Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 01:12 AM EDT

PDB ID	:	8FGD
Title	:	Structure of rat neuronal nitric oxide synthase R349A mutant heme domain in complex with 6-(5-(2-(diethylamino)ethyl)-2,3-difluorophenethyl)-4-methyl pyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-12-12
Resolution	:	1.78 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:

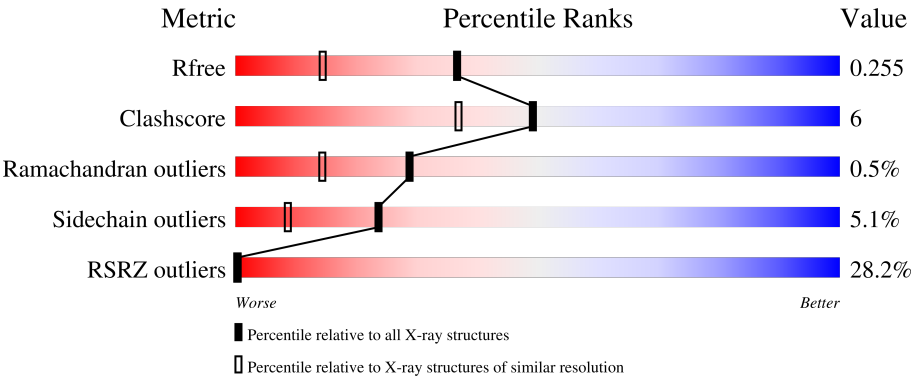
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	422	28% 81% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3519 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.

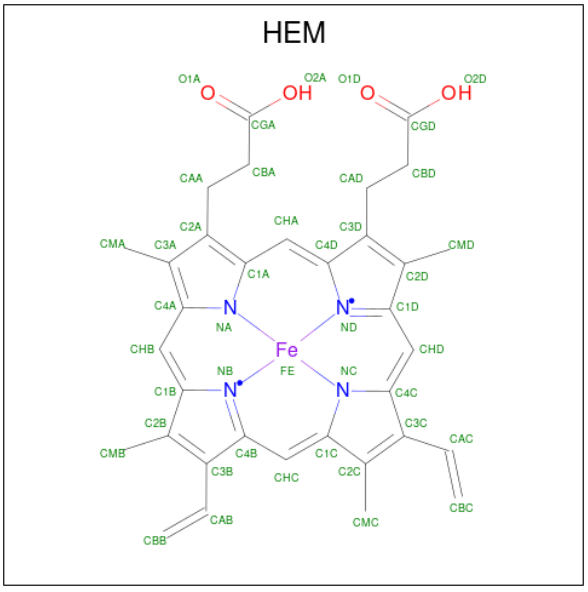
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3383	2163	581	617	22	0	2	0

There is a discrepancy between the modelled and reference sequences:

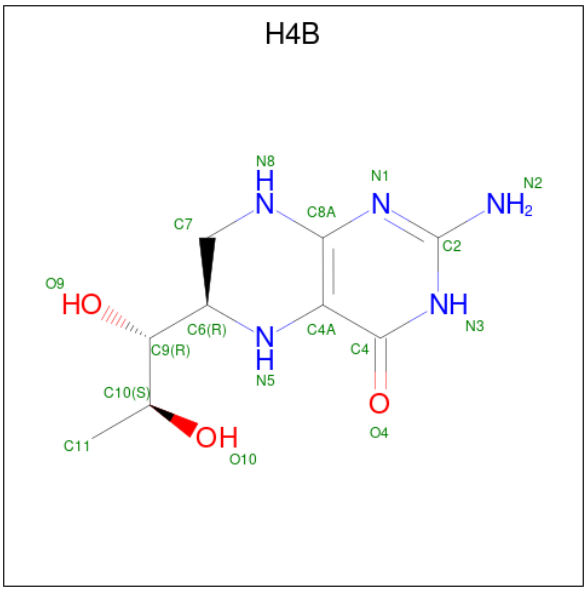
Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ALA	ARG	engineered mutation	UNP P29476

