



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:05 AM UTC

PDB ID : 4JSK / pdb_00004jsk
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6,6'-(pentane-1,5-diyl)bis(4-methylpyridin-2-amine)
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-03-22
Resolution : 2.28 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

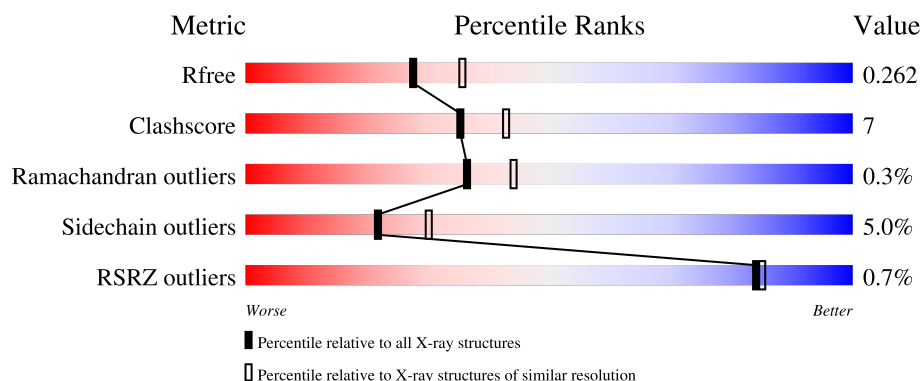
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	78% 12% • 9%
1	B	443	74% 15% • 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6769 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.

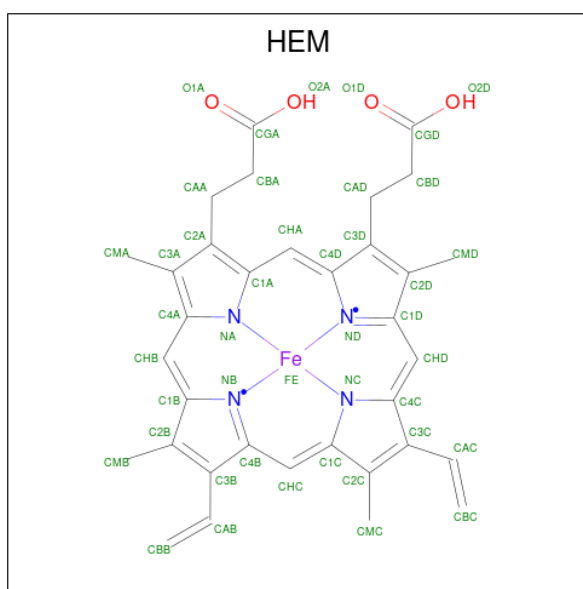
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	As	C	N	O	S	0	0	0
			3212	1	2043	564	588	16			
1	B	404	Total	As	C	N	O	S	0	0	0
			3221	1	2048	568	588	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

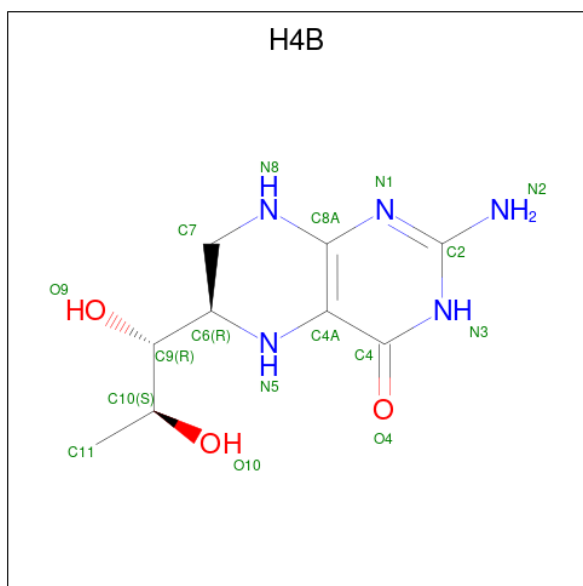
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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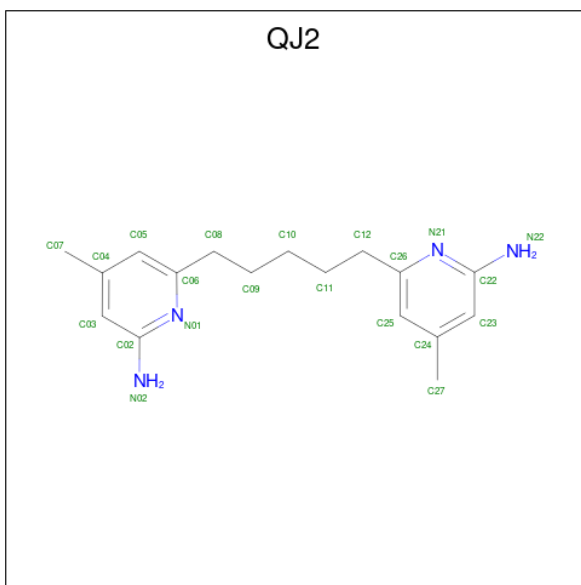
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



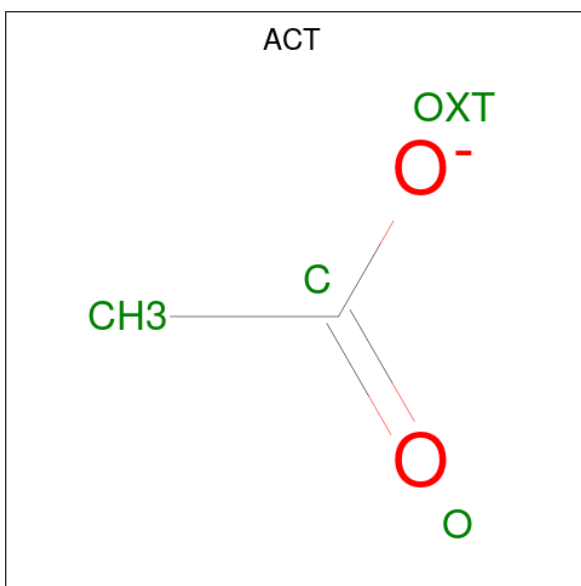
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6,6'-pentane-1,5-diylbis(4-methylpyridin-2-amine) (CCD ID: QJ2) (formula: $C_{17}H_{24}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	17	4		
4	B	1	Total	C	N	0	0
			21	17	4		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



