



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:28 PM UTC

PDB ID : 4KCK / pdb_00004kck
Title : Structure of neuronal nitric oxide synthase heme domain in complex with N-(3-(2-((3-(thiophene-2-carboximidamido)benzyl)amino)ethyl)phenyl)thiophene-2-carboximidamide
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-04-24
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

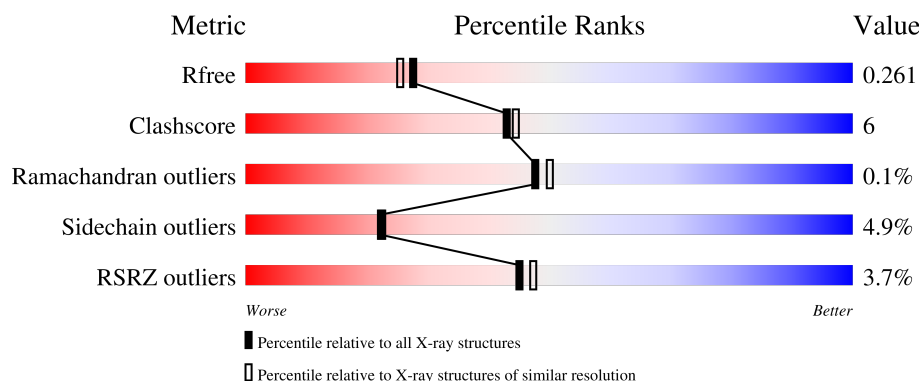
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	5% 78% 17% • •
1	B	422	3% 78% 18% • •

2 Entry composition [i](#)

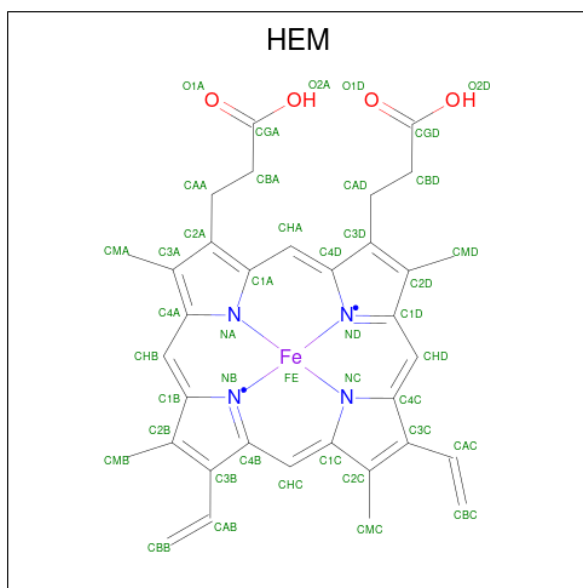
There are 7 unique types of molecules in this entry. The entry contains 7002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

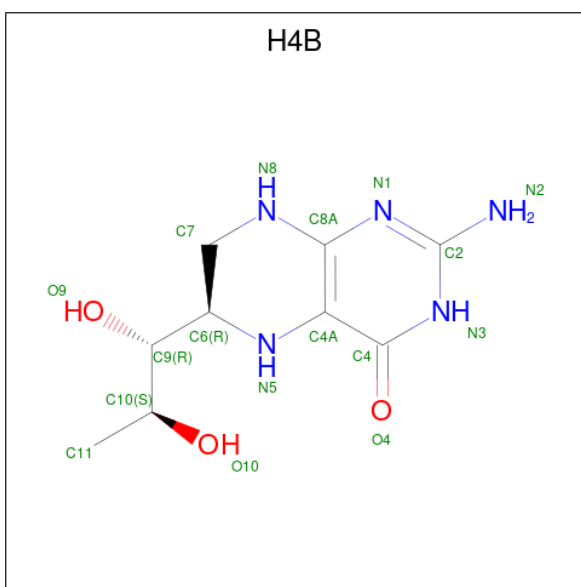
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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



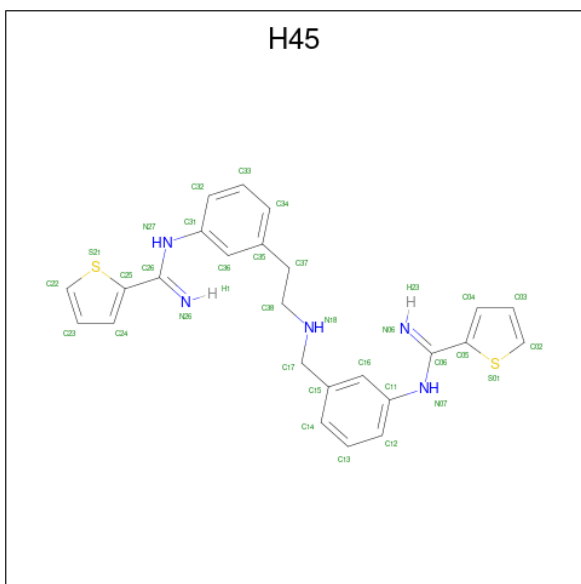
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: 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 N-(3-{2-[(3-{[(Z)-imino(thiophen-2-yl)methyl]amino}benzyl)amino]ethyl}phenyl)thiophene-2-carboximidamide (CCD ID: H45) (formula: C₂₅H₂₅N₅S₂).



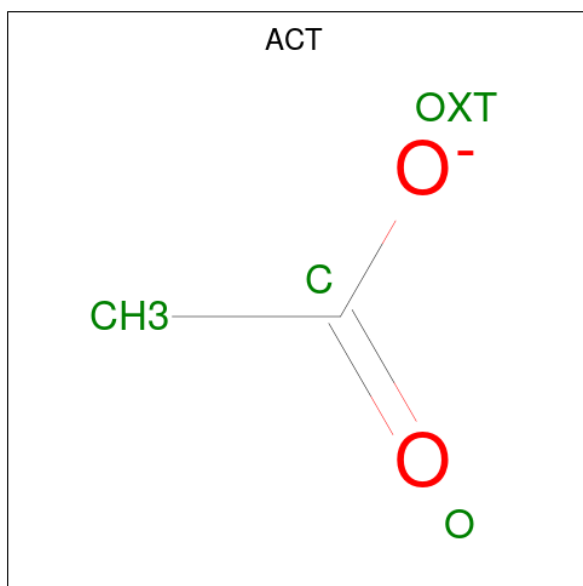
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			32	25	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	S	0	0
			32	25	5	2		

- Molecule 5 is ACETATE ION (CCD ID: 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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

