



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 02:57 PM EDT

PDB ID : 4JSM
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6-(((5-(((3-fluorophenethyl)amino)methyl)pyridin-3-yl)oxy)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-03-22
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

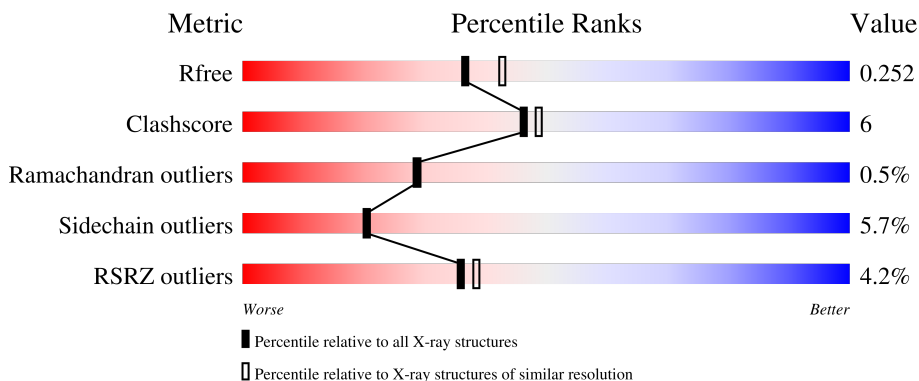
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

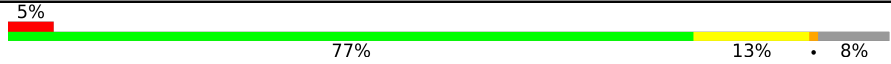
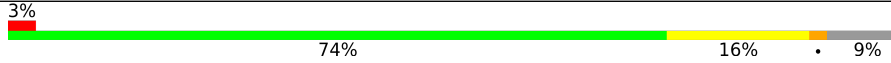
The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	 5% 77% 13% • 8%
1	B	443	 3% 74% 16% • 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6900 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	
			Total	As	C	N	O				S
1	A	406	3232	1	2055	570	590	16	0	0	0
1	B	405	3229	1	2054	569	589	16	0	0	0

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

Continued on next page...

Continued from previous page...

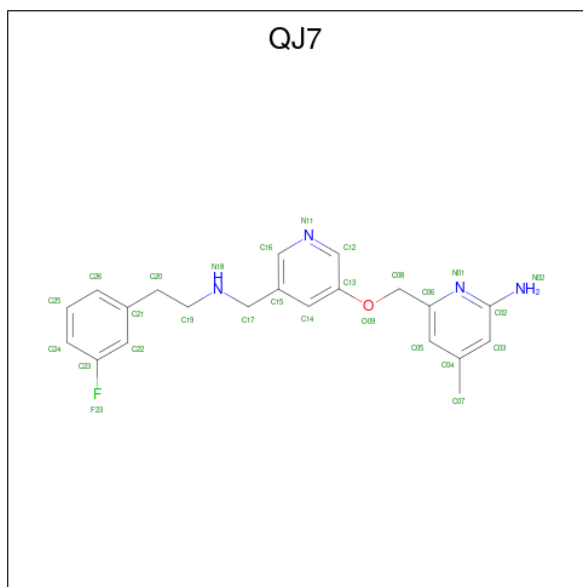
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

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



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

- Molecule 4 is 6-({[5-({[2-(3-fluorophenyl)ethyl]amino}methyl)pyridin-3-yl]oxy}methyl)-4-methylpyridin-2-amine (three-letter code: QJ7) (formula: $C_{21}H_{23}FN_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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


- Molecule 8 is water.