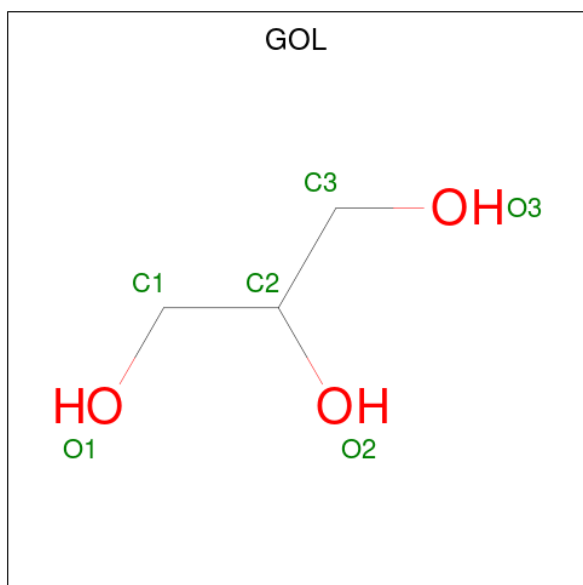
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	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		

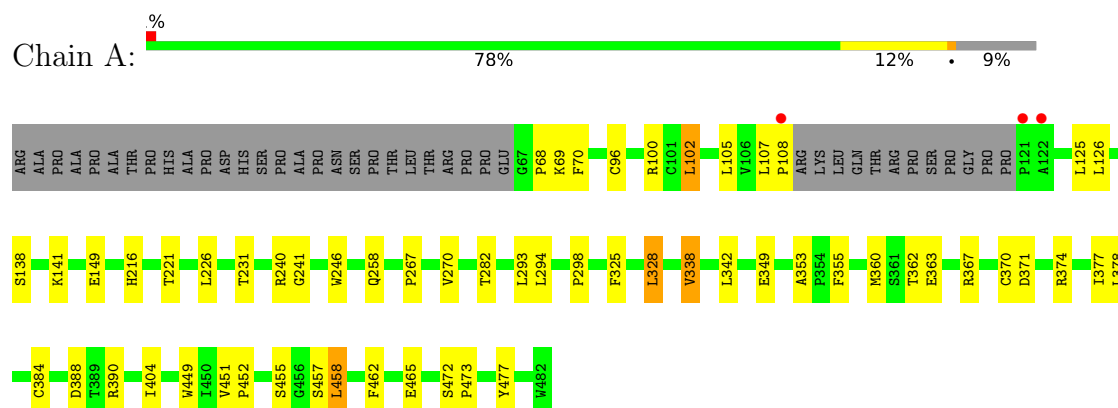
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	65	Total	O	0	0
			65	65		
8	B	80	Total	O	0	0
			80	80		

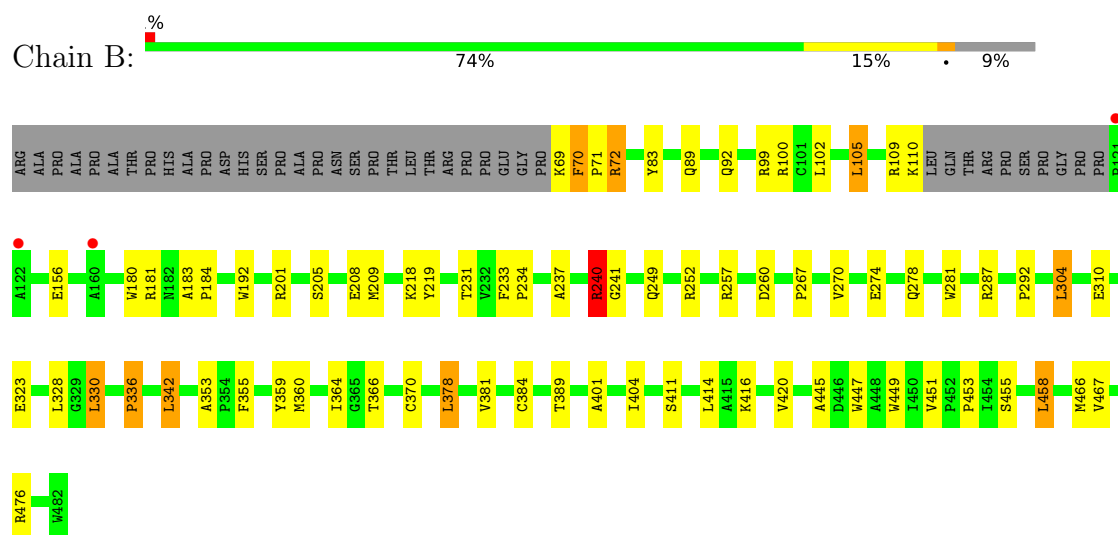
3 Residue-property plots [i](#)

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	58.43Å 106.57Å 156.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.90 – 2.28 42.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.90-2.28) 98.7 (42.90-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.258 0.217 , 0.262	Depositor DCC
R_{free} test set	2254 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6769	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, GOL, H4B, HEM, QJ2, ZN, CAS

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	0.88	1/3292 (0.0%)	0.99	1/4483 (0.0%)
1	B	0.90	0/3300	1.06	7/4491 (0.2%)
All	All	0.89	1/6592 (0.0%)	1.02	8/8974 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	VAL	CA-CB	5.19	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ALA	CA-C-N	-7.11	112.46	119.64
1	B	183	ALA	C-N-CA	-7.11	112.46	119.64
1	B	237	ALA	CA-C-N	6.82	128.36	119.84
1	B	237	ALA	C-N-CA	6.82	128.36	119.84
1	B	70	PHE	CA-C-N	6.00	126.31	119.83
1	B	70	PHE	C-N-CA	6.00	126.31	119.83
1	B	240	ARG	N-CA-C	5.74	116.97	107.73
1	A	70	PHE	N-CA-C	-5.26	99.94	109.09

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	3212	0	3114	39	0
1	B	3221	0	3130	55	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
4	A	21	0	24	1	0
4	B	21	0	24	1	0
5	A	8	0	6	0	0
5	B	8	0	6	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	65	0	0	2	0
8	B	80	0	0	8	0
All	All	6769	0	6410	97	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 7.