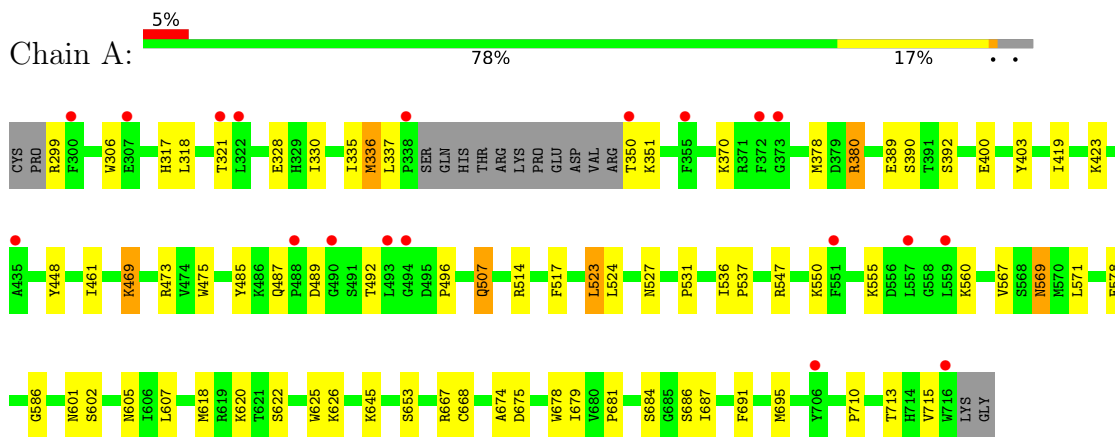
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	98	Total	O	0	0
			98	98		

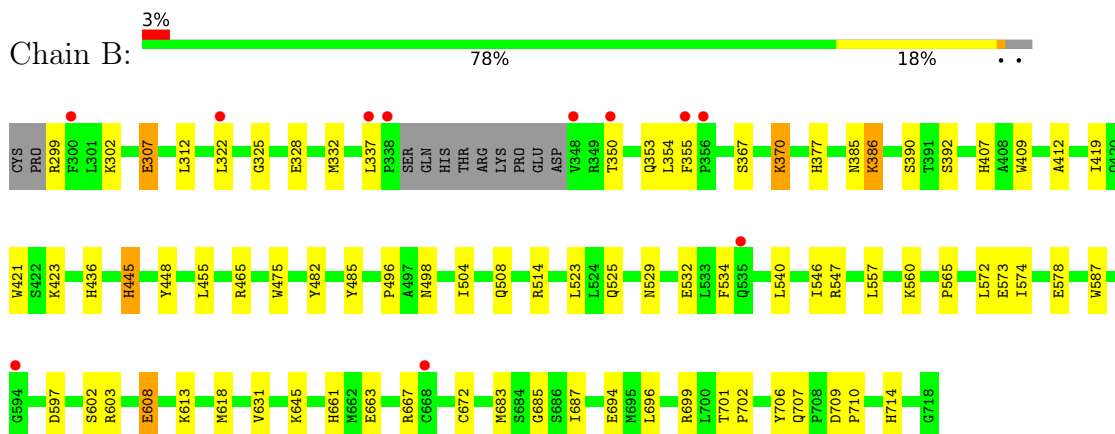
3 Residue-property plots [i](#)

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



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.92Å 111.06Å 165.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.19 – 2.10 92.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (92.19-2.10) 91.7 (92.19-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.264 0.215 , 0.261	Depositor DCC
R_{free} test set	2570 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ACT, H45, H4B, HEM, ZN

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	0.89	0/3406	0.96	4/4621 (0.1%)
1	B	1.03	8/3438 (0.2%)	1.04	5/4661 (0.1%)
All	All	0.96	8/6844 (0.1%)	1.00	9/9282 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	714	HIS	CG-CD2	6.29	1.42	1.35
1	B	445	HIS	CE1-NE2	5.88	1.38	1.32
1	B	445	HIS	CG-CD2	5.67	1.42	1.35
1	B	565	PRO	C-O	5.64	1.31	1.24
1	B	407	HIS	ND1-CE1	5.25	1.37	1.32
1	B	377	HIS	CG-ND1	-5.17	1.32	1.38
1	B	412	ALA	N-CA	5.05	1.52	1.46
1	B	436	HIS	CG-CD2	5.01	1.41	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	LEU	N-CA-C	6.90	118.59	111.14
1	A	681	PRO	CA-C-N	-6.33	114.37	120.83
1	A	681	PRO	C-N-CA	-6.33	114.37	120.83
1	A	461	ILE	N-CA-C	6.19	116.54	107.37
1	B	707	GLN	CA-C-N	-5.60	114.19	119.85
1	B	707	GLN	C-N-CA	-5.60	114.19	119.85
1	B	672	CYS	CA-C-N	-5.53	114.06	119.76
1	B	672	CYS	C-N-CA	-5.53	114.06	119.76
1	A	586	GLY	N-CA-C	-5.42	100.33	113.18

