B	299	ARG	4.4
1	A	392	SER	4.4
1	A	322	LEU	4.2
1	A	679	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	677	VAL	4.1
1	B	611	ALA	4.1
1	A	490	GLY	4.1
1	A	677	VAL	4.0
1	B	718	GLY	3.8
1	B	680	VAL	3.8
1	A	678	TRP	3.8
1	A	712	ASN	3.7
1	A	389	GLU	3.7
1	A	390	SER	3.7
1	A	486	LYS	3.6
1	A	349	ARG	3.6
1	B	619	ARG	3.5
1	A	479	LEU	3.5
1	A	393	THR	3.4
1	B	352	ASP	3.4
1	A	551	PHE	3.4
1	A	499	VAL	3.4
1	B	616	LEU	3.4
1	A	711	TRP	3.3
1	A	480	ILE	3.2
1	A	503	GLU	3.2
1	A	676	TRP	3.2
1	B	351	LYS	3.2
1	B	679	ILE	3.1
1	A	714	HIS	3.1
1	A	321	THR	3.1
1	A	354	LEU	3.1
1	A	619	ARG	3.1
1	B	678	TRP	3.0
1	A	467	ASP	3.0
1	B	309	ASP	3.0
1	A	469	LYS	3.0
1	A	609	GLU	3.0
1	A	611	ALA	3.0
1	A	386	LYS	2.9
1	A	567	VAL	2.9
1	A	505	CYS	2.9
1	A	385	ASN	2.9
1	A	466	THR	2.8
1	A	691	PHE	2.8
1	B	620	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	553	TRP	2.7
1	A	584	PHE	2.7
1	A	681	PRO	2.7
1	B	682	PRO	2.7
1	B	310	VAL	2.7
1	B	617	ASP	2.6
1	B	562	TYR	2.6
1	A	531	PRO	2.6
1	A	680	VAL	2.6
1	A	566	ALA	2.5
1	A	561	TRP	2.5
1	A	564	LEU	2.5
1	A	593	ILE	2.5
1	A	415	CYS	2.5
1	A	353	GLN	2.4
1	A	487	GLN	2.4
1	B	676	TRP	2.4
1	A	552	ASP	2.3
1	A	508	GLN	2.3
1	A	565	PRO	2.3
1	A	643	SER	2.3
1	A	591	THR	2.3
1	A	511	LYS	2.3
1	A	470	HIS	2.3
1	B	615	ASP	2.3
1	A	382	GLU	2.2
1	B	302	LYS	2.2
1	B	691	PHE	2.2
1	B	567	VAL	2.2
1	B	584	PHE	2.2
1	A	588	TYR	2.1
1	B	561	TRP	2.1
1	A	446	VAL	2.1
1	B	608	GLU	2.1
1	A	667	ARG	2.1
1	A	300	PHE	2.0
1	A	682	PRO	2.0
1	B	681	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

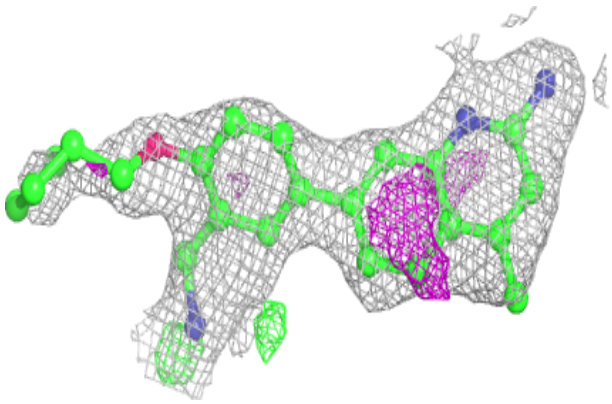
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

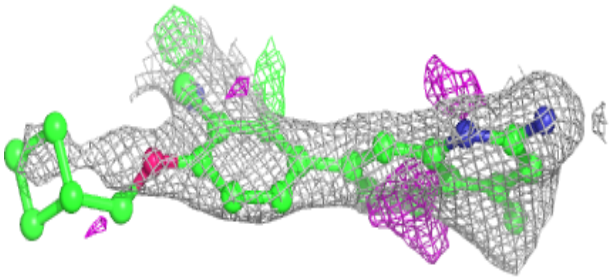
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	805	6/6	0.50	0.30	88,94,96,98	0
6	GOL	B	806	6/6	0.69	0.28	83,84,88,93	0
4	OUP	A	803	26/26	0.86	0.26	39,71,104,104	0
4	OUP	B	803	26/26	0.89	0.21	39,56,79,80	0
5	ACT	B	804	4/4	0.93	0.09	53,55,63,67	0
5	ACT	A	804	4/4	0.95	0.15	66,67,68,68	0
3	H4B	A	802	17/17	0.95	0.17	30,40,43,49	0
2	HEM	B	801	43/43	0.96	0.18	27,36,53,55	0
2	HEM	A	801	43/43	0.96	0.21	31,39,61,65	0
3	H4B	B	802	17/17	0.96	0.20	31,35,41,43	0
7	ZN	B	807	1/1	1.00	0.09	39,39,39,39	0

