



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:52 AM UTC

PDB ID : 4KCS / pdb_00004kcs
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with N-(3-((ethyl(3-fluorophenethyl)amino)methyl)phenyl)thiophene-2-carboximidamide
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2013-04-24
Resolution : 2.05 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

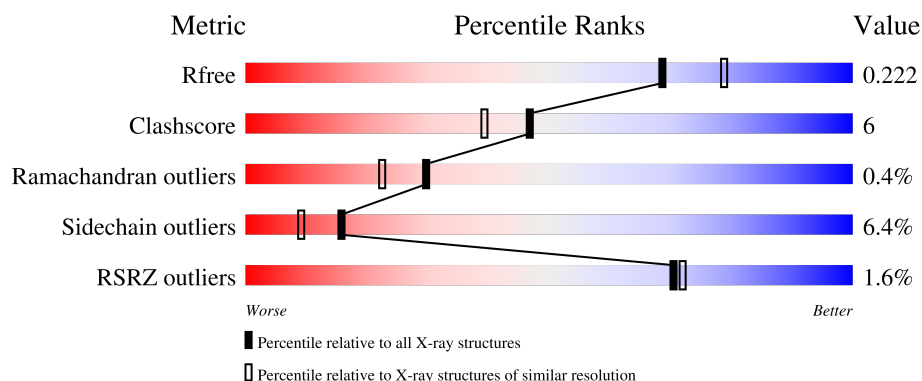
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

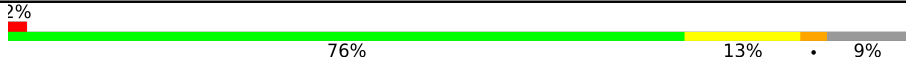
The reported resolution of this entry is 2.05 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	443	 2% 76% 13% 9%
1	B	443	 % 75% 14% 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6993 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.

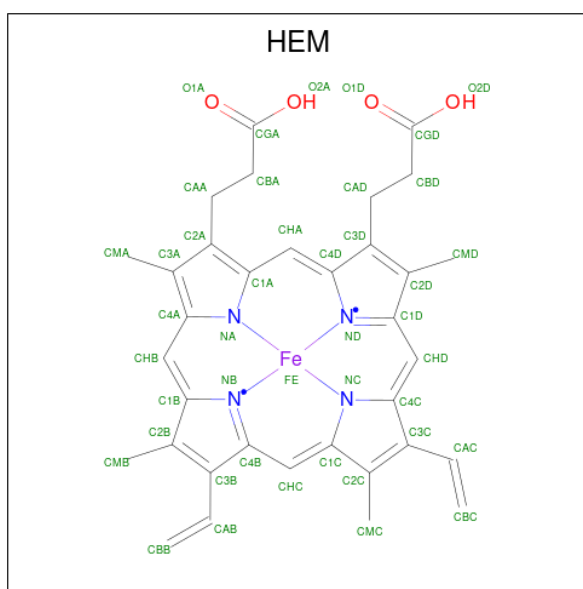
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473

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



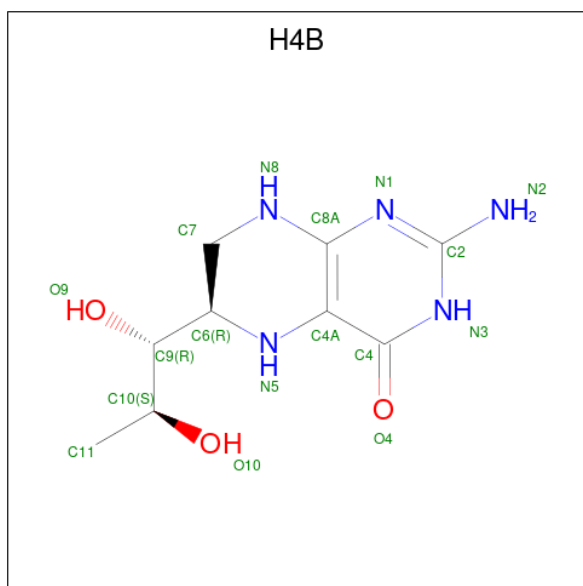
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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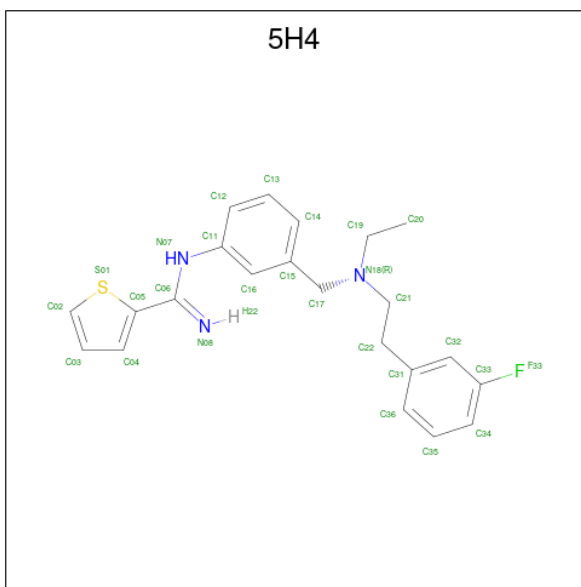
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



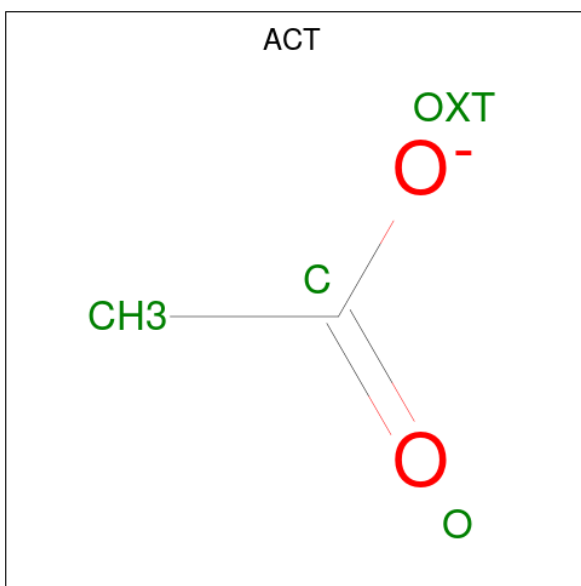
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[3-(ethyl[2-(3-fluorophenyl)ethyl]amino)methyl]phenyl]thiophene-2-carboximidamide (CCD ID: 5H4) (formula: $C_{22}H_{24}FN_3S$).