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



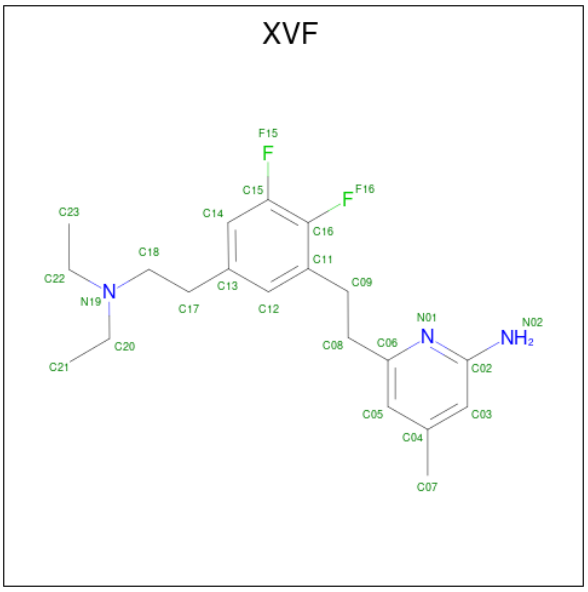
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

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



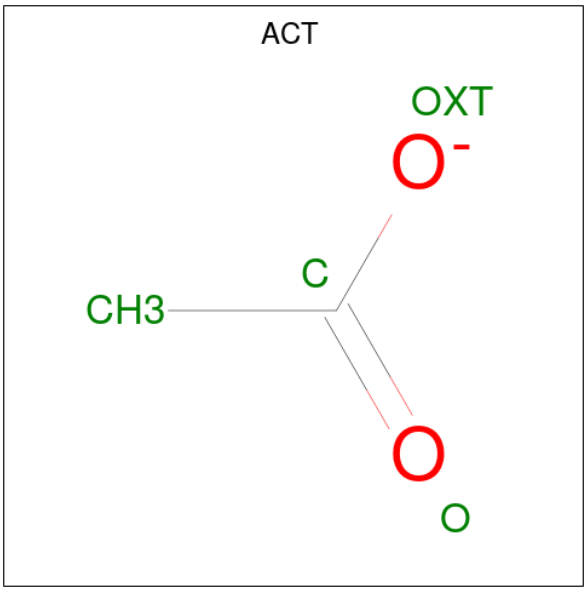
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0

- Molecule 4 is 6-(2-{5-[2-(diethylamino)ethyl]-2,3-difluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: XVF) (formula: $C_{20}H_{27}F_2N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
4	A	1	25	20	2	3	0	0

- 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 4 2 2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

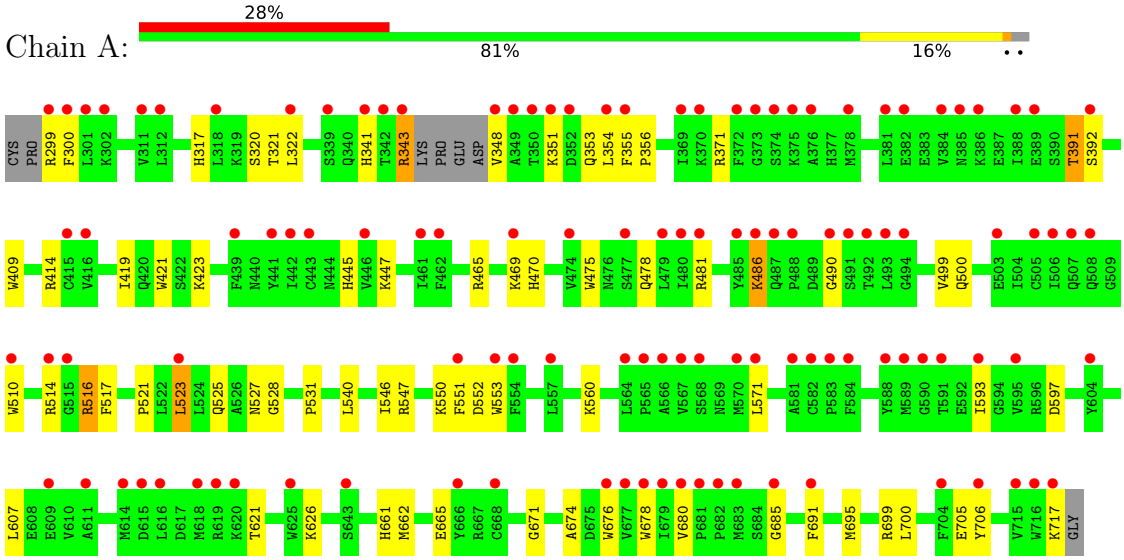
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	49.16Å 114.70Å 164.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.61 – 1.78 39.60 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.4 (39.61-1.78) 94.9 (39.60-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.216 , 0.253 0.221 , 0.255	Depositor DCC
R_{free} test set	2157 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	1.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: ZN, XVF, H4B, HEM, 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	0.36	0/3483	0.52	0/4724