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	3313	0	3221	45	0
1	B	3345	0	3259	37	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	32	0	23	3	0
4	B	32	0	24	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	53	0	0	1	0
7	B	98	0	0	1	0
All	All	7002	0	6623	83	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 (83) 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:336:MET:CE	1:A:678:TRP:HZ2	1.87	0.86
1:B:386:LYS:HE2	7:B:941:HOH:O	1.78	0.83
1:B:325:GLY:O	1:B:332:MET:HG3	1.81	0.80
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.63	0.80
1:A:336:MET:CE	1:A:678:TRP:CZ2	2.68	0.76
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.73	0.70
1:A:351:LYS:HE3	1:A:392:SER:HB3	1.79	0.65
1:A:469:LYS:HE3	1:A:469:LYS:HA	1.81	0.62
1:A:336:MET:HE2	1:A:678:TRP:HZ2	1.63	0.62
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.84	0.59
1:A:336:MET:HE1	1:A:678:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LEU:HD13	1:A:626:LYS:HG2	1.86	0.57
2:B:801:HEM:HBC2	2:B:801:HEM:CMC	2.34	0.57
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.20	0.57
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.05	0.56
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.87	0.56
1:A:675:ASP:O	1:A:679:ILE:HG12	2.06	0.56
1:B:547:ARG:H	1:B:547:ARG:HD3	1.72	0.55
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.90	0.53
1:B:701:THR:HA	1:B:702:PRO:C	2.32	0.53
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.90	0.53
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.91	0.52
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.45	0.51
1:B:587:TRP:H	2:B:801:HEM:HAB	1.75	0.51
1:B:448:TYR:CD2	1:B:448:TYR:C	2.88	0.51
1:A:524:LEU:O	1:A:531:PRO:HA	2.11	0.51
1:B:455:LEU:HD23	1:B:587:TRP:HB3	1.93	0.50
1:B:504:ILE:O	1:B:508:GLN:HG2	2.11	0.50
1:B:496:PRO:HB2	1:B:602:SER:O	2.13	0.49
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.27	0.48
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.94	0.48
1:A:686:SER:HA	1:A:691:PHE:CG	2.49	0.47
1:B:597:ASP:OD1	1:B:603:ARG:NH1	2.38	0.47
1:B:525:GLN:HG3	1:B:529:ASN:O	2.13	0.47
1:B:572:LEU:HD21	1:B:574:ILE:HD11	1.96	0.47
1:B:608:GLU:HG3	1:B:618:MET:HE1	1.94	0.47
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.44	0.47
2:A:801:HEM:HBC2	2:A:801:HEM:CMC	2.44	0.47
1:B:482:TYR:O	1:B:498:ASN:ND2	2.40	0.46
1:A:335:ILE:HA	1:B:694:GLU:HG2	1.97	0.46
1:B:302:LYS:HA	1:B:312:LEU:O	2.14	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.31	0.46
2:B:801:HEM:HBC2	2:B:801:HEM:HMC1	1.97	0.46
1:B:367:SER:O	1:B:370:LYS:HE3	2.15	0.46
1:A:536:ILE:O	1:A:537:PRO:C	2.58	0.45
1:A:403:TYR:CD2	1:A:403:TYR:C	2.95	0.45
1:A:547:ARG:HD3	1:A:547:ARG:H	1.82	0.45
1:B:547:ARG:HD3	1:B:547:ARG:N	2.31	0.45
1:A:492:THR:HG21	1:A:496:PRO:HA	1.98	0.45
1:A:306:TRP:HB3	4:B:803:H45:S21	2.58	0.44
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:SER:OG	4:A:803:H45:H3	2.18	0.43
1:A:569:ASN:HD22	1:A:569:ASN:H	1.66	0.43
1:A:567:VAL:HG21	4:A:803:H45:C14	2.48	0.43
1:B:465:ARG:NH1	1:B:578:GLU:OE1	2.51	0.43
2:B:801:HEM:C4B	4:B:803:H45:S01	3.12	0.42
1:A:448:TYR:CD2	1:A:448:TYR:C	2.96	0.42
1:B:546:ILE:HG12	1:B:560:LYS:HA	2.00	0.42
1:A:684:SER:HB3	1:A:687:ILE:HG12	2.00	0.42
1:A:321:THR:HG22	7:A:906:HOH:O	2.18	0.42
1:B:419:ILE:HD12	1:B:661:HIS:HB2	2.02	0.42
1:A:605:ASN:CG	1:A:605:ASN:O	2.60	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.98	0.42
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.55	0.42
1:B:322:LEU:HB3	1:B:699:ARG:HH21	1.83	0.42
1:A:567:VAL:HG23	4:A:803:H45:H26	2.01	0.41
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.55	0.41
1:A:469:LYS:NZ	1:A:715:VAL:HG22	2.35	0.41
1:A:507:GLN:HE21	1:A:507:GLN:HB3	1.67	0.41
1:B:557:LEU:HD21	1:B:613:LYS:HZ3	1.86	0.41
1:B:631:VAL:HG22	1:B:683:MET:HE1	2.02	0.41
1:A:378:MET:HA	1:A:378:MET:HE2	2.02	0.41
1:A:299:ARG:O	1:A:317:HIS:HE1	2.04	0.41
1:A:601:ASN:HB3	1:B:307:GLU:CD	2.45	0.41
1:B:355:PHE:CE1	1:B:385:ASN:HA	2.56	0.40
1:B:532:GLU:HB2	1:B:534:PHE:CE1	2.56	0.40
1:A:517:PHE:HB2	1:A:560:LYS:HE3	2.04	0.40
1:A:571:LEU:HD21	1:A:578:GLU:HB3	2.02	0.40
1:A:328:GLU:CD	1:A:328:GLU:H	2.30	0.40
1:A:299:ARG:O	1:A:317:HIS:CE1	2.75	0.40
1:A:550:LYS:HE3	1:A:550:LYS:HB2	1.69	0.40
1:B:709:ASP:HA	1:B:710:PRO:HD3	1.99	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	403/422 (96%)	389 (96%)	14 (4%)	0	100	100
1	B	407/422 (96%)	393 (97%)	13 (3%)	1 (0%)	43	44
All	All	810/844 (96%)	782 (96%)	27 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	685	GLY

5.3.2 Protein sidechains ⓘ

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	363/377 (96%)	341 (94%)	22 (6%)	17	15
1	B	366/377 (97%)	352 (96%)	14 (4%)	29	32
All	All	729/754 (97%)	693 (95%)	36 (5%)	22	22

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	MET
1	A	337	LEU
1	A	350	THR
1	A	370	LYS
1	A	380	ARG
1	A	389	GLU
1	A	390	SER
1	A	419	ILE
1	A	423	LYS
1	A	469	LYS
1	A	487	GLN
1	A	489	ASP

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Mol	Chain	Res	Type
1	A	507	GLN
1	A	523	LEU
1	A	527	ASN
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	622	SER
1	A	645	LYS
1	A	653	SER
1	A	713	THR
1	B	307	GLU
1	B	328	GLU
1	B	337	LEU
1	B	350	THR
1	B	353	GLN
1	B	370	LYS
1	B	386	LYS
1	B	390	SER
1	B	392	SER
1	B	423	LYS
1	B	540	LEU
1	B	573	GLU
1	B	608	GLU
1	B	645	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	353	GLN
1	A	407	HIS
1	A	425	GLN
1	A	454	ASN
1	A	470	HIS
1	A	507	GLN
1	A	508	GLN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	A	712	ASN
1	A	714	HIS
1	B	364	GLN

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Mol	Chain	Res	Type
1	B	436	HIS
1	B	454	ASN
1	B	487	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN
1	B	707	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	-	17,18,18	0.80	0	14,26,26	2.49	8 (57%)
3	H4B	B	802	-	17,18,18	1.14	2 (11%)	14,26,26	2.09	7 (50%)
5	ACT	A	804	-	3,3,3	0.81	0	3,3,3	0.65	0
5	ACT	B	804	-	3,3,3	0.79	0	3,3,3	0.81	0
2	HEM	A	801	1	50,50,50	2.58	22 (44%)	67,82,82	3.14	31 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	H45	A	803	-	35,35,35	1.22	3 (8%)	41,46,46	1.51	7 (17%)
4	H45	B	803	-	35,35,35	1.29	3 (8%)	41,46,46	1.62	7 (17%)
2	HEM	B	801	1	50,50,50	2.42	21 (42%)	67,82,82	3.25	27 (40%)