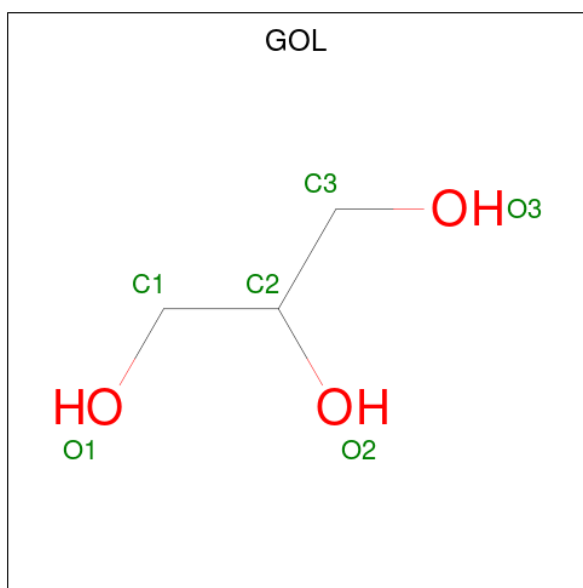
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	S	0	0
			27	22	1	3	1		
4	B	1	Total	C	F	N	S	0	0
			27	22	1	3	1		

- 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

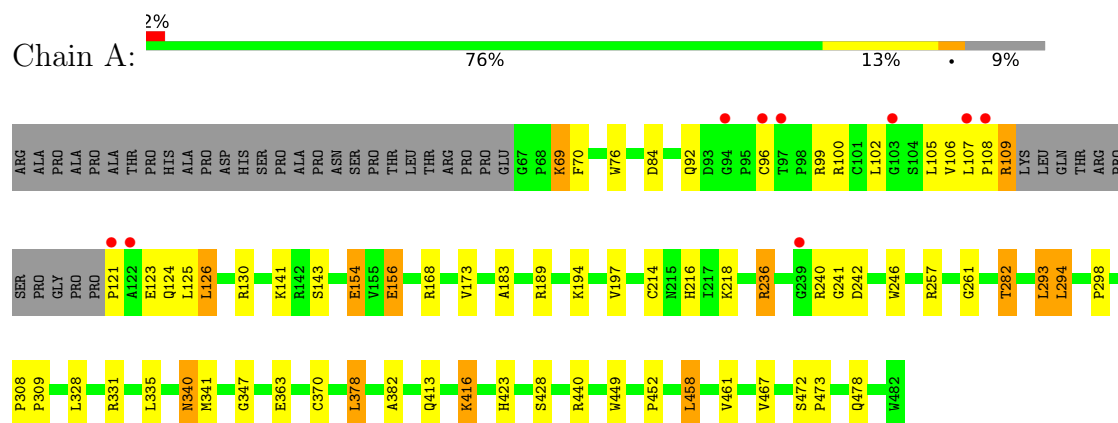
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	169	Total	O	0	0
			169	169		
8	B	177	Total	O	0	0
			177	177		

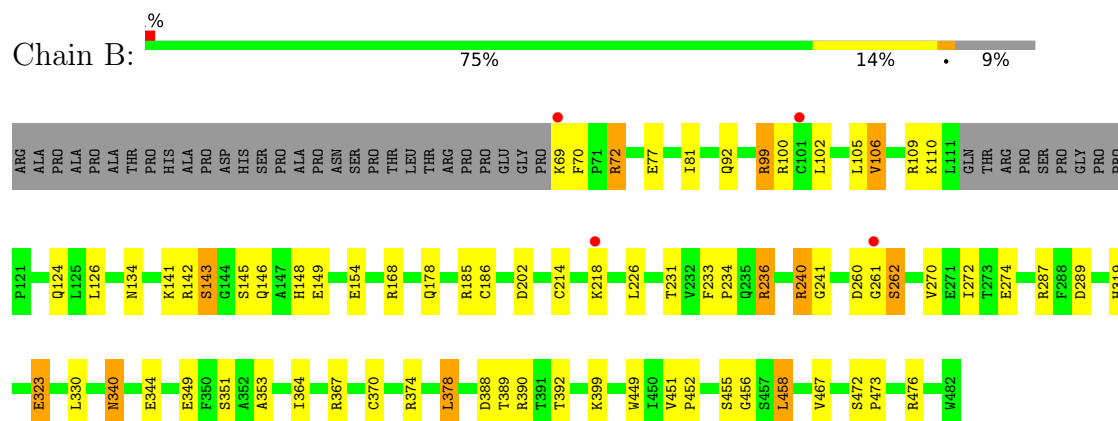
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.73Å 106.41Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 2.05 47.02 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.02-2.05) 99.1 (47.02-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.213 0.177 , 0.222	Depositor DCC
R_{free} test set	3041 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.1	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	0.97	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: CAS, GOL, 5H4, ACT, ZN, H4B, HEM

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	1.33	12/3303 (0.4%)	1.19	13/4497 (0.3%)
1	B	1.33	12/3308 (0.4%)	1.21	7/4502 (0.2%)
All	All	1.33	24/6611 (0.4%)	1.20	20/8999 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	LEU	C-O	-7.31	1.16	1.24
1	B	451	VAL	CA-C	7.07	1.60	1.53
1	A	428	SER	CA-C	6.94	1.62	1.52
1	B	77	GLU	CA-C	6.19	1.60	1.52
1	A	173	VAL	N-CA	6.16	1.53	1.46
1	B	374	ARG	CA-C	5.96	1.56	1.53
1	A	293	LEU	CA-C	-5.81	1.45	1.52
1	B	344	GLU	N-CA	5.78	1.53	1.46
1	A	197	VAL	C-O	-5.70	1.18	1.24
1	A	452	PRO	CA-CB	5.63	1.61	1.54
1	A	461	VAL	N-CA	5.59	1.53	1.46
1	B	451	VAL	C-O	-5.55	1.17	1.24
1	A	382	ALA	C-O	5.36	1.30	1.24
1	B	149	GLU	CA-CB	5.29	1.61	1.53
1	B	456	GLY	N-CA	5.29	1.53	1.45
1	A	96	CYS	N-CA	5.25	1.52	1.45
1	A	467	VAL	N-CA	5.22	1.52	1.46
1	B	364	ILE	N-CA	5.21	1.52	1.46
1	B	367	ARG	C-O	-5.16	1.18	1.24
1	B	319	HIS	C-O	-5.15	1.17	1.24
1	B	452	PRO	C-O	-5.12	1.18	1.24
1	A	440	ARG	C-O	-5.08	1.17	1.24
1	A	183	ALA	C-O	-5.07	1.18	1.24
1	B	289	ASP	CA-C	5.06	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	GLN	CA-C-N	-9.53	110.97	120.31
1	A	478	GLN	C-N-CA	-9.53	110.97	120.31
1	A	107	LEU	CA-C-N	-6.87	110.98	120.25
1	A	107	LEU	C-N-CA	-6.87	110.98	120.25
1	A	106	VAL	N-CA-C	6.85	116.97	110.53
1	B	319	HIS	CA-C-N	-6.84	112.58	119.56
1	B	319	HIS	C-N-CA	-6.84	112.58	119.56
1	B	240	ARG	N-CA-C	6.74	118.79	108.42
1	B	70	PHE	CA-C-N	-6.72	113.04	119.76
1	B	70	PHE	C-N-CA	-6.72	113.04	119.76
1	B	106	VAL	N-CA-C	6.09	116.87	110.72
1	A	189	ARG	N-CA-C	5.76	119.79	112.87
1	A	154	GLU	CB-CA-C	-5.67	101.38	110.79
1	B	467	VAL	N-CA-C	-5.65	100.20	108.11
1	A	141	LYS	N-CA-C	5.64	119.46	112.24
1	A	100	ARG	N-CA-C	5.46	117.39	108.55
1	A	341	MET	N-CA-C	5.45	118.58	110.52
1	A	458	LEU	N-CA-C	-5.32	106.75	113.18
1	A	363	GLU	N-CA-C	-5.30	105.58	111.36
1	A	347	GLY	N-CA-C	-5.09	109.02	115.08