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	3383	0	3298	38	0
2	A	43	0	30	4	0
3	A	17	0	15	0	0
4	A	25	0	0	0	0
5	A	4	0	3	1	0
6	A	1	0	0	0	0
7	A	46	0	0	1	0
All	All	3519	0	3346	40	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 6.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HH11	1:A:705:GLU:HG3	1.50	0.74
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.75	0.67
1:A:322:LEU:HD21	1:A:343:ARG:HH21	1.58	0.67
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.81	0.63
1:A:470:HIS:O	7:A:901:HOH:O	2.16	0.63
1:A:343:ARG:NH1	1:A:705:GLU:HG3	2.13	0.63
1:A:322:LEU:HD21	1:A:343:ARG:NH2	2.18	0.58
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.88	0.54
1:A:299:ARG:O	1:A:317:HIS:NE2	2.38	0.54
1:A:419:ILE:HG13	1:A:661:HIS:HB2	1.90	0.53
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.90	0.52
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.45	0.52
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.46	0.50
1:A:341:HIS:NE2	2:A:801:HEM:O1D	2.45	0.50
1:A:527:ASN:O	1:A:527:ASN:ND2	2.44	0.49
1:A:593:ILE:HA	1:A:597:ASP:HB2	1.95	0.48
1:A:525:GLN:HE21	1:A:528:GLY:HA2	1.81	0.46
1:A:607:LEU:HD13	1:A:626:LYS:HG2	1.98	0.46
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.98	0.46
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.51	0.46
1:A:351:LYS:HB3	1:A:392:SER:HB2	1.98	0.45
1:A:423:LYS:HB3	1:A:423:LYS:HE2	1.75	0.45
1:A:486:LYS:HE3	1:A:499:VAL:HG11	2.00	0.44
1:A:465:ARG:HH12	1:A:571:LEU:HD11	1.83	0.43
2:A:801:HEM:HBD2	2:A:801:HEM:HMD2	2.01	0.43
1:A:685:GLY:O	1:A:691:PHE:HB2	2.19	0.43
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.02	0.42
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.54	0.42
1:A:391:THR:O	1:A:392:SER:OG	2.33	0.42
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.32	0.42
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.35	0.42
1:A:516:ARG:HB3	1:A:517:PHE:H	1.75	0.41
1:A:355:PHE:N	1:A:356:PRO:HD2	2.35	0.41
1:A:445:HIS:CD2	1:A:445:HIS:C	2.94	0.41
1:A:419:ILE:HG22	5:A:804:ACT:H1	2.02	0.41
1:A:447:LYS:HD2	1:A:540:LEU:HD21	2.03	0.41
1:A:665:GLU:HB3	1:A:671:GLY:O	2.20	0.41
1:A:320:SER:HA	1:A:700:LEU:HD23	2.03	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.41
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.51	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	413/422 (98%)	384 (93%)	27 (6%)	2 (0%)	29 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	490	GLY

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	372/376 (99%)	353 (95%)	19 (5%)	24 9