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
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	4/14/54/54	-
4	H45	A	803	-	-	2/15/23/23	0/4/4/4
4	H45	B	803	-	-	1/15/23/23	0/4/4/4
2	HEM	B	801	1	-	2/14/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3C-C2C	5.93	1.49	1.37
2	A	801	HEM	FE-NB	5.32	2.11	1.94
2	B	801	HEM	C3C-C2C	5.17	1.47	1.37
2	A	801	HEM	FE-ND	5.16	2.10	1.94
2	B	801	HEM	C3D-C2D	5.02	1.47	1.36
2	A	801	HEM	CHD-C4C	4.72	1.47	1.38
2	B	801	HEM	FE-NB	4.63	2.09	1.94
2	B	801	HEM	CHD-C4C	4.62	1.47	1.38
2	A	801	HEM	C3D-C2D	4.49	1.46	1.36
2	A	801	HEM	CHC-C1C	4.20	1.46	1.38
2	B	801	HEM	FE-ND	4.20	2.07	1.94
2	B	801	HEM	C2A-C3A	4.00	1.49	1.38
2	A	801	HEM	C4D-ND	-3.94	1.33	1.40
2	B	801	HEM	C3B-C2B	3.85	1.45	1.37
2	B	801	HEM	CHC-C1C	3.80	1.45	1.38
2	A	801	HEM	C1C-NC	3.79	1.46	1.39
2	A	801	HEM	CHC-C4B	3.73	1.47	1.39
2	A	801	HEM	C4C-NC	3.68	1.46	1.39
2	A	801	HEM	C3B-C2B	3.55	1.44	1.37
2	B	801	HEM	C1B-NB	-3.46	1.34	1.40
2	B	801	HEM	CHC-C4B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	H45	C06-N07	-3.31	1.32	1.38
2	A	801	HEM	CHA-C4D	3.28	1.45	1.38
2	A	801	HEM	C1B-NB	-3.19	1.34	1.40
2	B	801	HEM	CHA-C1A	3.15	1.46	1.39
2	B	801	HEM	C4A-NA	3.12	1.45	1.39
2	A	801	HEM	C2A-C3A	2.99	1.46	1.38
2	B	801	HEM	CHA-C4D	2.98	1.44	1.38
2	A	801	HEM	CHD-C1D	2.90	1.45	1.39
2	B	801	HEM	C1C-NC	2.87	1.45	1.39
2	A	801	HEM	C4A-C3A	2.83	1.49	1.43
2	B	801	HEM	C4D-ND	-2.81	1.35	1.40
2	A	801	HEM	C4A-NA	2.80	1.44	1.39
2	B	801	HEM	C4C-NC	2.77	1.44	1.39
4	B	803	H45	C31-N27	-2.76	1.36	1.41
2	A	801	HEM	CHB-C4A	2.69	1.45	1.39
2	B	801	HEM	C1D-ND	-2.67	1.33	1.38
4	A	803	H45	C25-C26	2.64	1.50	1.45
2	B	801	HEM	C4D-C3D	2.51	1.49	1.45
2	A	801	HEM	CHB-C1B	2.49	1.43	1.38
2	B	801	HEM	C3B-C4B	2.45	1.49	1.44
2	B	801	HEM	CHB-C4A	2.44	1.44	1.39
2	A	801	HEM	C1B-C2B	2.32	1.49	1.44
4	A	803	H45	C06-N07	-2.32	1.34	1.38
3	B	802	H4B	C7-C6	2.25	1.54	1.52
2	A	801	HEM	C1A-NA	2.24	1.43	1.39
3	B	802	H4B	C2-N1	2.22	1.38	1.33
2	B	801	HEM	C1D-C2D	2.16	1.48	1.44
4	A	803	H45	C05-C06	2.14	1.49	1.45
2	A	801	HEM	C1D-C2D	2.14	1.48	1.44
4	B	803	H45	C26-N27	-2.09	1.34	1.38