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	3223	0	3127	32	0
1	B	3229	0	3141	36	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	27	0	23	2	0
4	B	27	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	169	0	0	3	0
8	B	177	0	0	5	0
All	All	6993	0	6426	74	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 (74) 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:108:PRO:HD3	8:A:735:HOH:O	1.67	0.94
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.51	0.88
1:A:126:LEU:HD23	1:A:130:ARG:NH2	1.95	0.82
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.65	0.76
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.72	0.72
1:B:214:CYS:SG	8:B:741:HOH:O	2.49	0.70
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.23	0.68
1:B:287:ARG:HD3	8:B:683:HOH:O	1.95	0.67
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.28	0.64
1:A:126:LEU:HD21	1:A:156:GLU:HB3	1.82	0.61
1:B:186:CYS:HB2	2:B:501:HEM:ND	2.18	0.58
1:B:240:ARG:HD2	1:B:241:GLY:O	2.04	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.31	0.58
1:A:121:PRO:O	1:A:124:GLN:HB3	2.05	0.57
1:A:449:TRP:HA	3:A:502:H4B:N1	2.19	0.57
1:B:323:GLU:H	1:B:323:GLU:CD	2.13	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.53	0.57
1:B:472:SER:HA	1:B:473:PRO:C	2.30	0.57
1:B:141:LYS:HB2	1:B:142:ARG:NH1	2.19	0.56
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.88	0.55
1:A:240:ARG:HD2	1:A:241:GLY:O	2.06	0.55
1:B:146:GLN:OE1	1:B:146:GLN:HA	2.07	0.55
1:B:186:CYS:HB2	2:B:501:HEM:C4D	2.41	0.55
1:A:109:ARG:CZ	1:B:72:ARG:HD3	2.39	0.53
1:A:214:CYS:O	1:A:218:LYS:HG3	2.07	0.53
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HB2	8:A:648:HOH:O	2.07	0.53
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.52
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.92	0.52
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.50	0.51
1:A:70:PHE:HB3	1:A:84:ASP:O	2.11	0.50
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.94	0.50
1:A:108:PRO:CD	8:A:735:HOH:O	2.42	0.50
1:B:340:ASN:HD22	1:B:340:ASN:H	1.60	0.49
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.94	0.49
1:A:282:THR:O	1:A:282:THR:HG22	2.13	0.49
1:B:145:SER:O	1:B:146:GLN:C	2.57	0.47
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.94	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.53	0.47
1:B:260:ASP:O	1:B:260:ASP:OD2	2.31	0.47
1:A:69:LYS:HA	1:A:69:LYS:HE2	1.97	0.47
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.15	0.47
4:A:503:5H4:C05	4:A:503:5H4:C12	2.92	0.47
1:B:455:SER:O	1:B:458:LEU:HB2	2.15	0.47
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.96	0.46
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.49	0.46
1:B:449:TRP:HA	3:B:502:H4B:N1	2.31	0.45
1:A:121:PRO:O	1:A:124:GLN:N	2.49	0.45
1:B:185:ARG:HG2	1:B:449:TRP:CG	2.51	0.45
1:B:399:LYS:NZ	8:B:743:HOH:O	2.51	0.44
1:B:260:ASP:O	1:B:262:SER:N	2.44	0.44
1:A:340:ASN:H	1:A:340:ASN:ND2	2.15	0.44
4:A:503:5H4:H11	4:A:503:5H4:H5	1.68	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.43
1:B:260:ASP:O	1:B:260:ASP:CG	2.58	0.43
1:A:340:ASN:HD22	1:A:340:ASN:N	2.13	0.43
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.53	0.43
1:B:388:ASP:CG	1:B:390:ARG:HH21	2.27	0.43
1:A:216:HIS:CD2	1:A:216:HIS:C	2.96	0.43
1:B:476:ARG:NH1	8:B:673:HOH:O	2.52	0.43
1:A:308:PRO:O	1:A:309:PRO:C	2.60	0.43
1:A:126:LEU:O	1:A:130:ARG:HG3	2.19	0.42
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.51	0.42
4:B:503:5H4:C12	4:B:503:5H4:C05	2.98	0.42
1:A:257:ARG:NH1	1:A:261:GLY:O	2.45	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.41
4:B:503:5H4:H5	4:B:503:5H4:H11	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLN:O	1:A:416:LYS:HE3	2.20	0.41
1:B:270:VAL:O	1:B:274:GLU:HG3	2.19	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.02	0.41
1:B:154:GLU:OE1	1:B:168:ARG:NH2	2.53	0.41
1:B:126:LEU:HD12	1:B:126:LEU:HA	1.85	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:B:272:ILE:HG22	8:B:666:HOH:O	2.21	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	400/443 (90%)	391 (98%)	9 (2%)	0	100	100
1	B	400/443 (90%)	376 (94%)	21 (5%)	3 (1%)	16	9
All	All	800/886 (90%)	767 (96%)	30 (4%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	SER
1	B	143	SER
1	B	261	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	343/375 (92%)	321 (94%)	22 (6%)	16	9
1	B	344/375 (92%)	322 (94%)	22 (6%)	16	9
All	All	687/750 (92%)	643 (94%)	44 (6%)	16	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	92	GLN
1	A	99	ARG
1	A	102	LEU
1	A	105	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	126	LEU
1	A	143	SER
1	A	156	GLU
1	A	194	LYS
1	A	236	ARG
1	A	282	THR
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	378	LEU
1	A	416	LYS
1	A	458	LEU
1	B	69	LYS
1	B	72	ARG
1	B	81	ILE
1	B	92	GLN
1	B	99	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	124	GLN
1	B	143	SER
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	202	ASP
1	B	218	LYS
1	B	226	LEU
1	B	236	ARG
1	B	323	GLU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	146	GLN
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	410	HIS
1	A	413	GLN
1	A	435	ASN
1	A	468	ASN
1	B	92	GLN
1	B	128	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	478	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CAS	A	384	1	5,8,9	0.93	0	1,9,11	0.80	0
1	CAS	B	384	1	5,8,9	1.08	0	1,9,11	0.78	0