All (97) 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:384:CAS:SG	1:B:384:CAS:AS	2.58	1.22
1:A:384:CAS:SG	1:A:384:CAS:AS	2.62	1.17
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.62	0.82
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.13	0.77
1:B:72:ARG:HG3	1:B:83:TYR:CE2	2.25	0.71
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.77	0.67
1:A:388:ASP:OD1	1:A:390:ARG:HG3	1.95	0.67
1:B:330:LEU:HB2	8:B:609:HOH:O	1.98	0.63
1:B:366:THR:O	1:B:370:CYS:HB2	2.00	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.82	0.61
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.81	0.61
1:B:449:TRP:HA	3:B:502:H4B:N1	2.16	0.60
1:A:231:THR:O	1:A:353:ALA:HA	2.02	0.60
1:B:453:PRO:HG3	8:B:652:HOH:O	2.03	0.59
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.85	0.59
1:B:72:ARG:HG3	1:B:83:TYR:HE2	1.68	0.58
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HMC1	2:B:501:HEM:CBC	2.31	0.58
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.41	0.55
1:A:363:GLU:OE1	4:A:503:QJ2:N01	2.40	0.55
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.87	0.55
1:B:304:LEU:C	1:B:304:LEU:HD23	2.32	0.55
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.89	0.55
1:A:258:GLN:HE21	1:A:258:GLN:HA	1.72	0.55
1:A:457:SER:HA	1:A:462:PHE:CG	2.43	0.54
1:A:68:PRO:O	1:B:109:ARG:NH2	2.40	0.54
1:A:378:LEU:HB2	8:A:602:HOH:O	2.07	0.53
1:B:342:LEU:C	1:B:342:LEU:HD23	2.34	0.53
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.50	0.52
1:B:267:PRO:O	1:B:270:VAL:HG23	2.08	0.52
1:A:240:ARG:HD3	1:A:241:GLY:O	2.10	0.52
8:A:644:HOH:O	1:B:109:ARG:HG2	2.10	0.52
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.91	0.51
1:A:360:MET:HE3	1:A:362:THR:OG1	2.11	0.51
1:A:458:LEU:HD21	1:B:401:ALA:CB	2.41	0.51
1:B:240:ARG:HD2	1:B:241:GLY:O	2.11	0.51
2:B:501:HEM:C1C	4:B:503:QJ2:H24	2.45	0.51
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.41	0.50
1:A:258:GLN:HA	1:A:258:GLN:NE2	2.27	0.50
1:A:267:PRO:HD2	1:A:374:ARG:HA	1.93	0.50
1:A:458:LEU:HD21	1:B:401:ALA:HB2	1.94	0.49
1:B:360:MET:HA	1:B:420:VAL:O	2.12	0.49
1:A:472:SER:HA	1:A:473:PRO:C	2.38	0.48
2:A:501:HEM:O1A	3:A:502:H4B:N3	2.43	0.48
1:B:72:ARG:HH11	1:B:72:ARG:HB3	1.77	0.48
1:B:72:ARG:CG	1:B:83:TYR:CE2	2.96	0.47
1:B:72:ARG:HH11	1:B:72:ARG:CB	2.27	0.47
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.81	0.47
1:B:72:ARG:HB3	1:B:72:ARG:NH1	2.30	0.47
1:B:219:TYR:CD2	1:B:219:TYR:C	2.93	0.46
1:B:355:PHE:CD1	2:B:501:HEM:CAC	2.98	0.46
1:B:384:CAS:AS	1:B:384:CAS:CB	3.22	0.46
1:B:455:SER:HB3	1:B:458:LEU:CD2	2.45	0.46
1:B:384:CAS:SG	1:B:384:CAS:CE2	3.04	0.46
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.67	0.46
1:A:102:LEU:CD1	1:B:467:VAL:HG13	2.45	0.46
1:A:377:ILE:HD11	1:A:404:ILE:HD13	1.98	0.46
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:TYR:OH	2:A:501:HEM:O1D	2.28	0.45
1:B:447:TRP:CE2	1:B:451:VAL:HG21	2.51	0.45
1:A:325:PHE:HA	1:A:328:LEU:HD22	1.97	0.45
1:B:231:THR:O	1:B:353:ALA:HA	2.16	0.45
1:B:184:PRO:HD2	8:B:602:HOH:O	2.15	0.45
1:A:107:LEU:HA	1:A:108:PRO:HD2	1.84	0.45
1:B:445:ALA:HB3	1:B:466:MET:HB3	1.97	0.45
1:B:310:GLU:OE1	1:B:310:GLU:N	2.50	0.44
1:B:455:SER:N	8:B:672:HOH:O	2.50	0.44
1:B:180:TRP:O	1:B:181:ARG:C	2.61	0.44
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.46	0.44
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.33	0.44
1:A:221:THR:O	1:A:226:LEU:HD12	2.18	0.44
1:A:258:GLN:HE21	1:A:258:GLN:CA	2.31	0.43
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.00	0.43
2:A:501:HEM:HHC	2:A:501:HEM:CBB	2.46	0.43
1:A:388:ASP:OD1	1:A:390:ARG:CG	2.64	0.43
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.59	0.43
1:B:304:LEU:C	1:B:304:LEU:CD2	2.92	0.42
1:B:336:PRO:HB3	1:B:359:TYR:CZ	2.54	0.42
1:B:414:LEU:C	1:B:416:LYS:H	2.28	0.42
1:B:281:TRP:CE2	1:B:292:PRO:HD3	2.55	0.42
1:B:360:MET:HE1	8:B:677:HOH:O	2.18	0.42
1:A:138:SER:O	1:A:141:LYS:HD3	2.20	0.42
1:A:449:TRP:HA	3:A:502:H4B:N1	2.35	0.42
1:A:355:PHE:CD1	2:A:501:HEM:HAC	2.55	0.42
1:B:99:ARG:HG2	1:B:100:ARG:HD2	2.01	0.42
1:A:96:CYS:HB2	8:B:610:HOH:O	2.19	0.41
1:B:208:GLU:O	1:B:209:MET:C	2.62	0.41
1:B:328:LEU:O	1:B:330:LEU:HD13	2.19	0.41
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.55	0.41
1:A:455:SER:O	1:A:458:LEU:HB2	2.20	0.41
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.56	0.41
1:B:205:SER:HB2	8:B:603:HOH:O	2.20	0.41
1:B:201:ARG:HB3	8:B:660:HOH:O	2.21	0.41
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.03	0.41
1:A:216:HIS:CD2	1:A:216:HIS:C	2.99	0.40
1:B:249:GLN:HB2	1:B:252:ARG:HD2	2.03	0.40
1:A:240:ARG:CD	1:A:241:GLY:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	399/443 (90%)	383 (96%)	16 (4%)	0	100	100
1	B	399/443 (90%)	372 (93%)	25 (6%)	2 (0%)	24	29
All	All	798/886 (90%)	755 (95%)	41 (5%)	2 (0%)	36	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ASP
1	B	336	PRO