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C2B-C1B	-11.17	98.03	106.41
2	B	801	HEM	C2B-C1B-NB	10.42	121.81	109.84
2	A	801	HEM	C3B-C2B-C1B	-9.00	99.65	106.41
2	B	801	HEM	C2D-C1D-ND	8.40	119.61	109.90
2	A	801	HEM	C3B-C4B-NB	8.39	115.50	109.47
2	A	801	HEM	C2B-C1B-NB	8.35	119.44	109.84
2	B	801	HEM	C3B-C4B-NB	7.73	115.02	109.47
2	A	801	HEM	C3D-C4D-ND	7.47	118.36	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C2D-C1D-ND	6.88	117.86	109.90
2	B	801	HEM	C3D-C4D-ND	6.66	117.48	110.17
2	A	801	HEM	C1D-C2D-C3D	-6.24	100.42	106.98
2	B	801	HEM	C1D-C2D-C3D	-6.20	100.45	106.98
3	A	802	H4B	C2-N1-C8A	5.64	123.31	113.36
2	B	801	HEM	C3C-C2C-C1C	-5.15	102.17	107.05
2	B	801	HEM	C1B-NB-C4B	-5.06	99.21	105.21
2	A	801	HEM	C3C-C2C-C1C	-5.04	102.28	107.05
2	A	801	HEM	CMD-C2D-C1D	4.78	132.50	125.03
4	B	803	H45	C06-C05-S01	-4.62	112.42	120.28
3	B	802	H4B	C2-N1-C8A	4.58	121.44	113.36
2	A	801	HEM	C4D-ND-C1D	-4.48	99.90	105.21
2	A	801	HEM	CHA-C4D-C3D	-4.29	117.31	125.23
2	A	801	HEM	C1B-NB-C4B	-4.26	100.16	105.21
2	B	801	HEM	C4D-ND-C1D	-4.23	100.20	105.21
2	B	801	HEM	CHD-C1D-C2D	-4.11	118.55	125.03
4	B	803	H45	C26-C25-S21	-4.09	113.33	120.28
2	A	801	HEM	C2A-C1A-NA	3.93	114.51	110.15
2	A	801	HEM	CHB-C1B-NB	-3.81	119.65	124.37
4	A	803	H45	C06-C05-S01	-3.74	113.92	120.28
2	A	801	HEM	CMB-C2B-C1B	3.71	130.84	125.03
4	B	803	H45	C24-C25-C26	3.62	135.81	128.65
2	B	801	HEM	CHB-C1B-C2B	-3.53	116.92	126.95
2	A	801	HEM	CMA-C3A-C4A	3.44	130.65	125.42
2	B	801	HEM	CHA-C4D-C3D	-3.38	118.99	125.23
4	A	803	H45	C03-C02-S01	-3.34	104.87	113.02
4	A	803	H45	C04-C05-C06	3.23	135.03	128.65
2	B	801	HEM	C4D-C3D-C2D	-3.19	102.25	106.89
2	B	801	HEM	CBA-CAA-C2A	-3.16	103.80	112.53
4	B	803	H45	C04-C05-C06	3.16	134.88	128.65
3	A	802	H4B	C4A-C4-N3	3.12	120.69	112.13
2	A	801	HEM	CBA-CAA-C2A	-3.10	103.97	112.53
3	A	802	H4B	C4-C4A-N5	3.04	124.55	116.27
2	A	801	HEM	CHD-C1D-C2D	-3.03	120.25	125.03
4	A	803	H45	C23-C22-S21	-2.96	105.79	113.02
2	B	801	HEM	CHB-C1B-NB	-2.94	120.74	124.37
2	A	801	HEM	CAD-CBD-CGD	-2.91	105.95	113.67
3	B	802	H4B	C4A-C4-N3	2.90	120.09	112.13
4	A	803	H45	C17-N18-C38	2.83	123.14	113.20
4	B	803	H45	C15-C17-N18	-2.82	103.91	112.79
2	B	801	HEM	C2C-C1C-NC	2.77	114.76	109.64
2	A	801	HEM	C2C-C1C-NC	2.71	114.64	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	H45	C24-C25-C26	2.70	133.98	128.65
2	A	801	HEM	CHC-C4B-C3B	-2.66	119.76	125.07
3	A	802	H4B	C2-N3-C4	-2.60	120.40	125.11
4	B	803	H45	C03-C02-S01	-2.59	106.69	113.02
2	A	801	HEM	CHD-C1D-ND	-2.54	121.69	124.42
2	A	801	HEM	C4A-NA-C1A	-2.52	101.71	105.82
2	B	801	HEM	CHD-C1D-ND	-2.52	121.71	124.42
3	B	802	H4B	O4-C4-C4A	-2.52	121.19	127.26
2	B	801	HEM	CHC-C4B-C3B	-2.52	120.04	125.07
2	B	801	HEM	CMC-C2C-C1C	2.50	129.14	124.73
2	B	801	HEM	C4C-NC-C1C	-2.49	101.76	105.82
2	B	801	HEM	CMD-C2D-C1D	2.49	128.93	125.03
2	A	801	HEM	CHC-C1C-C2C	-2.47	120.35	125.49
3	B	802	H4B	C4-C4A-N5	2.43	122.91	116.27
2	A	801	HEM	C4D-C3D-C2D	-2.42	103.37	106.89
3	A	802	H4B	N3-C2-N1	-2.42	118.90	123.32
3	B	802	H4B	O9-C9-C10	-2.35	104.67	109.14
2	A	801	HEM	C4C-NC-C1C	-2.33	102.02	105.82
2	B	801	HEM	O2D-CGD-CBD	2.33	121.35	114.00
3	A	802	H4B	O10-C10-C9	2.31	113.60	109.77
2	A	801	HEM	C4B-C3B-C2B	-2.30	105.17	107.28
2	B	801	HEM	CMB-C2B-C1B	2.25	128.55	125.03
2	B	801	HEM	C4A-C3A-C2A	-2.25	104.24	106.82
2	B	801	HEM	O1D-CGD-CBD	-2.23	116.02	123.09
3	B	802	H4B	N3-C2-N1	-2.22	119.26	123.32
3	A	802	H4B	N2-C2-N3	2.22	121.44	116.76
4	B	803	H45	C23-C22-S21	-2.21	107.62	113.02
2	A	801	HEM	C3A-C4A-NA	2.19	113.66	110.14
3	B	802	H4B	C2-N3-C4	-2.19	121.14	125.11
2	B	801	HEM	CHC-C1C-NC	-2.17	122.09	124.45
3	A	802	H4B	O4-C4-N3	-2.13	116.10	120.11
2	A	801	HEM	CHB-C1B-C2B	-2.13	120.91	126.95
2	A	801	HEM	O1D-CGD-CBD	-2.08	116.49	123.09
4	A	803	H45	C22-S21-C25	2.07	96.05	92.33
2	B	801	HEM	CMB-C2B-C3B	2.06	133.42	128.43
2	A	801	HEM	C4C-C3C-C2C	2.06	108.60	106.81
2	A	801	HEM	C1C-CHC-C4B	-2.04	121.69	126.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