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
1	CAS	A	384	1	-	0/0/7/9	-
1	CAS	B	384	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	504	-	3,3,3	0.71	0	3,3,3	1.00	0
6	GOL	B	505	-	5,5,5	0.36	0	5,5,5	1.19	0
3	H4B	B	502	-	17,18,18	1.00	1 (5%)	14,26,26	2.68	7 (50%)
3	H4B	A	502	-	17,18,18	1.02	1 (5%)	14,26,26	2.51	9 (64%)
2	HEM	A	501	1	50,50,50	1.70	9 (18%)	67,82,82	1.72	16 (23%)
4	5H4	B	503	-	29,29,29	1.31	4 (13%)	36,38,38	1.38	4 (11%)
2	HEM	B	501	1	50,50,50	1.46	11 (22%)	67,82,82	1.88	20 (29%)
5	ACT	A	504	-	3,3,3	1.50	0	3,3,3	0.74	0
6	GOL	A	505	-	5,5,5	0.52	0	5,5,5	1.30	0
4	5H4	A	503	-	29,29,29	1.16	2 (6%)	36,38,38	1.28	4 (11%)

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	505	-	-	0/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
3	H4B	A	502	-	-	1/8/17/17	0/2/2/2
2	HEM	A	501	1	-	0/14/54/54	-
4	5H4	B	503	-	-	2/15/19/19	0/3/3/3
2	HEM	B	501	1	-	1/14/54/54	-
6	GOL	A	505	-	-	0/4/4/4	-
4	5H4	A	503	-	-	3/15/19/19	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1B-NB	-5.67	1.30	1.40
2	A	501	HEM	FE-NB	4.97	2.10	1.94
2	A	501	HEM	FE-NC	3.62	2.07	1.95
4	B	503	5H4	C06-N07	-3.43	1.32	1.38
4	B	503	5H4	C11-N07	-3.16	1.35	1.41
2	B	501	HEM	FE-NC	3.08	2.05	1.95
2	A	501	HEM	C4B-NB	-2.96	1.33	1.38
2	A	501	HEM	C1D-C2D	2.86	1.50	1.44
4	A	503	5H4	C06-N07	-2.82	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1C-NC	-2.76	1.34	1.39
2	B	501	HEM	C2A-C3A	-2.74	1.31	1.38
2	B	501	HEM	FE-ND	-2.72	1.86	1.94
2	B	501	HEM	C4C-NC	-2.70	1.34	1.39
2	B	501	HEM	C1B-NB	-2.64	1.35	1.40
2	A	501	HEM	C3B-C4B	2.54	1.49	1.44
4	A	503	5H4	C05-C06	2.53	1.50	1.45
2	A	501	HEM	C1D-ND	-2.51	1.33	1.38
2	B	501	HEM	C4B-NB	-2.34	1.34	1.38
2	B	501	HEM	C1B-C2B	-2.33	1.39	1.44
3	B	502	H4B	C4-N3	-2.32	1.34	1.38
2	B	501	HEM	C3C-C4C	-2.28	1.42	1.46
3	A	502	H4B	O4-C4	2.28	1.27	1.23
2	A	501	HEM	C3C-C2C	2.17	1.41	1.37
2	A	501	HEM	C4D-ND	-2.14	1.36	1.40
4	B	503	5H4	C32-C33	2.13	1.41	1.37
4	B	503	5H4	C16-C15	-2.06	1.35	1.39
2	B	501	HEM	C1C-C2C	-2.02	1.41	1.45
2	B	501	HEM	CAD-C3D	2.00	1.56	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C11-C10-C9	5.36	118.68	112.11
3	B	502	H4B	O4-C4-C4A	-5.13	114.89	127.26
2	A	501	HEM	C1B-NB-C4B	4.36	110.37	105.21
3	B	502	H4B	C2-N3-C4	-4.26	117.39	125.11
2	B	501	HEM	CHC-C4B-NB	3.97	128.70	124.42
3	B	502	H4B	C2-N1-C8A	3.95	120.33	113.36
2	B	501	HEM	C1A-CHA-C4D	-3.90	117.08	126.25
4	B	503	5H4	C15-C17-N18	3.89	121.10	113.15
2	B	501	HEM	CHD-C1D-C2D	-3.75	119.11	125.03
2	A	501	HEM	CHC-C4B-NB	3.71	128.41	124.42
2	A	501	HEM	CHD-C1D-ND	3.68	128.38	124.42
2	A	501	HEM	C1A-CHA-C4D	-3.67	117.62	126.25
2	B	501	HEM	CHA-C4D-C3D	-3.64	118.52	125.23
3	B	502	H4B	C4A-C4-N3	3.49	121.73	112.13
2	A	501	HEM	CHA-C4D-C3D	-3.47	118.83	125.23
4	A	503	5H4	C15-C17-N18	3.46	120.23	113.15
3	A	502	H4B	O4-C4-C4A	-3.41	119.03	127.26
2	B	501	HEM	CHA-C4D-ND	3.41	128.58	124.37
2	A	501	HEM	CHD-C1D-C2D	-3.33	119.76	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C4B-NB	-3.29	107.11	109.47
2	B	501	HEM	CHD-C1D-ND	3.28	127.96	124.42
2	B	501	HEM	CAD-C3D-C4D	3.25	130.37	124.70
2	B	501	HEM	CMD-C2D-C1D	3.21	130.04	125.03
3	B	502	H4B	N2-C2-N3	3.19	123.50	116.76
2	B	501	HEM	CMB-C2B-C1B	3.06	129.81	125.03
2	A	501	HEM	C3D-C4D-ND	2.95	113.40	110.17
4	A	503	5H4	C34-C33-C32	-2.81	119.52	123.23
2	B	501	HEM	C4D-ND-C1D	-2.74	101.97	105.21
3	A	502	H4B	C2-N3-C4	-2.72	120.17	125.11
3	A	502	H4B	N2-C2-N3	2.70	122.47	116.76
2	B	501	HEM	CBA-CAA-C2A	-2.68	105.13	112.53
2	B	501	HEM	C4C-CHD-C1D	-2.63	120.43	126.02
4	B	503	5H4	C05-C06-N07	2.59	121.25	116.12
2	A	501	HEM	CHB-C1B-NB	2.59	127.56	124.37
2	A	501	HEM	CHA-C4D-ND	2.57	127.55	124.37
4	B	503	5H4	C04-C05-S01	2.57	117.22	111.23
3	B	502	H4B	N2-C2-N1	-2.51	114.78	119.67
3	A	502	H4B	O9-C9-C10	2.50	113.91	109.14
2	B	501	HEM	C2D-C1D-ND	2.50	112.79	109.90
4	B	503	5H4	C02-S01-C05	-2.49	87.86	92.33
3	A	502	H4B	C4A-C4-N3	2.49	118.97	112.13
2	A	501	HEM	O2A-CGA-O1A	-2.48	116.96	123.33
2	B	501	HEM	C3D-C4D-ND	2.48	112.89	110.17
3	B	502	H4B	O9-C9-C6	2.42	115.08	109.28
2	B	501	HEM	O2A-CGA-CBA	2.39	121.54	114.00
3	A	502	H4B	C2-N1-C8A	2.38	117.55	113.36
2	B	501	HEM	CMB-C2B-C3B	-2.33	122.80	128.43
2	B	501	HEM	CHD-C4C-NC	2.29	126.95	124.45
4	A	503	5H4	C05-C06-N07	2.28	120.65	116.12
2	B	501	HEM	C3B-C4B-NB	-2.25	107.85	109.47
2	B	501	HEM	CBD-CAD-C3D	2.23	118.71	112.53
3	A	502	H4B	N2-C2-N1	-2.20	115.37	119.67
2	A	501	HEM	CAA-CBA-CGA	2.20	119.50	113.67
4	A	503	5H4	C12-C11-C16	-2.20	117.00	119.66
2	A	501	HEM	CMA-C3A-C4A	2.19	128.75	125.42
3	A	502	H4B	C4-C4A-N5	2.18	122.20	116.27
2	B	501	HEM	CAB-C3B-C2B	-2.13	121.50	128.43
2	A	501	HEM	CMB-C2B-C1B	2.11	128.32	125.03
2	A	501	HEM	C4B-C3B-C2B	-2.08	105.36	107.28
2	A	501	HEM	CAD-C3D-C4D	2.08	128.32	124.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