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	342/375 (91%)	331 (97%)	11 (3%)	34	49
1	B	343/375 (92%)	320 (93%)	23 (7%)	15	19
All	All	685/750 (91%)	651 (95%)	34 (5%)	22	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	102	LEU
1	A	105	LEU
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	126	LEU
1	A	149	GLU
1	A	270	VAL
1	A	282	THR
1	A	293	LEU
1	A	328	LEU
1	A	458	LEU
1	B	69	LYS
1	B	72	ARG
1	B	89	GLN
1	B	92	GLN
1	B	102	LEU
1	B	105	LEU
1	B	110	LYS
1	B	156	GLU
1	B	218	LYS
1	B	240	ARG
1	B	257	ARG
1	B	274	GLU
1	B	278	GLN
1	B	287	ARG
1	B	304	LEU
1	B	323	GLU
1	B	330	LEU
1	B	342	LEU
1	B	378	LEU
1	B	389	THR
1	B	411	SER
1	B	458	LEU
1	B	476	ARG

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	166	HIS
1	A	178	GLN
1	A	191	GLN
1	A	258	GLN
1	A	278	GLN
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	405	ASN
1	A	413	GLN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
1	B	296	GLN
1	B	405	ASN

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	1.17	0	1,9,11	1.03	0
1	CAS	B	384	1	5,8,9	1.16	0	1,9,11	0.44	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	1	0
1	B	384	CAS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	502	-	17,18,18	0.91	0	14,26,26	1.99	4 (28%)
5	ACT	A	504	-	3,3,3	0.87	0	3,3,3	0.57	0
3	H4B	B	502	-	17,18,18	1.02	1 (5%)	14,26,26	1.89	5 (35%)
5	ACT	A	505	-	3,3,3	0.74	0	3,3,3	1.00	0
2	HEM	B	501	1	50,50,50	1.84	13 (26%)	67,82,82	1.49	11 (16%)
5	ACT	B	505	-	3,3,3	0.92	0	3,3,3	0.30	0
4	QJ2	B	503	-	22,22,22	0.72	0	27,29,29	1.68	7 (25%)
6	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.54	0
4	QJ2	A	503	-	22,22,22	0.99	1 (4%)	27,29,29	2.34	9 (33%)
6	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.47	0
5	ACT	B	504	-	3,3,3	0.92	0	3,3,3	0.30	0
2	HEM	A	501	1	50,50,50	1.61	8 (16%)	67,82,82	1.29	7 (10%)

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	502	-	-	0/8/17/17	0/2/2/2
3	H4B	B	502	-	-	1/8/17/17	0/2/2/2
2	HEM	B	501	1	-	0/14/54/54	-
4	QJ2	B	503	-	-	3/8/8/8	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
4	QJ2	A	503	-	-	5/8/8/8	0/2/2/2
6	GOL	A	506	-	-	3/4/4/4	-
2	HEM	A	501	1	-	0/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	6.72	1.51	1.36
2	A	501	HEM	C3D-C2D	5.84	1.49	1.36
2	B	501	HEM	FE-ND	3.46	2.05	1.94
2	B	501	HEM	CAB-C3B	3.38	1.56	1.47
2	A	501	HEM	CAC-C3C	3.12	1.55	1.47
2	B	501	HEM	CMD-C2D	2.88	1.56	1.50
2	B	501	HEM	FE-NC	2.77	2.04	1.95
2	A	501	HEM	CMC-C2C	2.75	1.56	1.50
2	B	501	HEM	FE-NA	2.68	2.04	1.95
4	A	503	QJ2	C03-C04	2.63	1.43	1.39
2	A	501	HEM	FE-NA	2.58	2.03	1.95
2	B	501	HEM	CAC-C3C	2.56	1.54	1.47
3	B	502	H4B	C4-N3	-2.52	1.34	1.38
2	A	501	HEM	CAB-C3B	2.50	1.54	1.47
2	B	501	HEM	FE-NB	-2.47	1.87	1.94
2	B	501	HEM	CMA-C3A	2.46	1.55	1.50
2	A	501	HEM	CMD-C2D	2.44	1.55	1.50
2	B	501	HEM	C3B-C2B	-2.32	1.32	1.37
2	A	501	HEM	CMA-C3A	2.31	1.55	1.50
2	B	501	HEM	C4B-NB	2.30	1.43	1.38
2	B	501	HEM	C2A-C3A	-2.26	1.33	1.38
2	B	501	HEM	C3C-C4C	-2.25	1.42	1.46
2	A	501	HEM	FE-NC	2.15	2.02	1.95