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	321	THR
1	A	343	ARG
1	A	348	VAL
1	A	353	GLN
1	A	354	LEU
1	A	371	ARG
1	A	391	THR
1	A	469	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	LYS
1	A	500	GLN
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	552	ASP
1	A	621	THR
1	A	662	MET
1	A	717	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\|>2$
3	H4B	A	802	-	16,18,18	0.86	0	11,26,26	2.49	5 (45%)
4	XVF	A	803	-	26,26,26	2.04	1 (3%)	34,35,35	1.78	8 (23%)
5	ACT	A	804	-	3,3,3	0.76	0	3,3,3	0.75	0
2	HEM	A	801	1	41,50,50	1.52	6 (14%)	45,82,82	1.68	10 (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
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	XVF	A	803	-	-	5/14/14/14	0/2/2/2
2	HEM	A	801	1	-	5/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	XVF	C11-C16	10.19	1.49	1.38
2	A	801	HEM	C3C-CAC	3.61	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.48	1.35	1.40
2	A	801	HEM	FE-NB	3.39	2.13	1.96
2	A	801	HEM	CAB-C3B	2.70	1.54	1.47
2	A	801	HEM	CMD-C2D	2.18	1.55	1.50
2	A	801	HEM	CMB-C2B	2.10	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	CBA-CAA-C2A	-5.19	103.75	112.62
3	A	802	H4B	C8A-C4A-C4	4.84	118.87	114.57
4	A	803	XVF	C08-C06-N01	4.04	121.97	115.95
4	A	803	XVF	C02-N01-C06	3.98	121.12	118.10
4	A	803	XVF	C13-C14-C15	3.33	121.53	119.37
4	A	803	XVF	F16-C16-C11	3.32	121.36	117.85
4	A	803	XVF	C05-C06-N01	-3.27	119.43	122.90
3	A	802	H4B	C4-C4A-N5	3.02	121.66	119.12
2	A	801	HEM	C4B-CHC-C1C	2.99	126.50	122.56
3	A	802	H4B	N1-C2-N3	-2.95	120.80	125.42
2	A	801	HEM	CMC-C2C-C3C	2.88	130.07	124.68
3	A	802	H4B	C2-N3-C4	2.88	120.50	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	XVF	N02-C02-N01	2.79	120.90	116.49
3	A	802	H4B	C2-N1-C8A	2.69	120.57	114.54
4	A	803	XVF	C17-C13-C14	-2.67	116.16	120.54
2	A	801	HEM	C4D-ND-C1D	2.61	107.77	105.07
2	A	801	HEM	CAD-C3D-C2D	2.29	132.14	127.88
2	A	801	HEM	CAD-C3D-C4D	-2.25	120.72	124.66
2	A	801	HEM	CBD-CAD-C3D	2.22	118.79	112.63
2	A	801	HEM	C1B-NB-C4B	2.12	107.26	105.07
2	A	801	HEM	C4C-CHD-C1D	2.10	125.33	122.56
2	A	801	HEM	CAD-CBD-CGD	-2.08	109.12	113.60
4	A	803	XVF	C08-C06-C05	-2.00	118.57	121.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2D-C3D-CAD-CBD
4	A	803	XVF	C06-C08-C09-C11
2	A	801	HEM	C4D-C3D-CAD-CBD
4	A	803	XVF	C13-C17-C18-N19
4	A	803	XVF	C12-C13-C17-C18
4	A	803	XVF	C14-C13-C17-C18
4	A	803	XVF	C17-C18-N19-C20
2	A	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

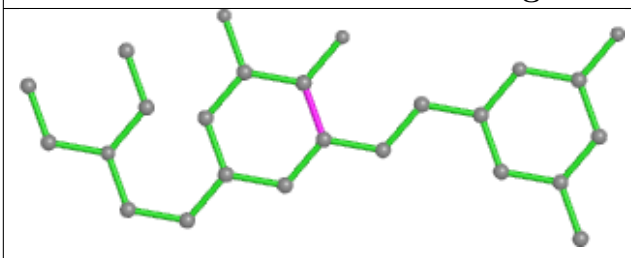
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	ACT	1	0
2	A	801	HEM	4	0

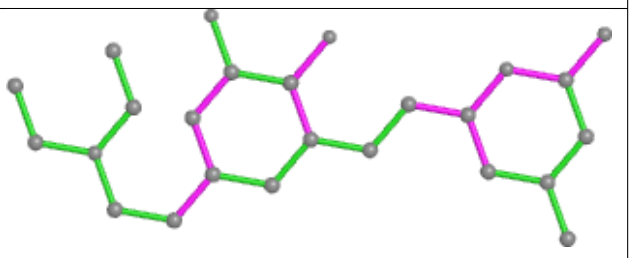
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