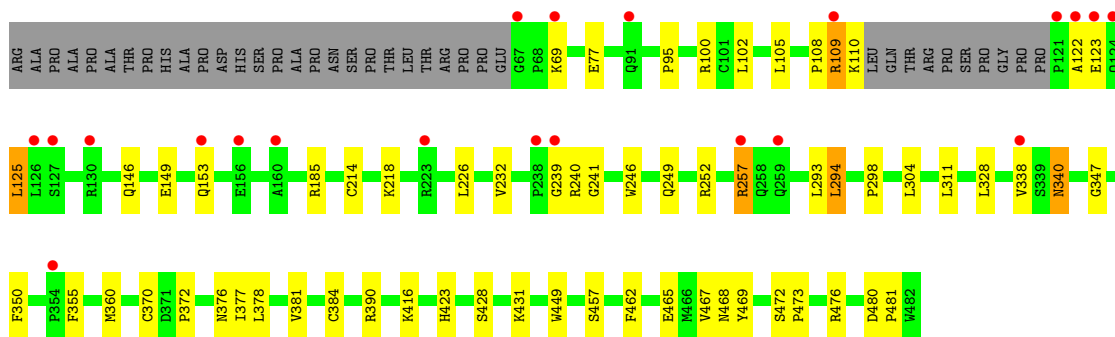
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	127	Total O 127 127	0	0
8	B	117	Total O 117 117	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

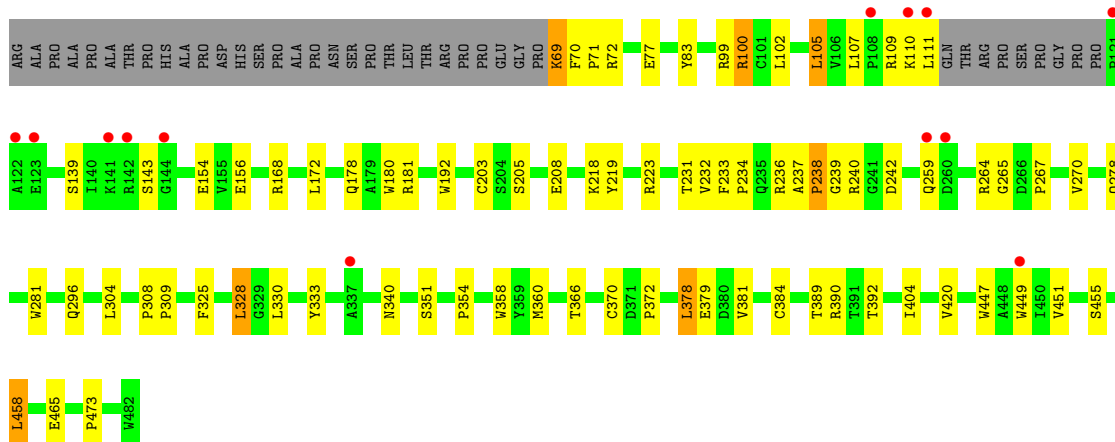
- Molecule 1: Nitric oxide synthase, endothelial

Chain A: 



- Molecule 1: Nitric oxide synthase, endothelial

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.28Å 106.44Å 157.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.13 – 2.25 39.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.13-2.25) 99.5 (39.30-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.24Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.244 0.200 , 0.252	Depositor DCC
R_{free} test set	2334 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.603	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6900	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, QJ7, HEM, GOL, H4B, 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	0.76	1/3312 (0.0%)	0.76	1/4508 (0.0%)
1	B	0.78	2/3308 (0.1%)	0.77	0/4502
All	All	0.77	3/6620 (0.0%)	0.77	1/9010 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	TYR	CD2-CE2	6.76	1.49	1.39
1	B	203	CYS	CB-SG	-6.71	1.70	1.82
1	A	428	SER	CB-OG	5.11	1.48	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