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	QJ2	C02-N01-C06	6.63	123.03	118.07
4	A	503	QJ2	C22-N21-C26	5.77	122.39	118.07
4	B	503	QJ2	C22-N21-C26	4.77	121.63	118.07
3	A	502	H4B	C2-N1-C8A	4.55	121.39	113.36
2	B	501	HEM	CMD-C2D-C1D	3.78	130.94	125.03
2	B	501	HEM	C1D-C2D-C3D	-3.74	103.04	106.98
2	B	501	HEM	C3B-C2B-C1B	3.67	109.17	106.41
4	A	503	QJ2	C07-C04-C05	-3.60	116.05	120.92
3	B	502	H4B	C2-N1-C8A	3.48	119.50	113.36
4	A	503	QJ2	C09-C08-C06	3.29	122.86	113.09
2	B	501	HEM	CHD-C4C-NC	3.11	127.84	124.45
3	B	502	H4B	O4-C4-C4A	-3.00	120.03	127.26
2	A	501	HEM	CBA-CAA-C2A	-2.99	104.26	112.53
4	A	503	QJ2	C05-C06-N01	-2.98	119.33	122.73
2	B	501	HEM	CBA-CAA-C2A	-2.98	104.31	112.53
3	A	502	H4B	C4-C4A-N5	2.95	124.31	116.27
3	B	502	H4B	C4A-C4-N3	2.93	120.19	112.13
4	B	503	QJ2	C09-C08-C06	2.92	121.75	113.09
2	B	501	HEM	C4D-ND-C1D	2.91	108.66	105.21
2	A	501	HEM	CMD-C2D-C1D	2.89	129.56	125.03
2	A	501	HEM	CHB-C1B-NB	2.78	127.81	124.37
2	B	501	HEM	CBD-CAD-C3D	-2.75	104.92	112.53
3	A	502	H4B	C4A-C4-N3	2.71	119.57	112.13
4	B	503	QJ2	C02-N01-C06	2.68	120.07	118.07
4	A	503	QJ2	C11-C12-C26	-2.63	105.30	113.09
2	A	501	HEM	CMA-C3A-C4A	2.58	129.35	125.42
3	A	502	H4B	N3-C2-N1	-2.43	118.88	123.32
2	A	501	HEM	C1D-C2D-C3D	-2.38	104.47	106.98
2	B	501	HEM	CAD-C3D-C4D	2.37	128.82	124.70
4	A	503	QJ2	C10-C09-C08	-2.35	103.94	113.74
4	B	503	QJ2	C10-C09-C08	-2.33	104.02	113.74
4	A	503	QJ2	C25-C26-N21	-2.29	120.12	122.73
4	A	503	QJ2	C05-C04-C03	2.25	120.62	118.11
4	B	503	QJ2	C11-C12-C26	-2.24	106.44	113.09
3	B	502	H4B	C4-C4A-N5	2.24	122.37	116.27
2	B	501	HEM	CAD-C3D-C2D	-2.23	123.69	127.87
3	B	502	H4B	N3-C2-N1	-2.23	119.25	123.32
2	A	501	HEM	C4A-CHB-C1B	-2.15	121.20	126.25
4	B	503	QJ2	C25-C26-N21	-2.13	120.30	122.73
2	A	501	HEM	C2D-C1D-ND	2.08	112.31	109.90
2	B	501	HEM	CHB-C1B-NB	2.06	126.91	124.37
2	B	501	HEM	CBC-CAC-C3C	-2.02	117.41	127.53
4	B	503	QJ2	C25-C24-C23	2.02	120.36	118.11

There are no chirality outliers.

All (14) torsion outliers are listed below:

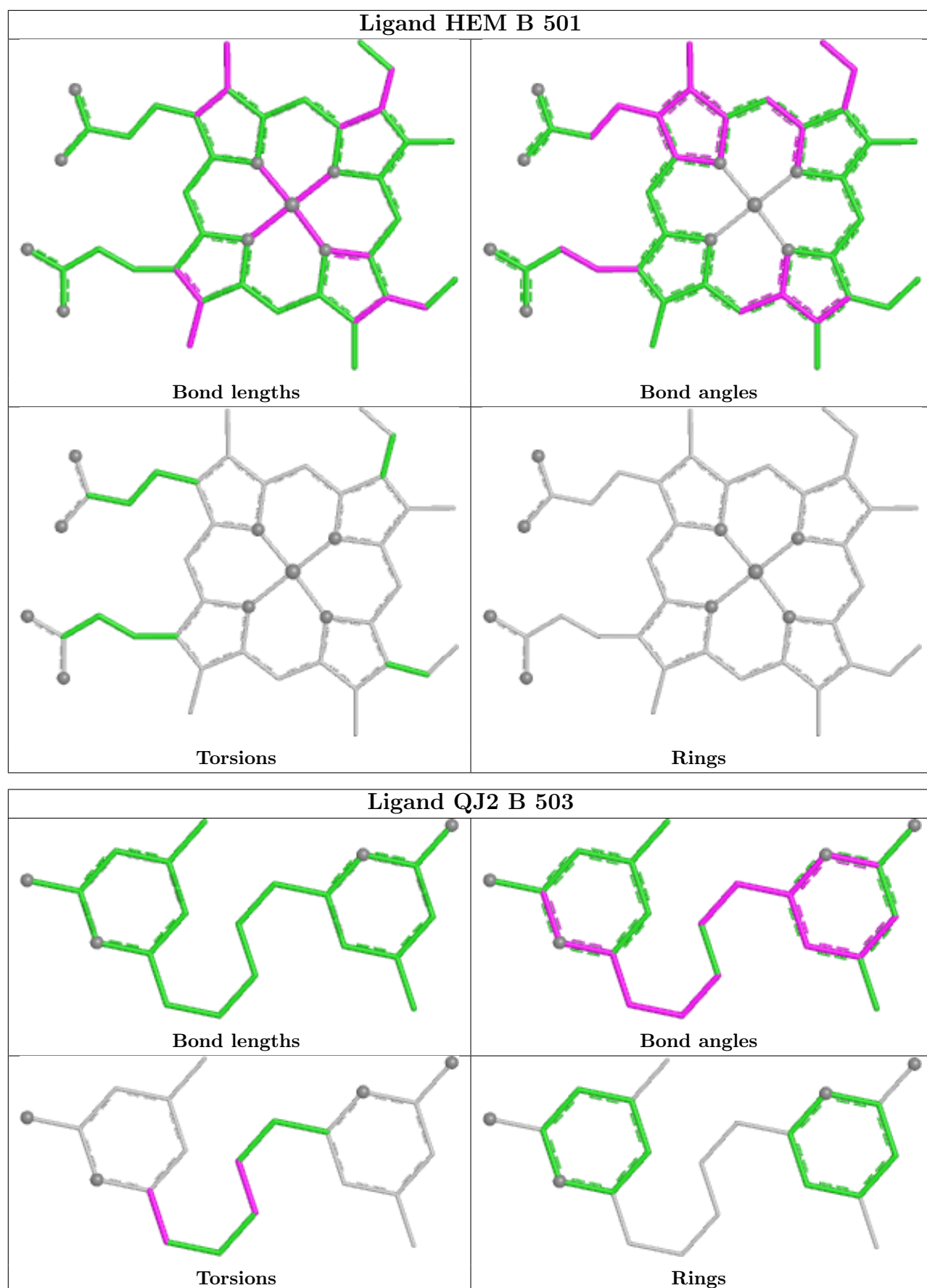
Mol	Chain	Res	Type	Atoms
6	B	506	GOL	C1-C2-C3-O3
6	A	506	GOL	O1-C1-C2-C3
4	A	503	QJ2	C09-C10-C11-C12
4	B	503	QJ2	C09-C10-C11-C12
6	A	506	GOL	O2-C2-C3-O3
6	A	506	GOL	O1-C1-C2-O2
6	B	506	GOL	O2-C2-C3-O3
4	A	503	QJ2	N01-C06-C08-C09
4	B	503	QJ2	C05-C06-C08-C09
4	A	503	QJ2	C11-C12-C26-N21
4	B	503	QJ2	N01-C06-C08-C09
4	A	503	QJ2	C05-C06-C08-C09
4	A	503	QJ2	C11-C12-C26-C25
3	B	502	H4B	N5-C6-C9-O9