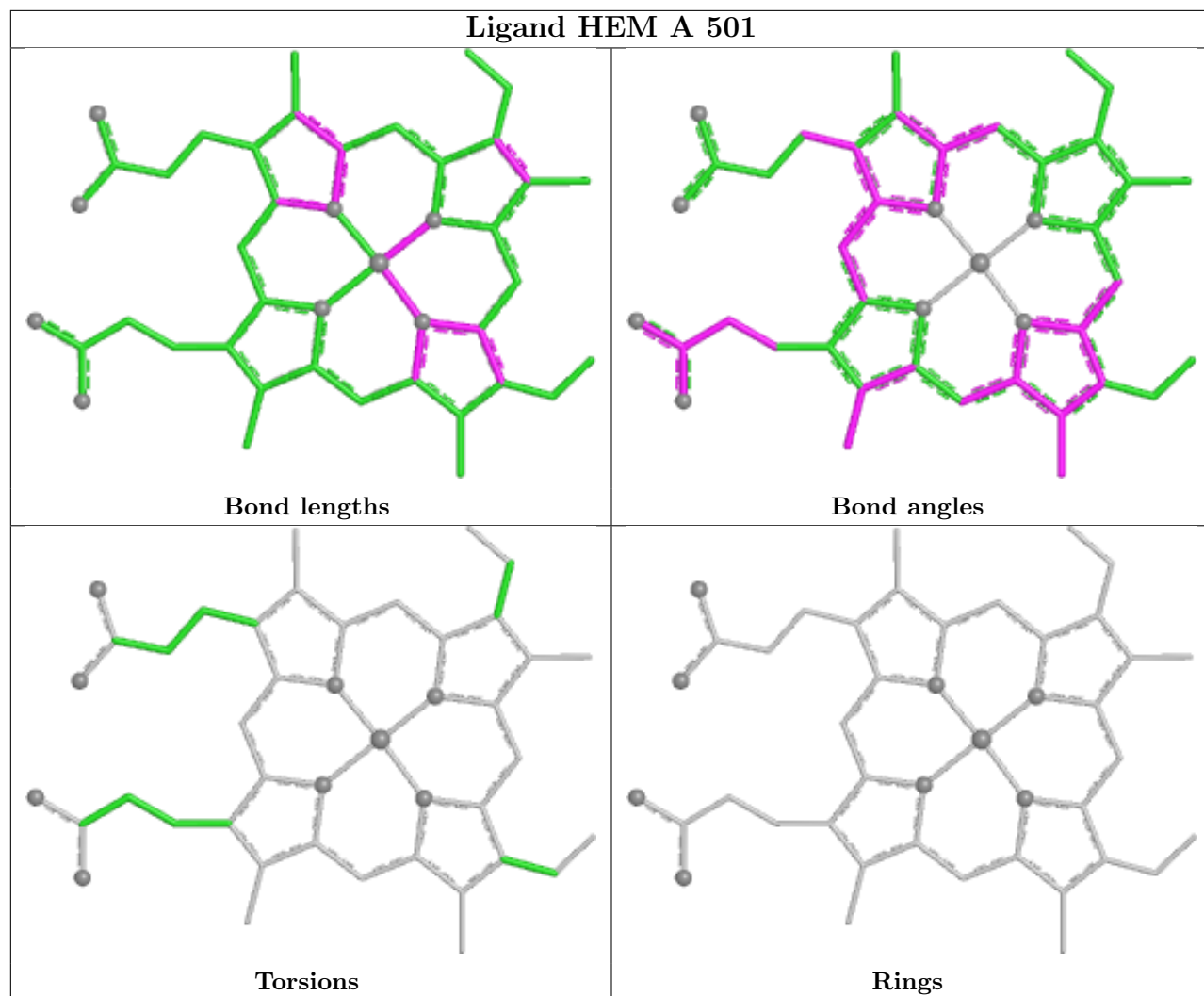
Mol	Chain	Res	Type	Atoms
4	A	503	5H4	N18-C21-C22-C31
4	B	503	5H4	N18-C21-C22-C31
4	B	503	5H4	C15-C17-N18-C21
2	B	501	HEM	C4B-C3B-CAB-CBB
4	A	503	5H4	C20-C19-N18-C17
4	A	503	5H4	C20-C19-N18-C21
3	A	502	H4B	C7-C6-C9-O9