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	3232	0	3140	39	0
1	B	3229	0	3141	44	0
2	A	43	0	30	2	0
2	B	43	0	30	3	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	1	0
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	1	0
7	A	1	0	0	0	0
8	A	127	0	0	5	0
8	B	117	0	0	3	0
All	All	6900	0	6439	82	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 (82) 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	2.51	1.29
1:A:384:CAS:SG	1:A:384:CAS:AS	2.53	1.26
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.67	0.74
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.58	0.68
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.94	0.67
1:A:476:ARG:HD2	8:A:602:HOH:O	1.96	0.65
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.79	0.64
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.78	0.64
8:A:719:HOH:O	1:B:109:ARG:HD3	1.99	0.63
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.82	0.61
1:B:366:THR:O	1:B:370:CYS:HB2	2.00	0.61
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HD11	4:B:505:QJ7:C25	2.31	0.60
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.83	0.60
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.15	0.59
1:B:325:PHE:O	1:B:328:LEU:HB2	2.02	0.59
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.85	0.59
1:B:178:GLN:HB3	1:B:473:PRO:HG2	1.87	0.57
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.45	0.57
1:A:149:GLU:O	1:A:153:GLN:HG3	2.05	0.57
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.87	0.56
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.35	0.56
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.88	0.55
1:A:239:GLY:N	8:A:670:HOH:O	2.42	0.53
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.38	0.53
1:B:455:SER:HB3	1:B:458:LEU:HB2	1.91	0.51
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.92	0.51
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.93	0.50
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.51	0.50
1:B:72:ARG:HB2	1:B:83:TYR:CE2	2.45	0.50
1:B:358:TRP:H	2:B:501:HEM:HAB	1.77	0.50
1:A:377:ILE:HD12	1:A:381:VAL:HG21	1.94	0.50
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.33	0.49
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.48	0.49
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.48	0.48
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.44	0.48
1:A:457:SER:HA	1:A:462:PHE:CG	2.49	0.48
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.96	0.48
1:A:378:LEU:HB2	8:A:601:HOH:O	2.13	0.48
1:B:265:GLY:O	1:B:267:PRO:HD3	2.14	0.48
1:B:259:GLN:HG2	8:B:690:HOH:O	2.14	0.47
1:B:205:SER:OG	1:B:208:GLU:HG3	2.14	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.47
1:A:384:CAS:AS	1:A:384:CAS:CB	3.22	0.47
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.61	0.47
1:B:360:MET:HA	1:B:420:VAL:O	2.15	0.46
1:A:372:PRO:HA	1:A:376:ASN:ND2	2.31	0.46
1:A:423:HIS:HB2	1:B:392:THR:HB	1.98	0.46
1:B:231:THR:O	1:B:354:PRO:HD2	2.15	0.46
1:B:449:TRP:HA	3:B:502:H4B:N1	2.29	0.46
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.26	0.46
1:A:340:ASN:H	1:A:340:ASN:HD22	1.64	0.45
1:B:72:ARG:HB2	1:B:83:TYR:HE2	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.99	0.45
1:A:125:LEU:HD23	1:A:347:GLY:HA3	1.99	0.45
1:A:338:VAL:HG23	4:A:503:QJ7:H21	1.98	0.45
1:A:476:ARG:CD	8:A:602:HOH:O	2.62	0.45
1:B:154:GLU:OE1	1:B:168:ARG:NH2	2.50	0.45
1:B:69:LYS:HA	1:B:69:LYS:NZ	2.32	0.44
1:B:110:LYS:HE3	1:B:110:LYS:HB3	1.83	0.44
1:B:308:PRO:HA	1:B:309:PRO:HD3	1.87	0.44
1:A:214:CYS:O	1:A:218:LYS:HG3	2.17	0.44
1:A:240:ARG:HD2	1:A:241:GLY:O	2.17	0.44
1:B:384:CAS:AS	1:B:384:CAS:CB	3.25	0.44
1:A:467:VAL:HG12	1:A:469:TYR:HD1	1.82	0.44
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.86	0.43
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.53	0.43
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.99	0.43
1:B:390:ARG:HE	1:B:390:ARG:HB2	1.67	0.43
1:B:455:SER:N	8:B:621:HOH:O	2.52	0.42
1:A:355:PHE:CD1	2:A:501:HEM:HAC	2.54	0.42
1:B:237:ALA:HA	1:B:238:PRO:HD2	1.71	0.42
1:A:249:GLN:HB2	1:A:252:ARG:HG2	2.01	0.41
1:A:480:ASP:HA	1:A:481:PRO:HD3	1.84	0.41
1:A:95:PRO:HB3	1:A:108:PRO:HB2	2.02	0.41
1:A:338:VAL:CG2	4:A:503:QJ7:H21	2.50	0.41
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.56	0.41
1:A:232:VAL:CG1	1:A:350:PHE:CD2	3.04	0.41
6:B:504:GOL:H11	8:B:696:HOH:O	2.20	0.41
1:A:360:MET:HE2	1:A:360:MET:HB3	1.92	0.40
1:A:449:TRP:HA	3:A:502:H4B:N1	2.36	0.40
1:B:219:TYR:CD2	1:B:219:TYR:C	2.94	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	401/443 (90%)	387 (96%)	12 (3%)	2 (0%)	29	29
1	B	400/443 (90%)	384 (96%)	14 (4%)	2 (0%)	29	29
All	All	801/886 (90%)	771 (96%)	26 (3%)	4 (0%)	29	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	122	ALA
1	B	328	LEU
1	B	238	PRO