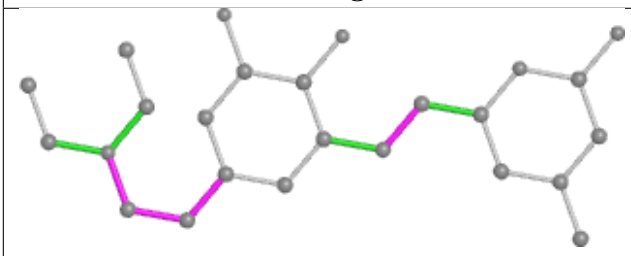
Ligand XVF A 803



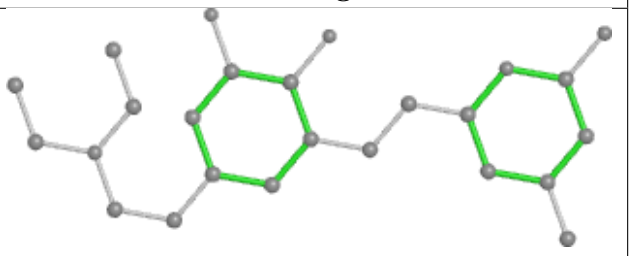
Bond lengths



Bond angles

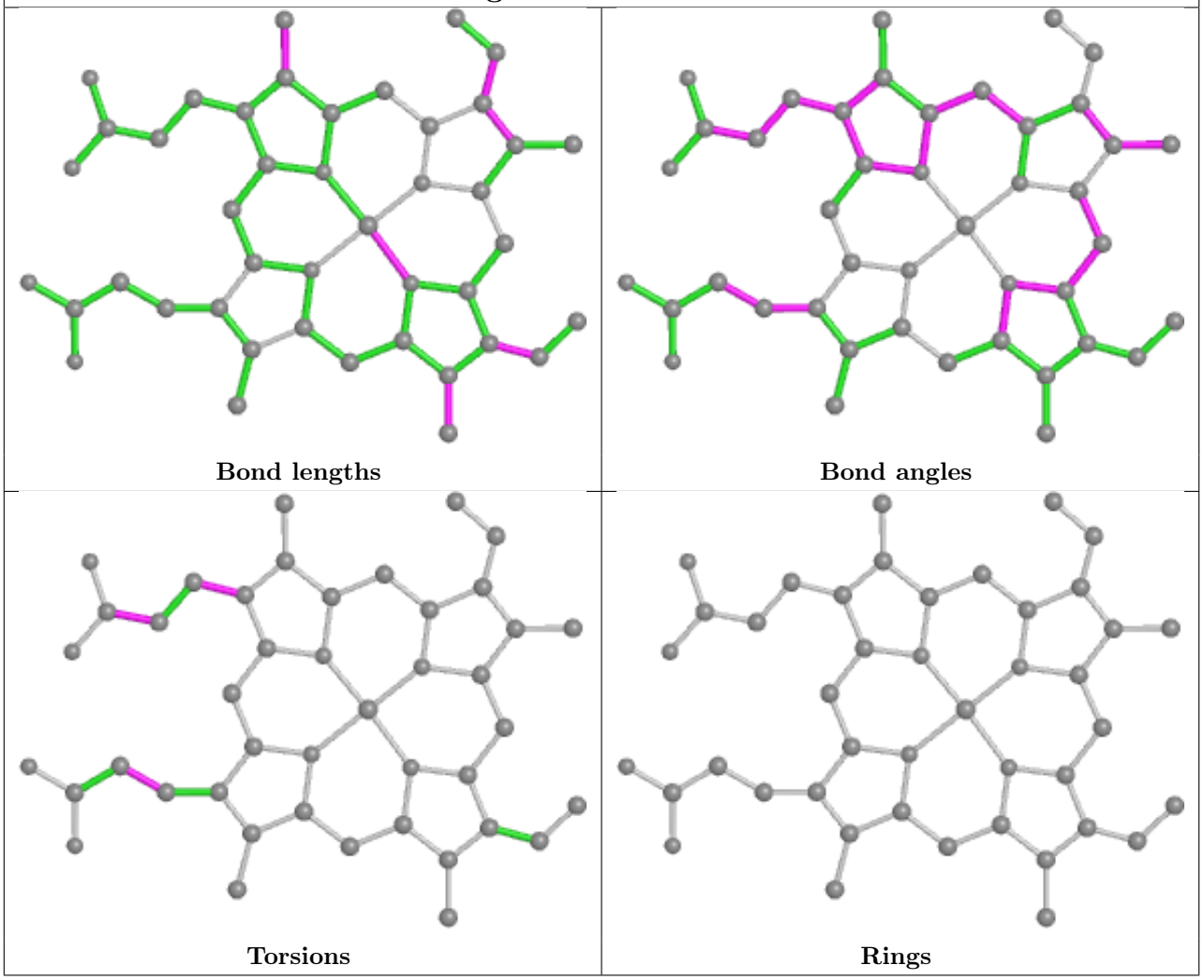


Torsions



Rings

Ligand HEM A 801



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	415/422 (98%)	1.40	117 (28%)	0	0	39, 73, 128, 175	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	7.7
1	A	551	PHE	7.6
1	A	615	ASP	7.4
1	A	488	PRO	6.9
1	A	493	LEU	6.7
1	A	348	VAL	6.4
1	A	370	LYS	5.9
1	A	506	ILE	5.5
1	A	351	LYS	5.3
1	A	611	ALA	5.0
1	A	566	ALA	4.9
1	A	355	PHE	4.9
1	A	505	CYS	4.5
1	A	677	VAL	4.5
1	A	554	PHE	4.4
1	A	479	LEU	4.3
1	A	706	TYR	4.3
1	A	491	SER	4.3
1	A	343	ARG	4.2
1	A	584	PHE	4.2
1	A	373	GLY	4.2
1	A	553	TRP	4.2
1	A	300	PHE	4.1
1	A	691	PHE	4.1
1	A	349	ALA	4.1
1	A	381	LEU	4.0
1	A	487	GLN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	372	PHE	3.9
1	A	299	ARG	3.8
1	A	568	SER	3.8
1	A	388	ILE	3.8
1	A	442	ILE	3.8
1	A	354	LEU	3.8
1	A	571	LEU	3.8
1	A	492	THR	3.7
1	A	716	TRP	3.7
1	A	490	GLY	3.7
1	A	704	PHE	3.7
1	A	582	CYS	3.7
1	A	378	MET	3.6
1	A	384	VAL	3.6
1	A	567	VAL	3.5
1	A	350	THR	3.5
1	A	679	ILE	3.4
1	A	389	GLU	3.4
1	A	620	LYS	3.3
1	A	485	TYR	3.3
1	A	616	LEU	3.3
1	A	680	VAL	3.3
1	A	374	SER	3.3