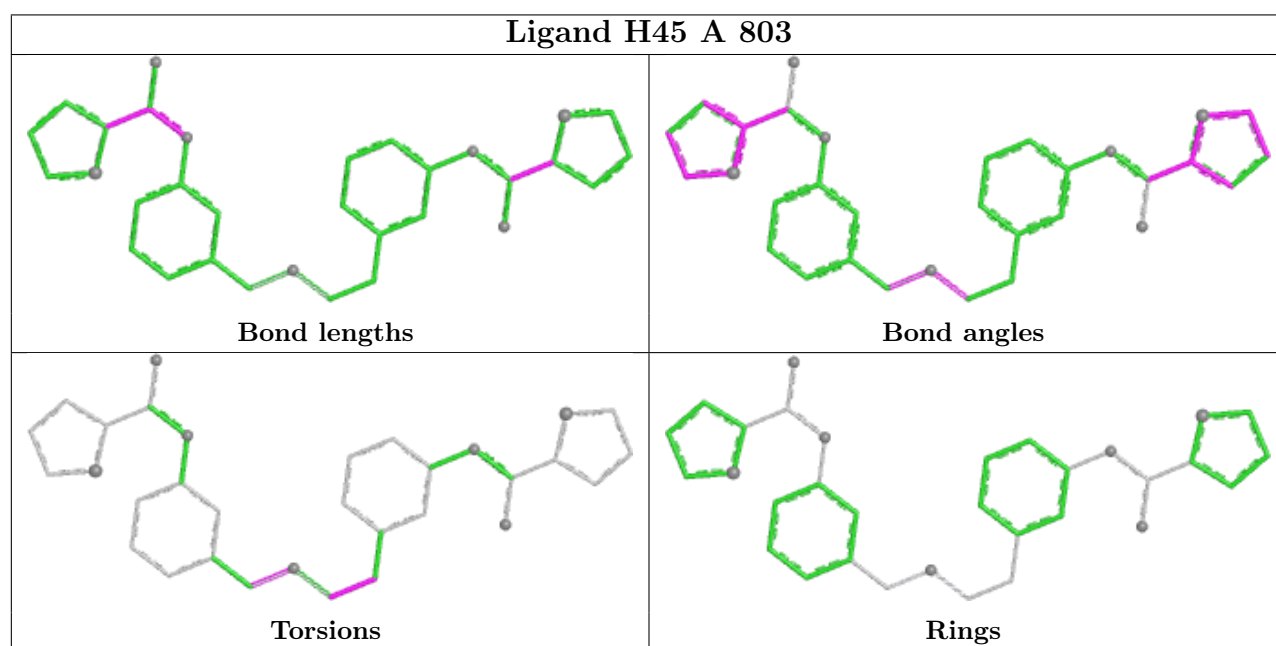
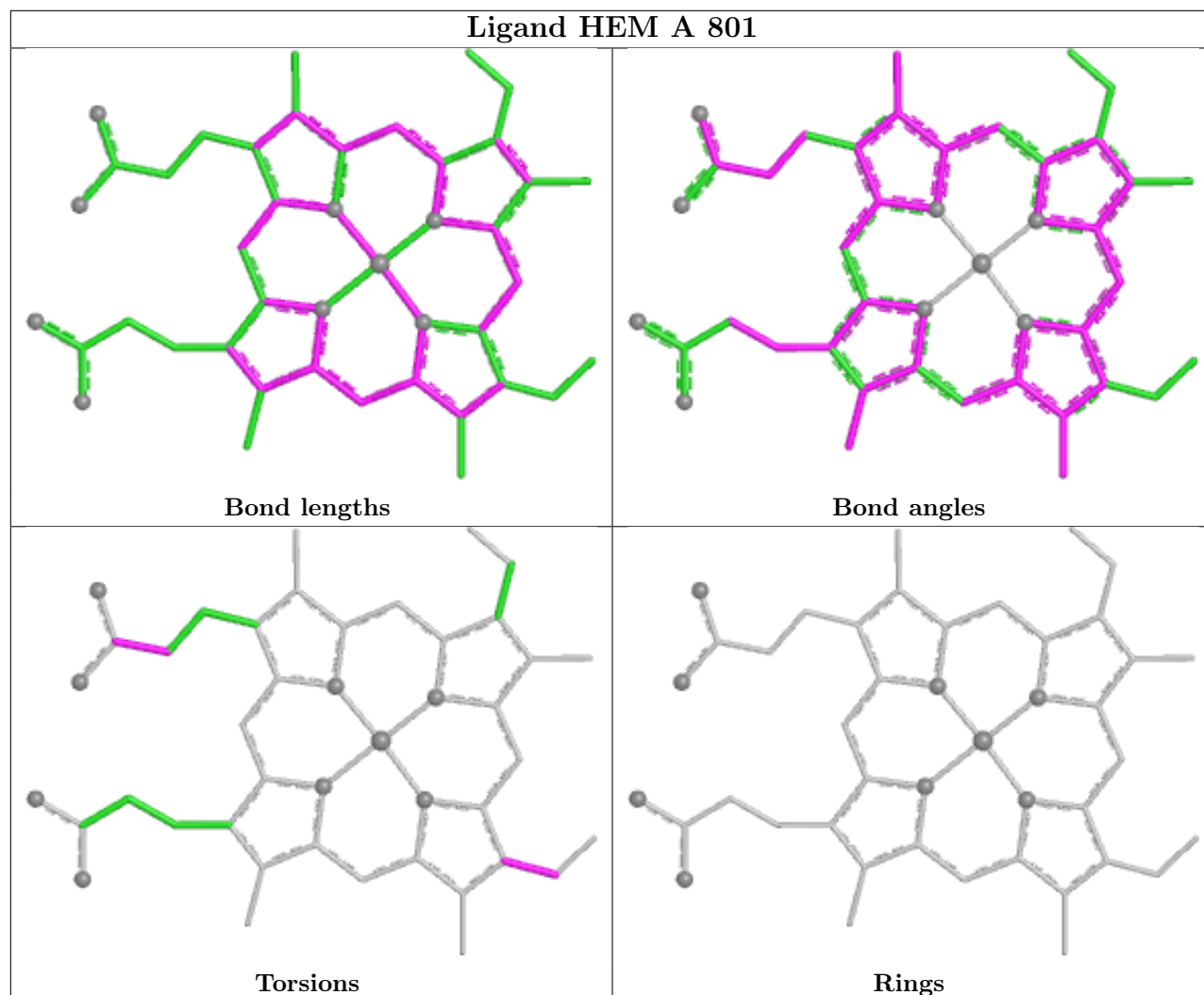
Mol	Chain	Res	Type	Atoms
4	A	803	H45	C35-C37-C38-N18
4	A	803	H45	C15-C17-N18-C38
4	B	803	H45	C35-C37-C38-N18
2	A	801	HEM	C2B-C3B-CAB-CBB
2	B	801	HEM	C2B-C3B-CAB-CBB
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
2	A	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

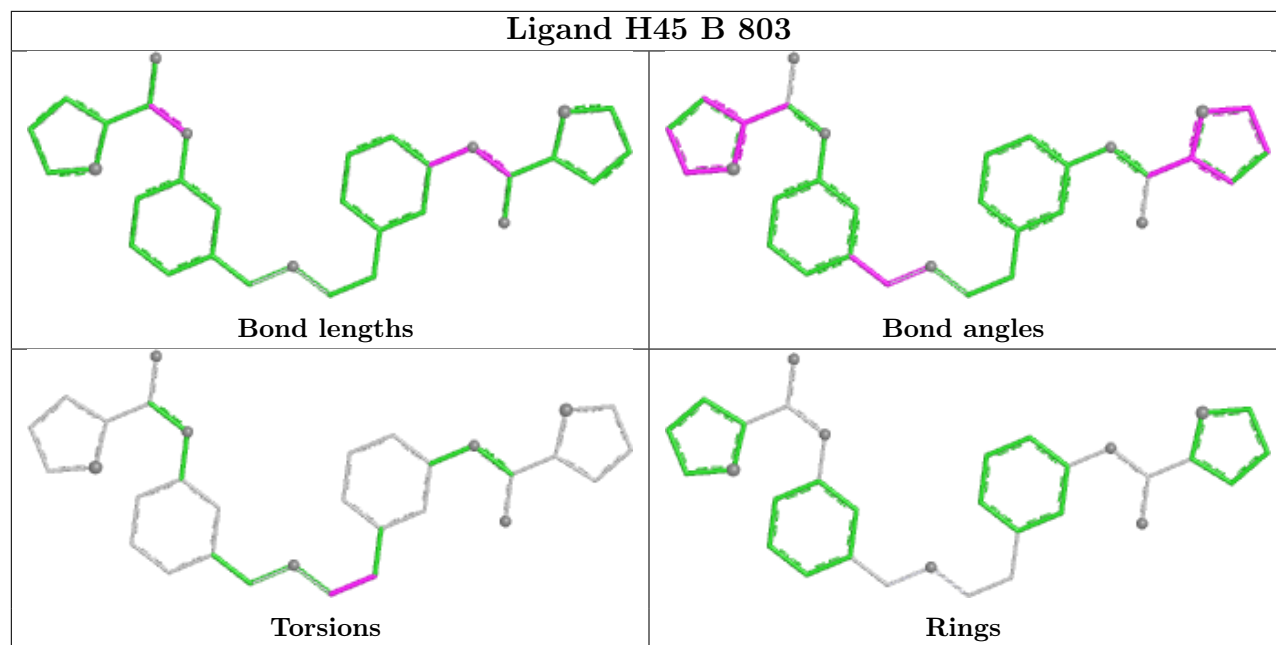
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	2	0
4	A	803	H45	3	0
4	B	803	H45	2	0
2	B	801	HEM	5	0