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	344/375 (92%)	326 (95%)	18 (5%)	23	24
1	B	344/375 (92%)	323 (94%)	21 (6%)	18	18
All	All	688/750 (92%)	649 (94%)	39 (6%)	20	20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	110	LYS
1	A	123	GLU
1	A	125	LEU
1	A	146	GLN
1	A	226	LEU
1	A	257	ARG
1	A	293	LEU
1	A	294	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	311	LEU
1	A	328	LEU
1	A	340	ASN
1	A	416	LYS
1	A	431	LYS
1	A	468	ASN
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	111	LEU
1	B	139	SER
1	B	143	SER
1	B	156	GLU
1	B	218	LYS
1	B	223	ARG
1	B	240	ARG
1	B	264	ARG
1	B	270	VAL
1	B	278	GLN
1	B	296	GLN
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	379	GLU
1	B	389	THR
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	91	GLN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	405	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1.32	0	1,9,11	0.53	0
1	CAS	B	384	1	5,8,9	1.22	0	1,9,11	0.23	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	2	0
1	B	384	CAS	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	A	502	-	16,18,18	1.14	2 (12%)	11,26,26	3.19	7 (63%)
3	H4B	B	502	-	16,18,18	1.05	1 (6%)	11,26,26	3.06	7 (63%)
4	QJ7	B	505	-	29,29,29	0.91	3 (10%)	37,38,38	1.75	8 (21%)
5	ACT	B	503	-	3,3,3	0.83	0	3,3,3	0.48	0
5	ACT	A	504	-	3,3,3	0.83	0	3,3,3	0.44	0
4	QJ7	A	503	-	29,29,29	0.88	0	37,38,38	1.60	8 (21%)
2	HEM	B	501	1	41,50,50	2.03	7 (17%)	45,82,82	1.75	9 (20%)
6	GOL	B	504	-	5,5,5	0.65	0	5,5,5	1.64	2 (40%)
6	GOL	A	505	-	5,5,5	0.55	0	5,5,5	1.15	0
2	HEM	A	501	1	41,50,50	1.82	6 (14%)	45,82,82	1.46	8 (17%)