1	A	480	ILE	3.2
1	A	318	LEU	3.2
1	A	375	LYS	3.1
1	A	583	PRO	3.1
1	A	682	PRO	3.1
1	A	341	HIS	3.1
1	A	676	TRP	3.1
1	A	503	GLU	3.0
1	A	678	TRP	3.0
1	A	302	LYS	3.0
1	A	385	ASN	3.0
1	A	301	LEU	3.0
1	A	590	GLY	2.9
1	A	715	VAL	2.9
1	A	591	THR	2.9
1	A	515	GLY	2.9
1	A	565	PRO	2.9
1	A	461	ILE	2.9
1	A	619	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	683	MET	2.8
1	A	339	SER	2.8
1	A	494	GLY	2.8
1	A	382	GLU	2.7
1	A	352	ASP	2.7
1	A	668[A]	CYS	2.7
1	A	666	TYR	2.7
1	A	392	SER	2.7
1	A	643	SER	2.7
1	A	386	LYS	2.7
1	A	510	TRP	2.7
1	A	564	LEU	2.7
1	A	609	GLU	2.7
1	A	443	CYS	2.6
1	A	342	THR	2.6
1	A	477	SER	2.6
1	A	581	ALA	2.6
1	A	681	PRO	2.5
1	A	614	MET	2.5
1	A	507	GLN	2.5
1	A	474	VAL	2.5
1	A	717	LYS	2.4
1	A	311	VAL	2.4
1	A	618	MET	2.4
1	A	588	TYR	2.4
1	A	481	ARG	2.4
1	A	508	GLN	2.4
1	A	441	TYR	2.4
1	A	322	LEU	2.3
1	A	570	MET	2.3
1	A	312	LEU	2.3
1	A	416	VAL	2.3
1	A	514	ARG	2.3
1	A	593	ILE	2.2
1	A	462	PHE	2.2
1	A	589	MET	2.2
1	A	685	GLY	2.2
1	A	604	TYR	2.1
1	A	469	LYS	2.1
1	A	376	ALA	2.1
1	A	625	TRP	2.1
1	A	415	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	486	LYS	2.1
1	A	446	VAL	2.1
1	A	523	LEU	2.1
1	A	557	LEU	2.1
1	A	595	VAL	2.0
1	A	439	PHE	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)