There are no ring outliers.

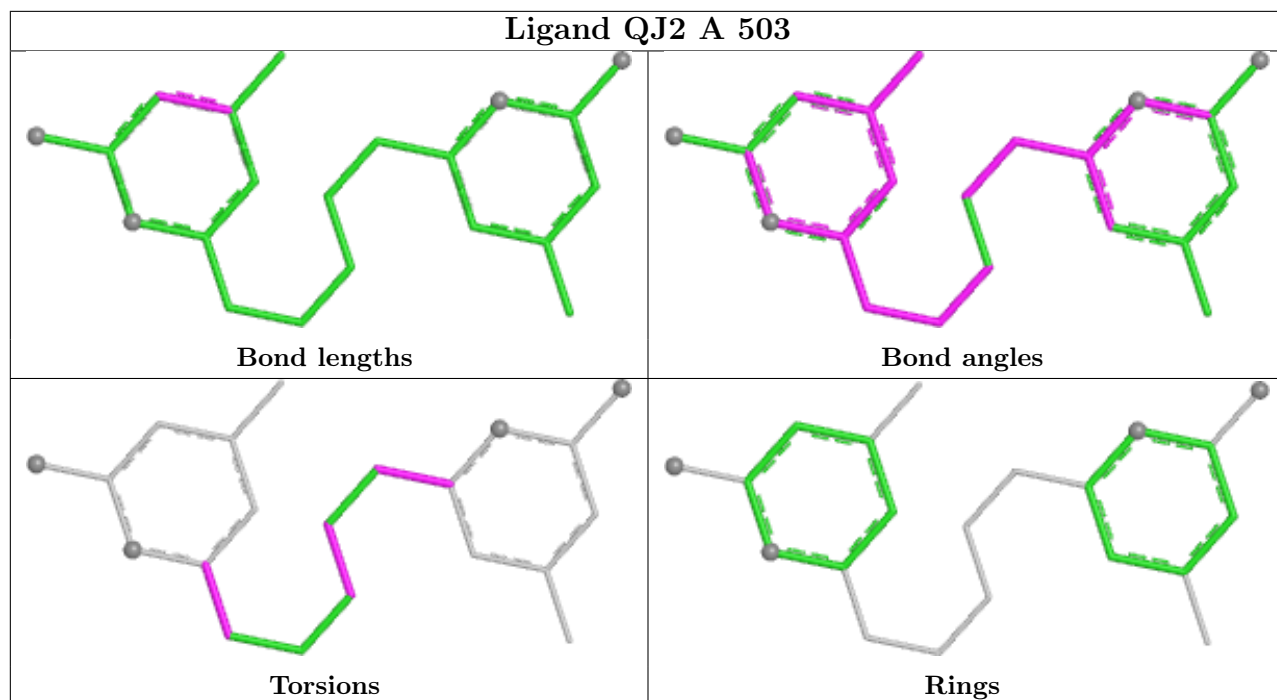
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	H4B	2	0
3	B	502	H4B	1	0
2	B	501	HEM	6	0
4	B	503	QJ2	1	0
4	A	503	QJ2	1	0
2	A	501	HEM	5	0