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	-	-	0/8/17/17	0/2/2/2
4	QJ7	B	505	-	-	1/12/12/12	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QJ7	A	503	-	-	0/12/12/12	0/3/3/3
2	HEM	B	501	1	-	2/12/54/54	-
6	GOL	B	504	-	-	1/4/4/4	-
6	GOL	A	505	-	-	1/4/4/4	-
2	HEM	A	501	1	-	2/12/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	7.87	1.53	1.36
2	A	501	HEM	C3D-C2D	6.35	1.50	1.36
2	B	501	HEM	C3C-C2C	-4.88	1.33	1.40
2	B	501	HEM	C3C-CAC	3.64	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.43	1.35	1.40
2	B	501	HEM	CAB-C3B	3.39	1.56	1.47
2	A	501	HEM	C3C-CAC	3.35	1.54	1.47
2	A	501	HEM	C1B-NB	-3.28	1.34	1.40
2	A	501	HEM	CAB-C3B	2.88	1.55	1.47
2	B	501	HEM	CMD-C2D	2.67	1.56	1.50
3	B	502	H4B	C4A-C4	-2.55	1.38	1.41
2	B	501	HEM	CMB-C2B	2.26	1.55	1.50
4	B	505	QJ7	C24-C23	2.25	1.41	1.37
3	A	502	H4B	O4-C4	2.19	1.30	1.24
2	B	501	HEM	FE-ND	2.17	2.07	1.96
2	A	501	HEM	C3B-C2B	-2.09	1.33	1.37
3	A	502	H4B	C4-N3	2.06	1.36	1.33
4	B	505	QJ7	C12-C13	2.05	1.41	1.38
4	B	505	QJ7	C22-C23	2.00	1.41	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C8A-C4A-C4	6.37	120.23	114.57
4	B	505	QJ7	C02-N01-C06	5.28	122.10	118.10
3	B	502	H4B	C4-C4A-N5	5.11	123.41	119.12
2	B	501	HEM	CBA-CAA-C2A	-5.02	104.05	112.62
3	A	502	H4B	C2-N3-C4	4.62	123.27	115.93
3	B	502	H4B	C2-N3-C4	4.53	123.12	115.93
2	B	501	HEM	C4D-ND-C1D	4.50	109.72	105.07
3	B	502	H4B	N1-C2-N3	-4.49	118.37	125.42
4	A	503	QJ7	C02-N01-C06	4.13	121.23	118.10
2	B	501	HEM	C3B-C2B-C1B	3.97	109.43	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C4-C4A-N5	3.88	122.37	119.12
2	A	501	HEM	C3B-C2B-C1B	3.64	109.19	106.49
2	A	501	HEM	C4D-ND-C1D	3.58	108.77	105.07
3	B	502	H4B	N2-C2-N1	3.55	122.77	117.25
4	B	505	QJ7	C05-C06-N01	-3.52	119.17	122.90
4	A	503	QJ7	C14-C15-C16	3.51	120.10	116.71
3	A	502	H4B	N1-C2-N3	-3.44	120.03	125.42
2	B	501	HEM	CMD-C2D-C1D	3.42	130.25	125.04
4	B	505	QJ7	O09-C08-C06	3.27	118.21	109.42
4	B	505	QJ7	C12-N11-C16	3.23	121.88	117.48
2	B	501	HEM	CBD-CAD-C3D	-3.16	103.85	112.63
4	A	503	QJ7	O09-C08-C06	3.13	117.86	109.42
4	B	505	QJ7	C14-C15-C16	3.09	119.69	116.71
3	B	502	H4B	C8A-C4A-C4	2.96	117.20	114.57
2	B	501	HEM	C1D-C2D-C3D	-2.95	103.85	106.96
4	A	503	QJ7	C24-C23-C22	-2.93	119.48	123.29
6	B	504	GOL	O3-C3-C2	-2.93	96.14	110.20
4	B	505	QJ7	C24-C23-C22	-2.91	119.51	123.29
3	A	502	H4B	C4A-C4-N3	-2.83	115.97	124.01
2	B	501	HEM	CHC-C4B-NB	2.77	127.44	124.43
3	B	502	H4B	C2-N1-C8A	2.65	120.49	114.54
4	A	503	QJ7	C12-N11-C16	2.62	121.05	117.48
2	A	501	HEM	CBA-CAA-C2A	-2.58	108.21	112.62
3	A	502	H4B	C2-N1-C8A	2.55	120.26	114.54
4	A	503	QJ7	C04-C05-C06	-2.54	118.66	120.32
4	A	503	QJ7	C08-C06-C05	2.52	124.58	121.08
4	A	503	QJ7	C21-C22-C23	2.45	121.04	118.81
2	A	501	HEM	C2C-C3C-C4C	2.44	108.60	106.90
4	B	505	QJ7	C19-C20-C21	-2.43	107.23	112.87
2	A	501	HEM	CHB-C1B-NB	2.37	127.31	124.38
3	A	502	H4B	N2-C2-N3	2.28	120.79	117.25
4	B	505	QJ7	C15-C16-N11	-2.21	119.41	123.72
2	A	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	B	501	HEM	CHA-C4D-ND	2.12	127.00	124.38
2	B	501	HEM	C2C-C3C-C4C	2.05	108.33	106.90
2	A	501	HEM	CMD-C2D-C1D	2.05	128.16	125.04
2	A	501	HEM	CHA-C4D-ND	2.04	126.90	124.38
3	B	502	H4B	C4A-N5-C6	-2.03	115.63	121.16
6	B	504	GOL	O1-C1-C2	-2.02	100.53	110.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