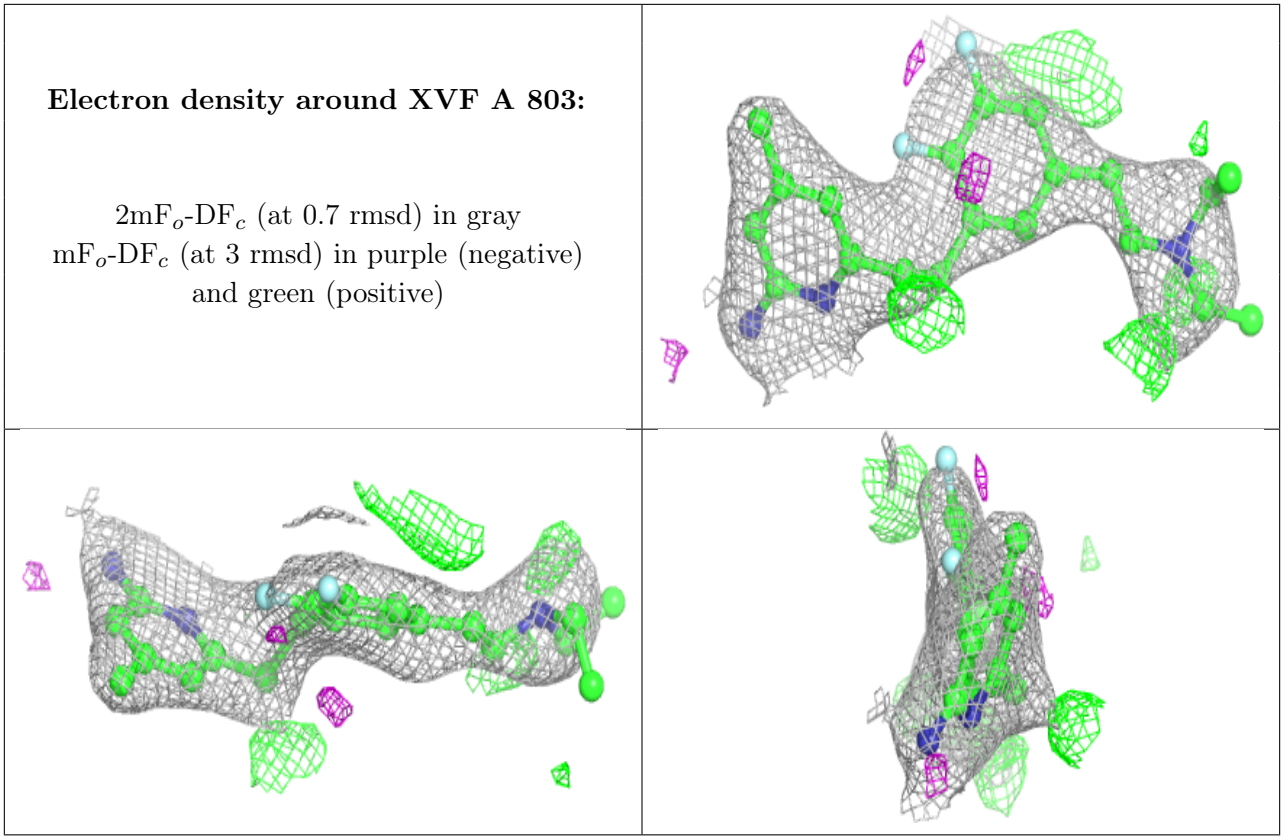
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	XVF	A	803	25/25	0.93	0.29	40,79,95,98	0
5	ACT	A	804	4/4	0.95	0.20	105,105,107,108	0
2	HEM	A	801	43/43	0.97	0.19	36,47,62,66	0
3	H4B	A	802	17/17	0.98	0.21	40,45,54,55	0
6	ZN	A	805	1/1	0.99	0.16	43,43,43,43	1