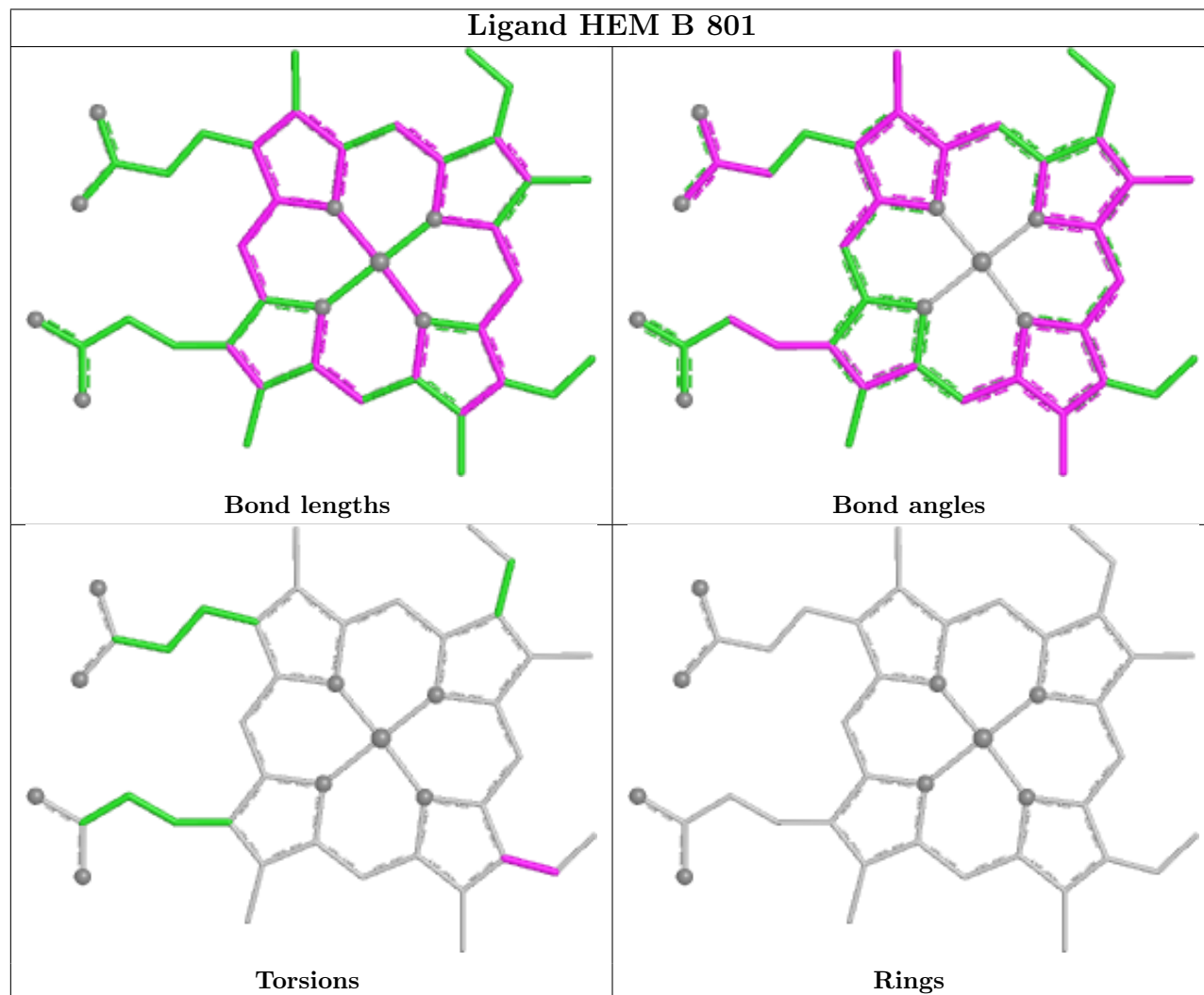
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 H45 B 803



Ligand HEM B 801



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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	407/422 (96%)	0.76	19 (4%) 36 38	34, 63, 107, 145	0
1	B	411/422 (97%)	0.52	11 (2%) 56 59	32, 51, 82, 103	0
All	All	818/844 (96%)	0.64	30 (3%) 45 47	32, 56, 98, 145	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	4.3
1	A	300	PHE	4.2
1	B	322	LEU	3.8
1	B	300	PHE	3.6
1	A	322	LEU	3.4
1	A	350	THR	3.4
1	A	557	LEU	3.1
1	A	355	PHE	2.9
1	A	373	GLY	2.9
1	B	348	VAL	2.8
1	B	350	THR	2.8
1	B	338	PRO	2.7
1	A	716	TRP	2.7
1	A	488	PRO	2.6
1	B	594	GLY	2.5
1	A	307	GLU	2.5
1	B	355	PHE	2.5
1	B	535	GLN	2.4
1	A	559	LEU	2.3
1	A	321	THR	2.3
1	A	494	GLY	2.3
1	A	435	ALA	2.2
1	A	706	TYR	2.2
1	B	356	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	2.1
1	A	490	GLY	2.1
1	B	668	CYS	2.1
1	A	493	LEU	2.1
1	B	337	LEU	2.1
1	A	372	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

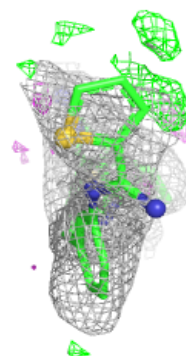
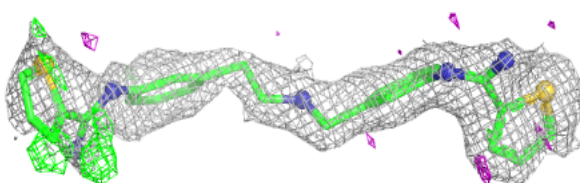
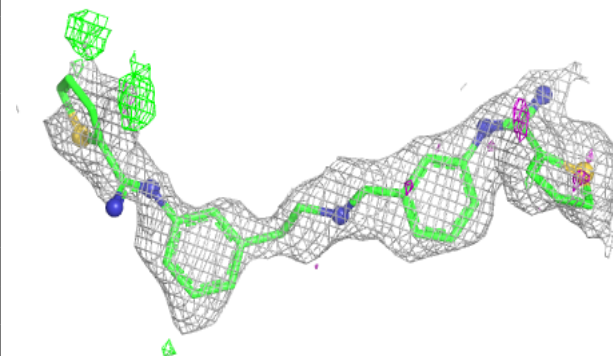
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	H45	B	803	32/32	0.85	0.14	34,50,97,101	0
4	H45	A	803	32/32	0.89	0.12	39,52,91,93	0
5	ACT	A	804	4/4	0.90	0.17	72,73,75,76	0
5	ACT	B	804	4/4	0.90	0.15	65,68,69,74	0
3	H4B	A	802	17/17	0.93	0.08	37,40,46,46	0
3	H4B	B	802	17/17	0.93	0.09	37,39,48,48	0
2	HEM	B	801	43/43	0.96	0.09	32,35,45,47	0
2	HEM	A	801	43/43	0.97	0.08	38,42,47,54	0
6	ZN	A	805	1/1	1.00	0.02	50,50,50,50	0