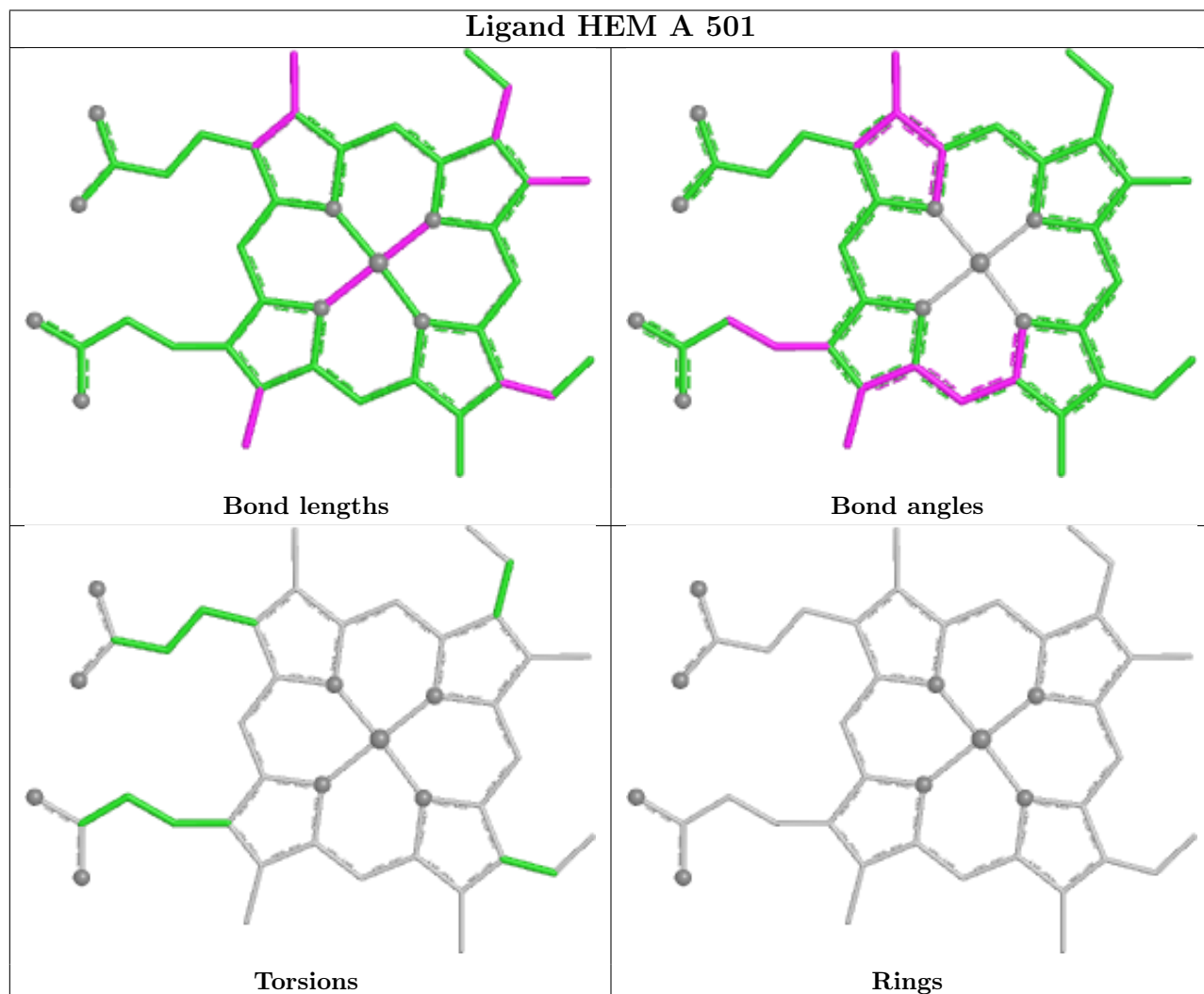
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 QJ2 A 503



Ligand HEM A 501



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	403/443 (90%)	0.04	3 (0%) 84 85	35, 55, 81, 99	0
1	B	403/443 (90%)	0.04	3 (0%) 84 85	37, 56, 84, 103	0
All	All	806/886 (90%)	0.04	6 (0%) 84 85	35, 56, 83, 103	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	3.9
1	B	121	PRO	3.8
1	A	108	PRO	3.6
1	A	121	PRO	3.2
1	B	122	ALA	2.3
1	B	160	ALA	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	0.91	0.12	70,72,98,98	0
1	CAS	A	384	9/10	0.93	0.11	59,60,93,94	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

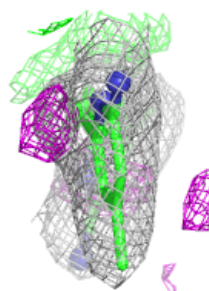
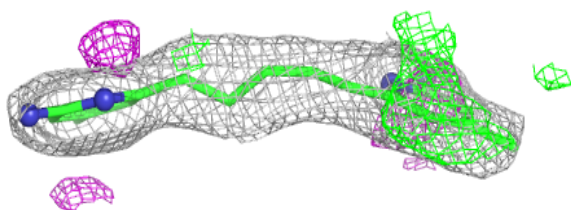
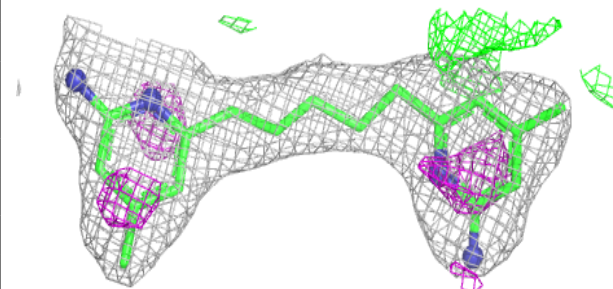
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	506	6/6	0.83	0.20	80,82,82,84	0
4	QJ2	B	503	21/21	0.88	0.13	40,49,62,63	0
6	GOL	B	506	6/6	0.88	0.14	68,70,71,72	0
4	QJ2	A	503	21/21	0.91	0.10	37,52,77,78	0
5	ACT	A	504	4/4	0.91	0.12	60,62,62,64	0
3	H4B	A	502	17/17	0.93	0.07	43,47,50,53	0
5	ACT	B	505	4/4	0.93	0.08	48,49,50,50	0
5	ACT	B	504	4/4	0.94	0.10	61,61,62,62	0
3	H4B	B	502	17/17	0.96	0.07	39,44,47,49	0
5	ACT	A	505	4/4	0.96	0.06	51,56,56,56	0
2	HEM	A	501	43/43	0.97	0.08	33,42,53,60	0
2	HEM	B	501	43/43	0.97	0.07	36,43,53,56	0
7	ZN	A	507	1/1	0.99	0.02	48,48,48,48	0

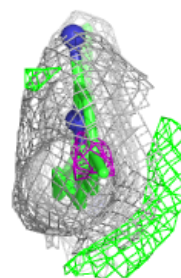
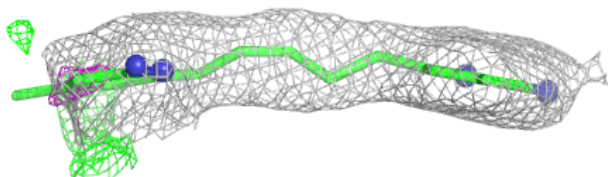
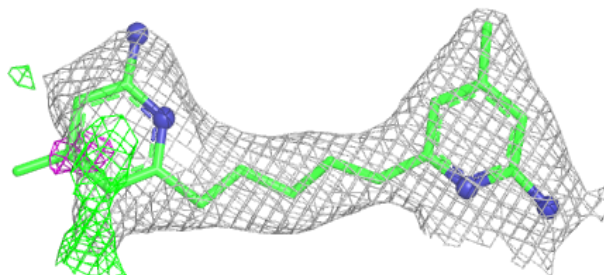
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QJ2 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)