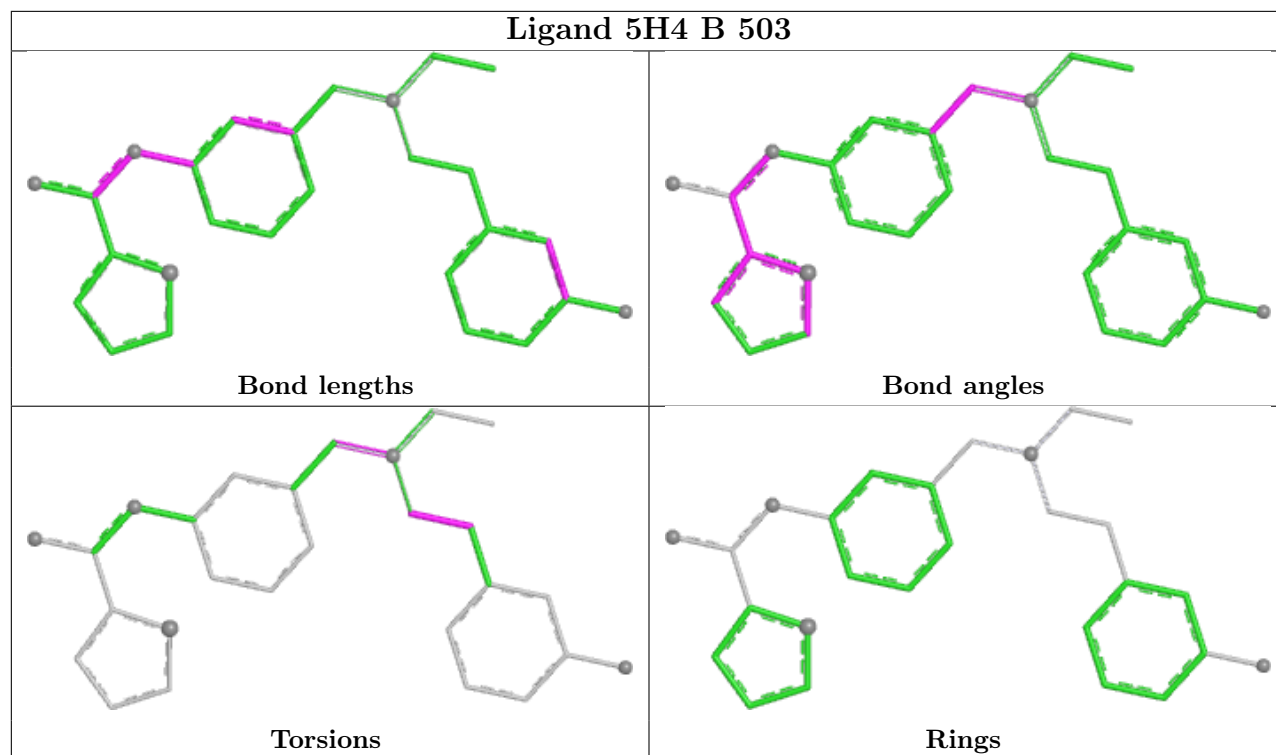
There are no ring outliers.

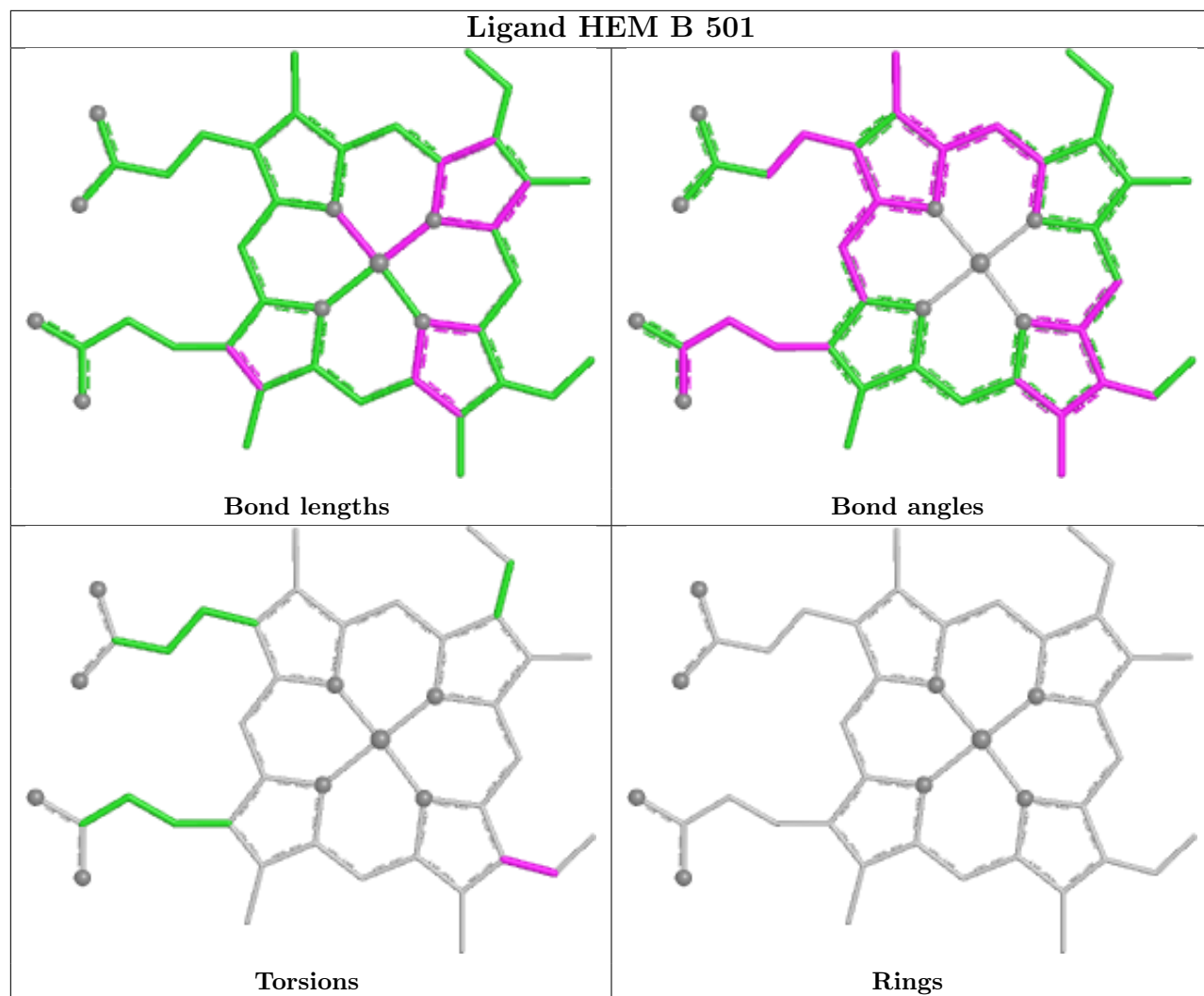
6 monomers are involved in 13 short contacts:

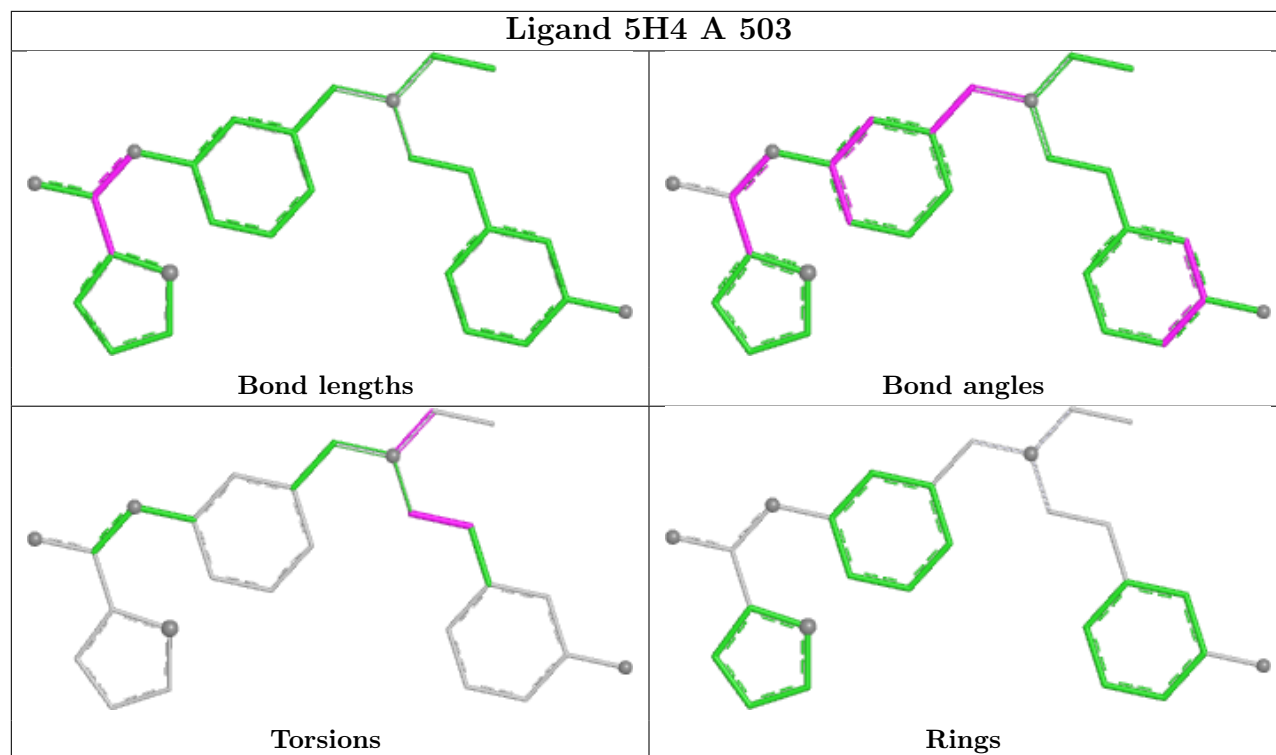
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	H4B	1	0
3	A	502	H4B	1	0
2	A	501	HEM	2	0
4	B	503	5H4	2	0
2	B	501	HEM	5	0
4	A	503	5H4	2	0

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.









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 [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, 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	404/443 (91%)	-0.01	9 (2%) 62 64	30, 42, 69, 98	0
1	B	404/443 (91%)	0.04	4 (0%) 79 81	29, 43, 72, 105	0
All	All	808/886 (91%)	0.01	13 (1%) 70 72	29, 43, 71, 105	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	GLY	3.2
1	A	121	PRO	2.7
1	A	103	GLY	2.5
1	A	108	PRO	2.5
1	A	97	THR	2.4
1	B	69	LYS	2.3
1	B	261	GLY	2.3
1	A	96	CYS	2.3
1	A	239	GLY	2.3
1	A	107	LEU	2.2
1	A	122	ALA	2.1
1	B	218	LYS	2.0
1	B	101	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAS	B	384	9/10	0.95	0.12	43,48,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CAS	A	384	9/10	0.97	0.08	40,42,63,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

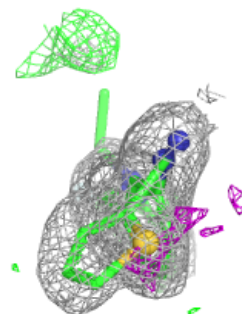
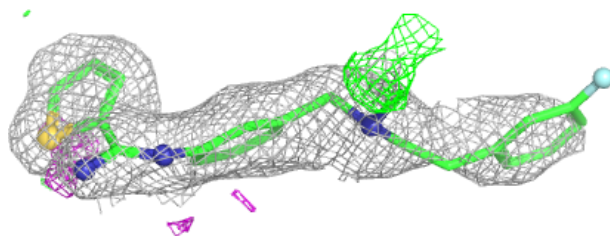
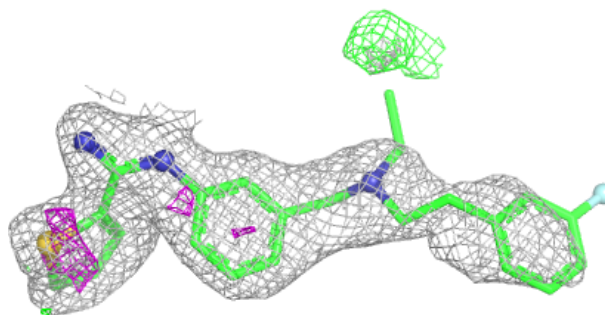
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	504	4/4	0.87	0.12	41,42,46,59	0
6	GOL	A	505	6/6	0.88	0.21	60,66,73,73	0
5	ACT	B	504	4/4	0.90	0.14	47,48,55,60	0
6	GOL	B	505	6/6	0.90	0.15	58,66,76,86	0
4	5H4	A	503	27/27	0.91	0.13	28,43,96,105	0
4	5H4	B	503	27/27	0.94	0.12	27,40,95,99	0
3	H4B	B	502	17/17	0.96	0.07	33,36,48,54	0
2	HEM	B	501	43/43	0.97	0.07	29,34,45,48	0
3	H4B	A	502	17/17	0.97	0.06	34,38,43,45	0
2	HEM	A	501	43/43	0.97	0.08	30,36,40,42	0
7	ZN	A	506	1/1	0.99	0.10	48,48,48,48	0