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

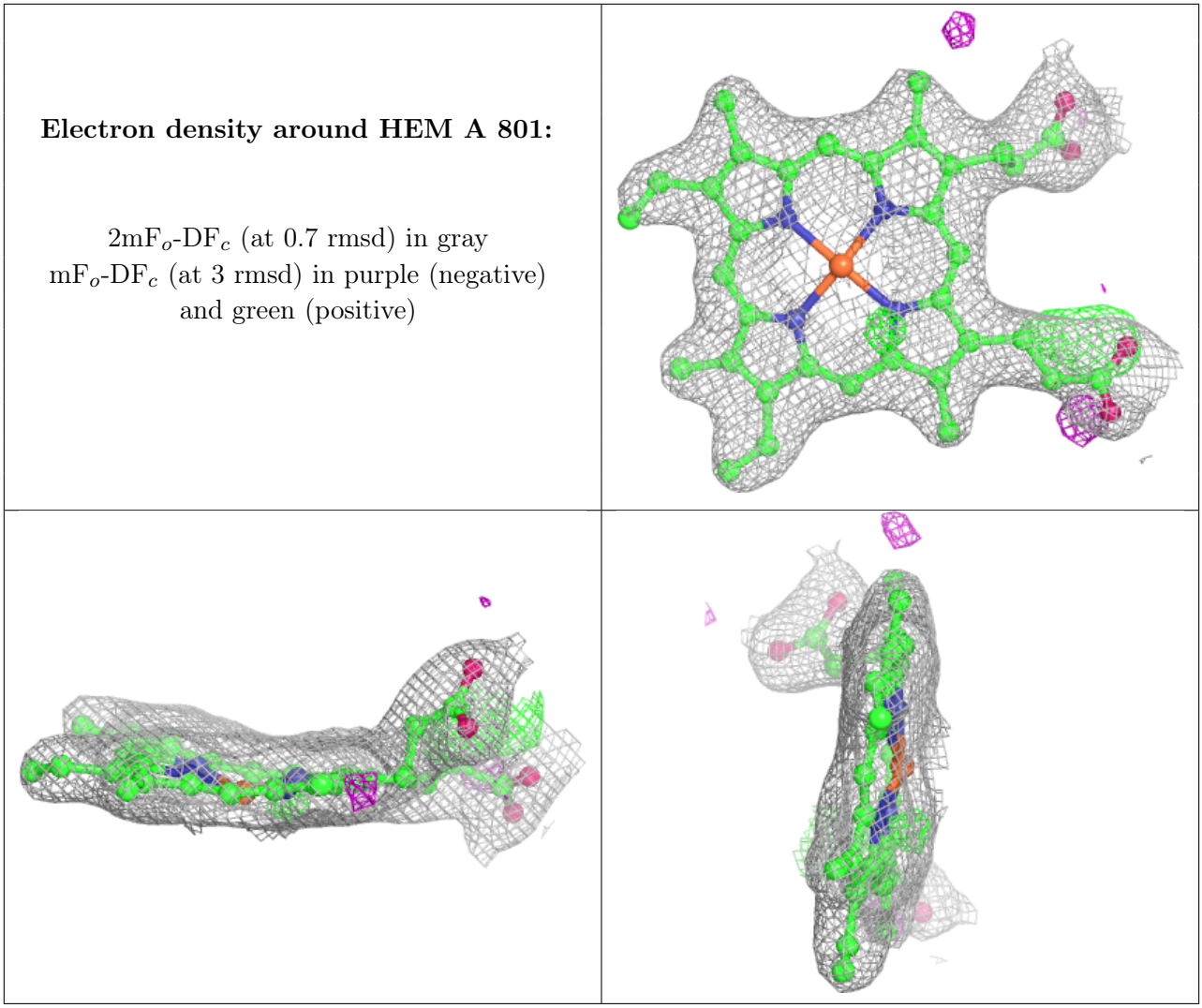
Electron density around XVF A 803:

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



Electron density around 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

There are no such residues in this entry.