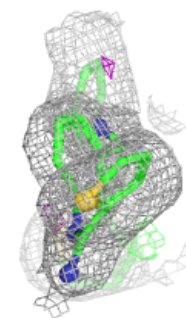
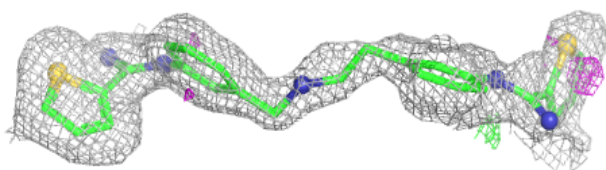
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H45 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)

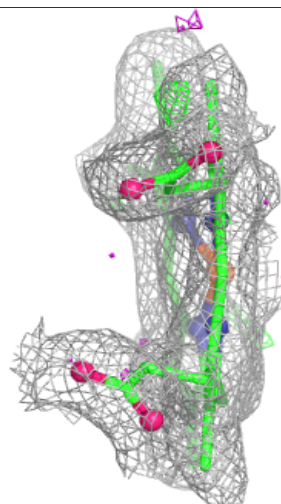
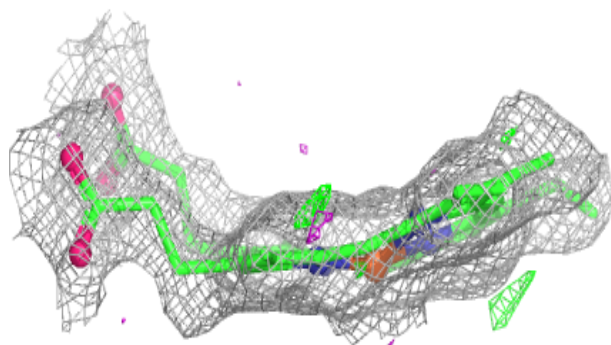
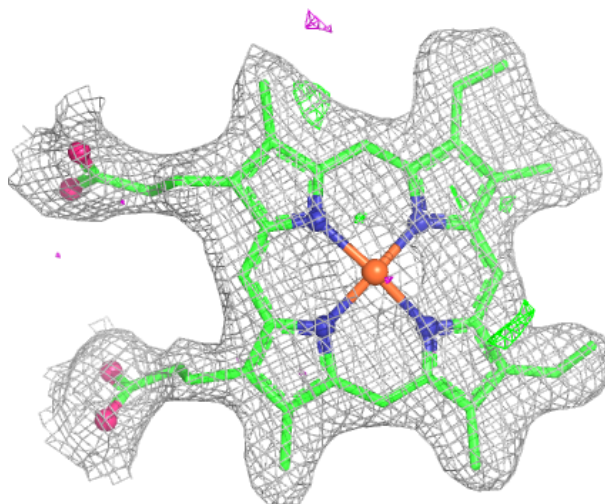
**Electron density around H45 A 803:**

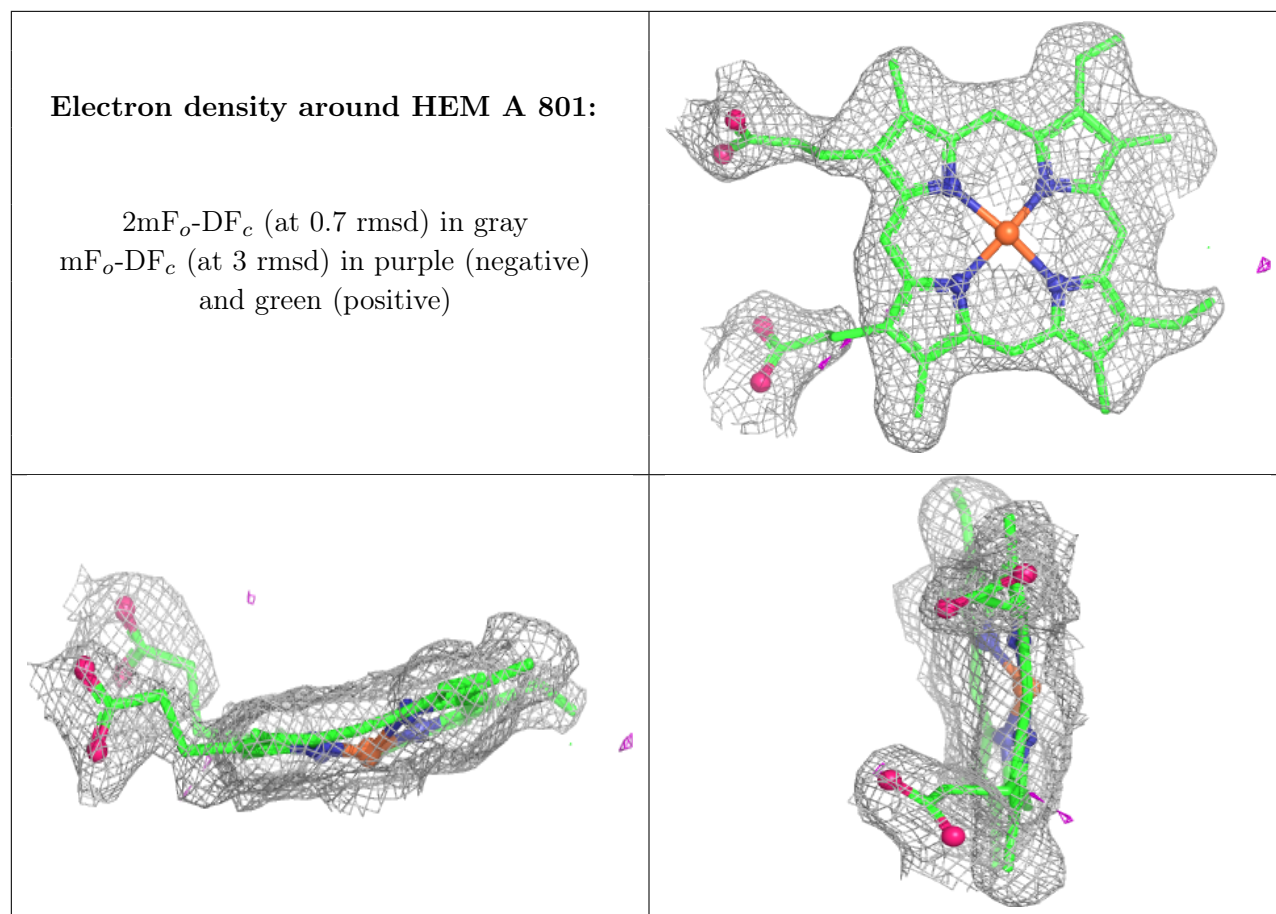
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.