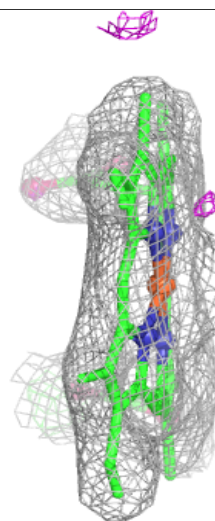
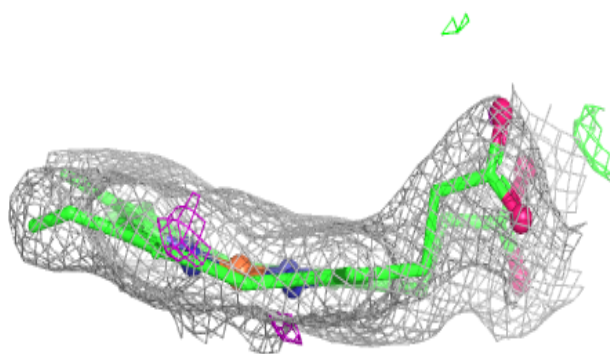
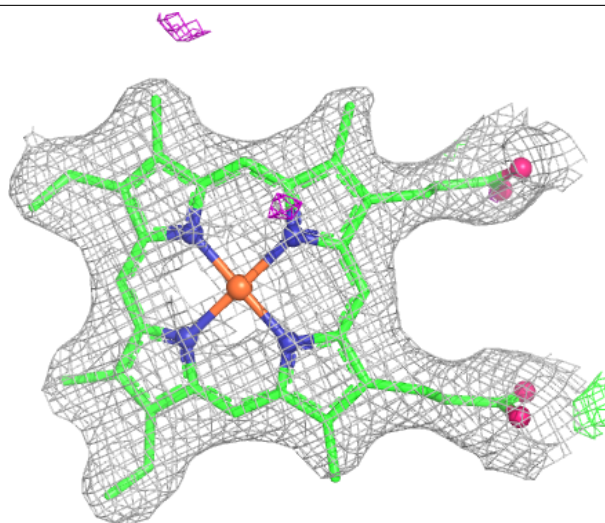
**Electron density around QJ2 A 503:**

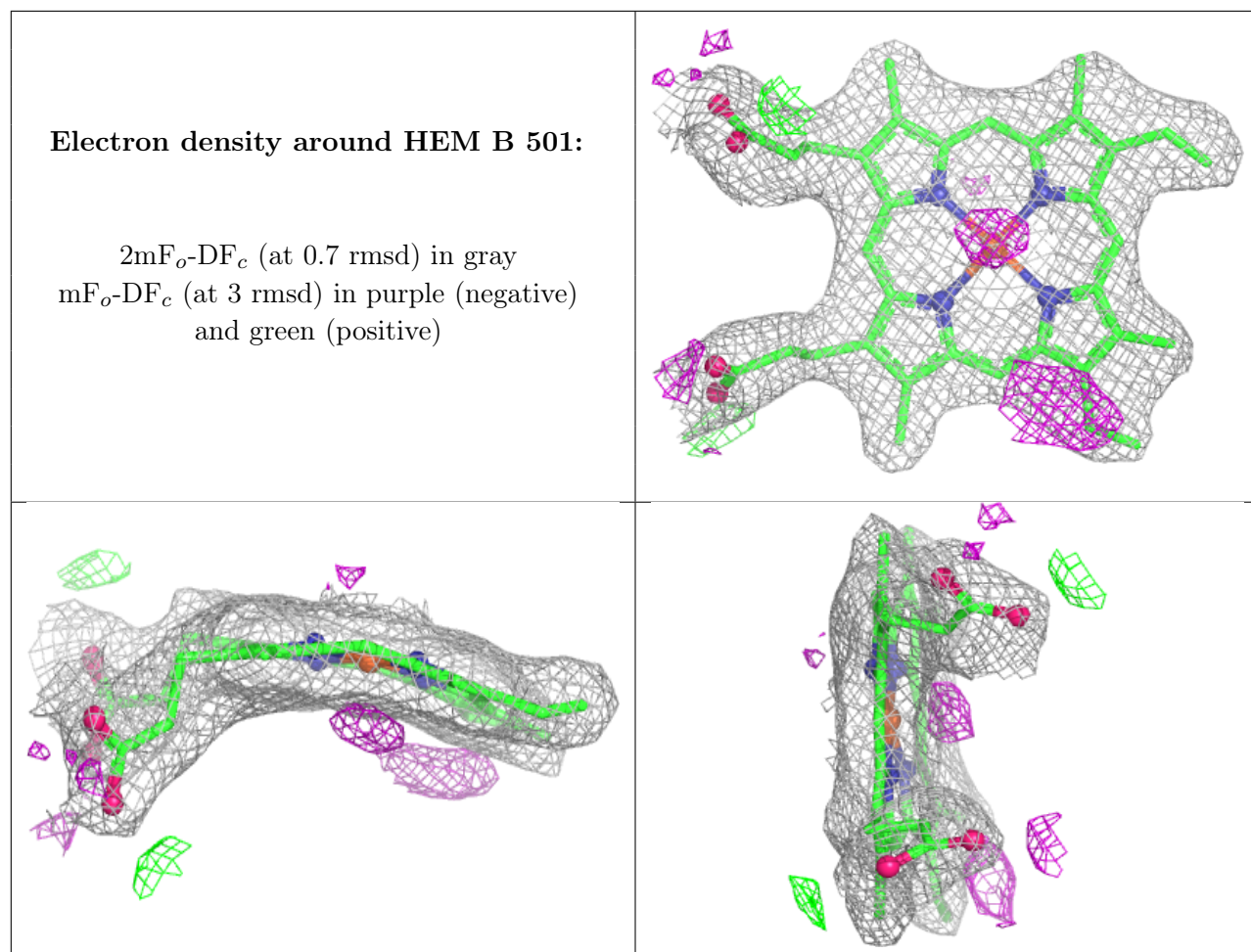
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 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.