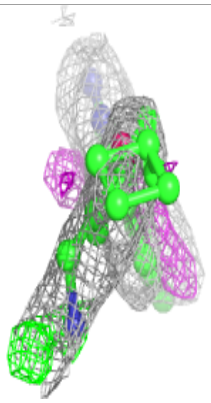
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OUP A 803:

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

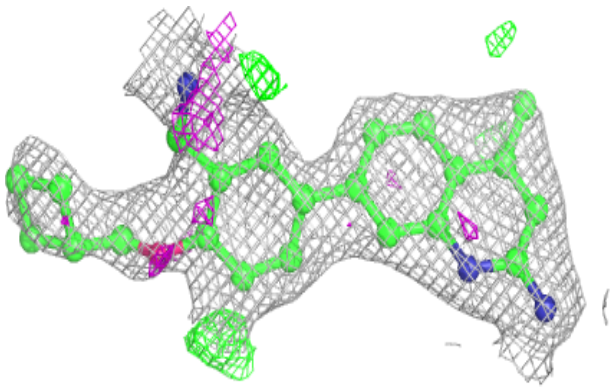


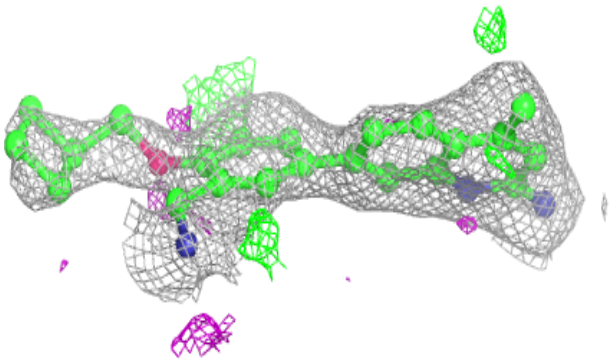


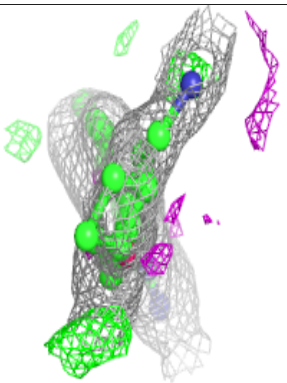


Electron density around OUP B 803:

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

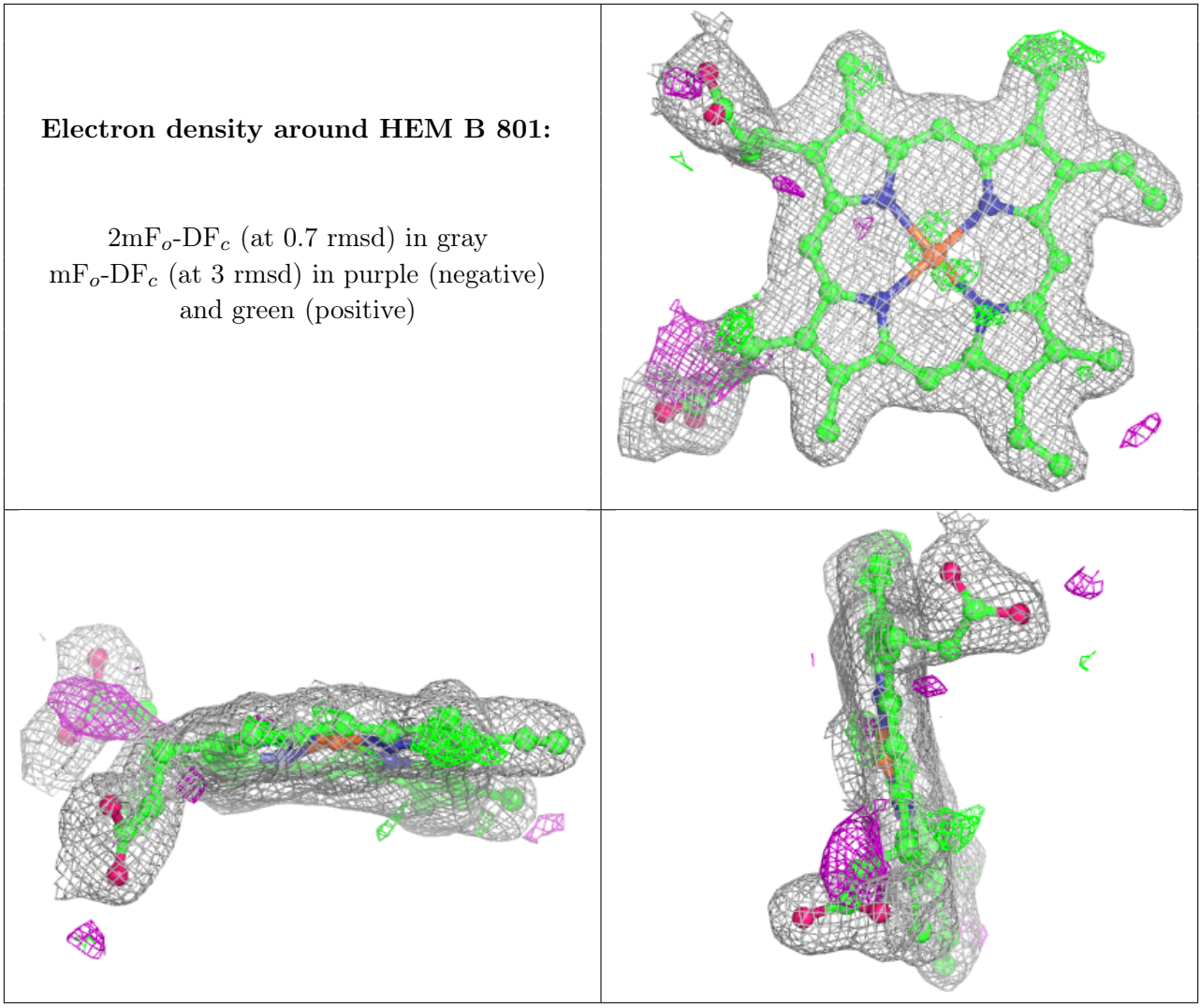






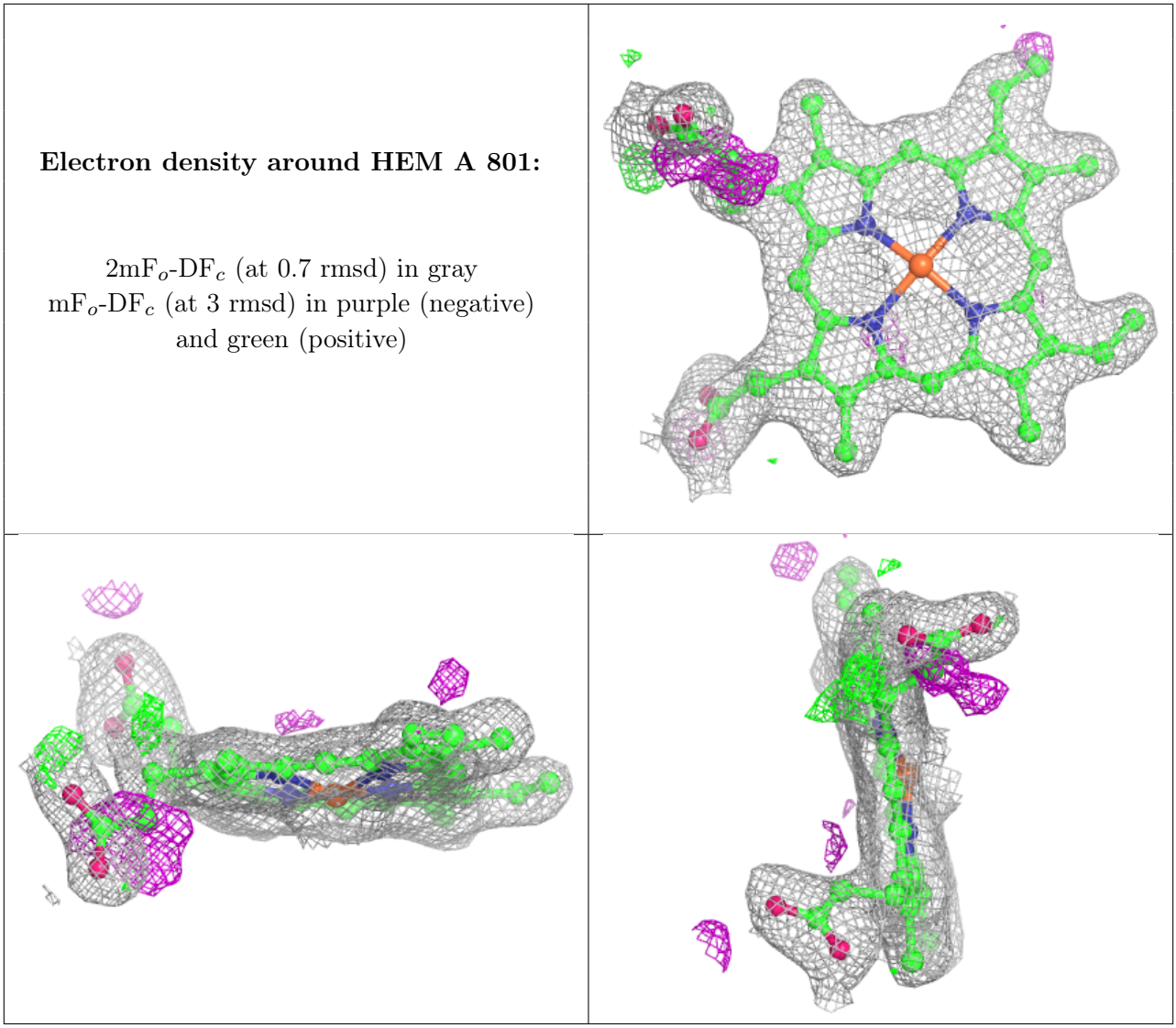
Electron density around HEM B 801:

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



Electron density around HEM A 801:

$2mF_o$-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.