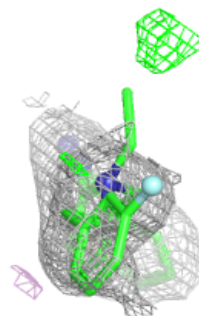
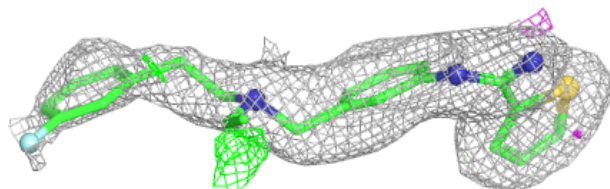
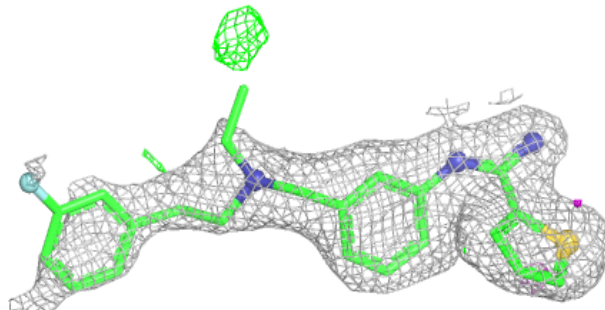
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5H4 A 503:

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

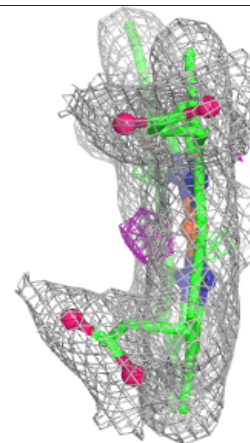
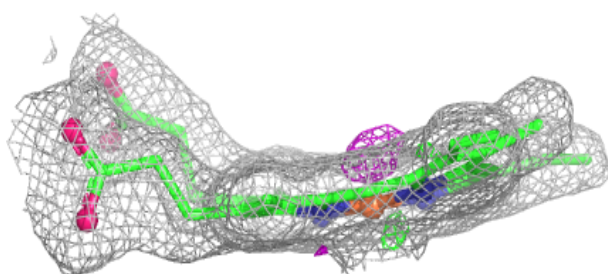
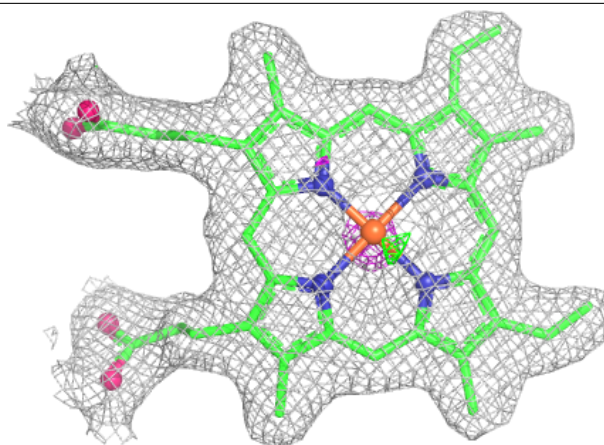
**Electron density around 5H4 B 503:**

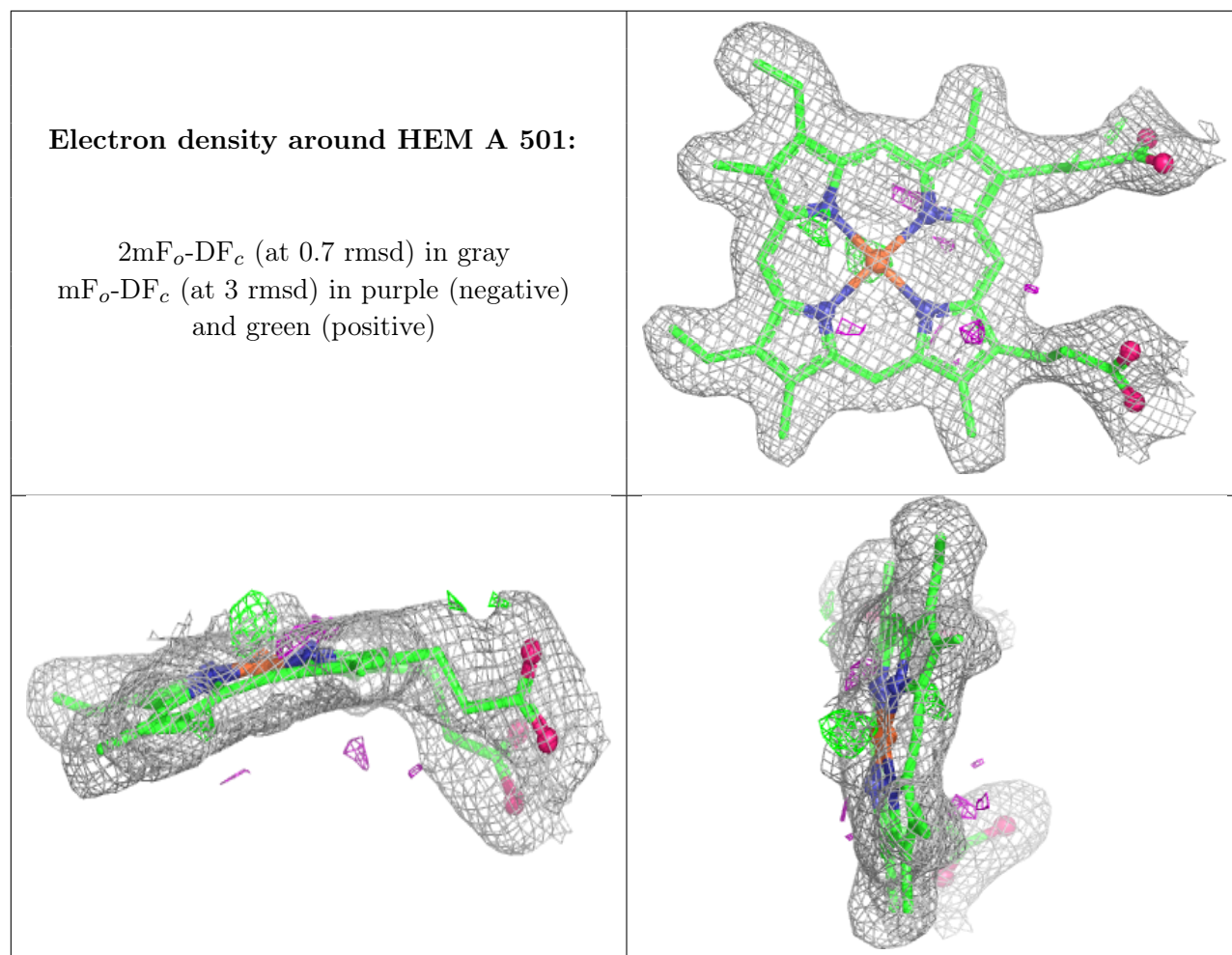
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

$2mF_o - DF_c$ (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.