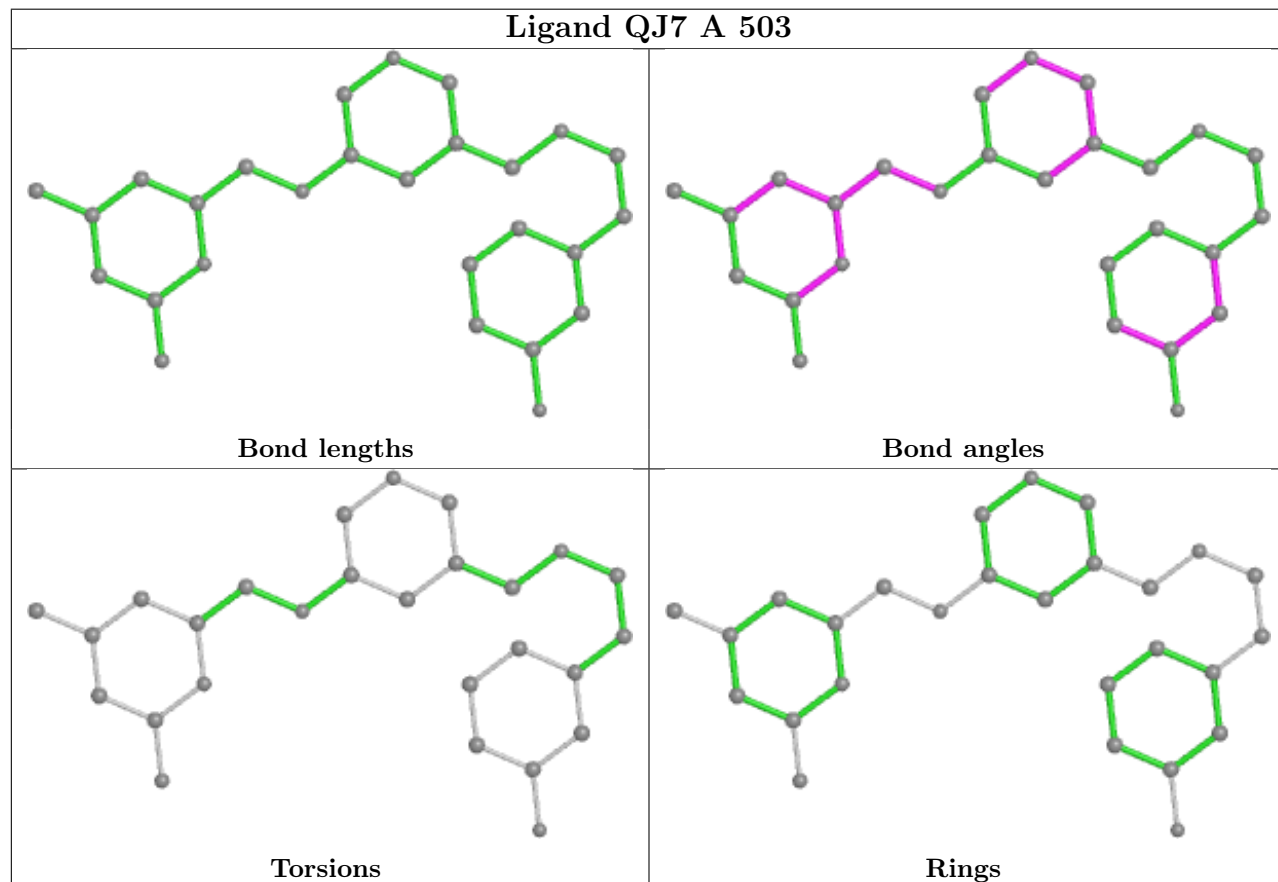
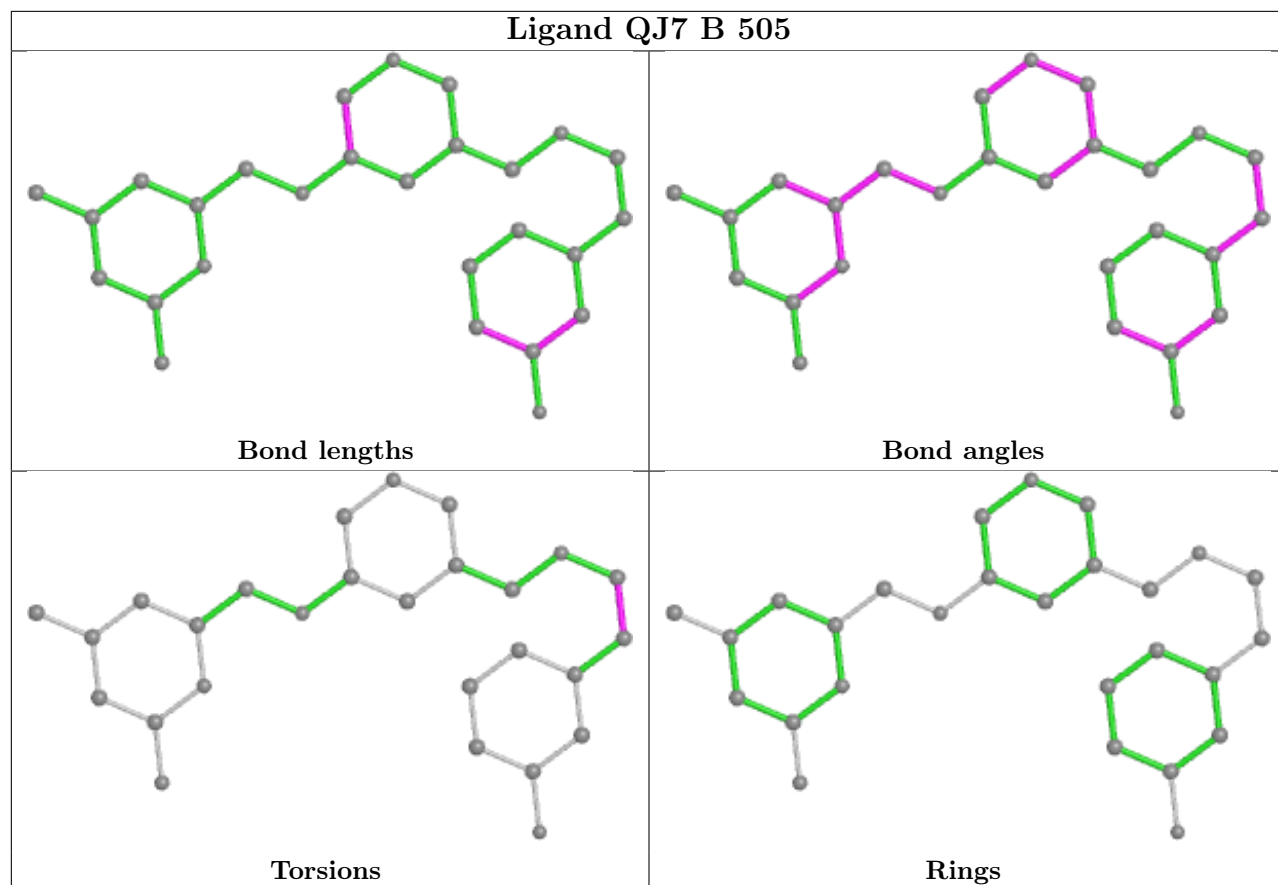
Mol	Chain	Res	Type	Atoms
4	B	505	QJ7	N18-C19-C20-C21
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
6	B	504	GOL	C1-C2-C3-O3
2	A	501	HEM	CAA-CBA-CGA-O2A
6	A	505	GOL	O1-C1-C2-C3
2	A	501	HEM	CAA-CBA-CGA-O1A

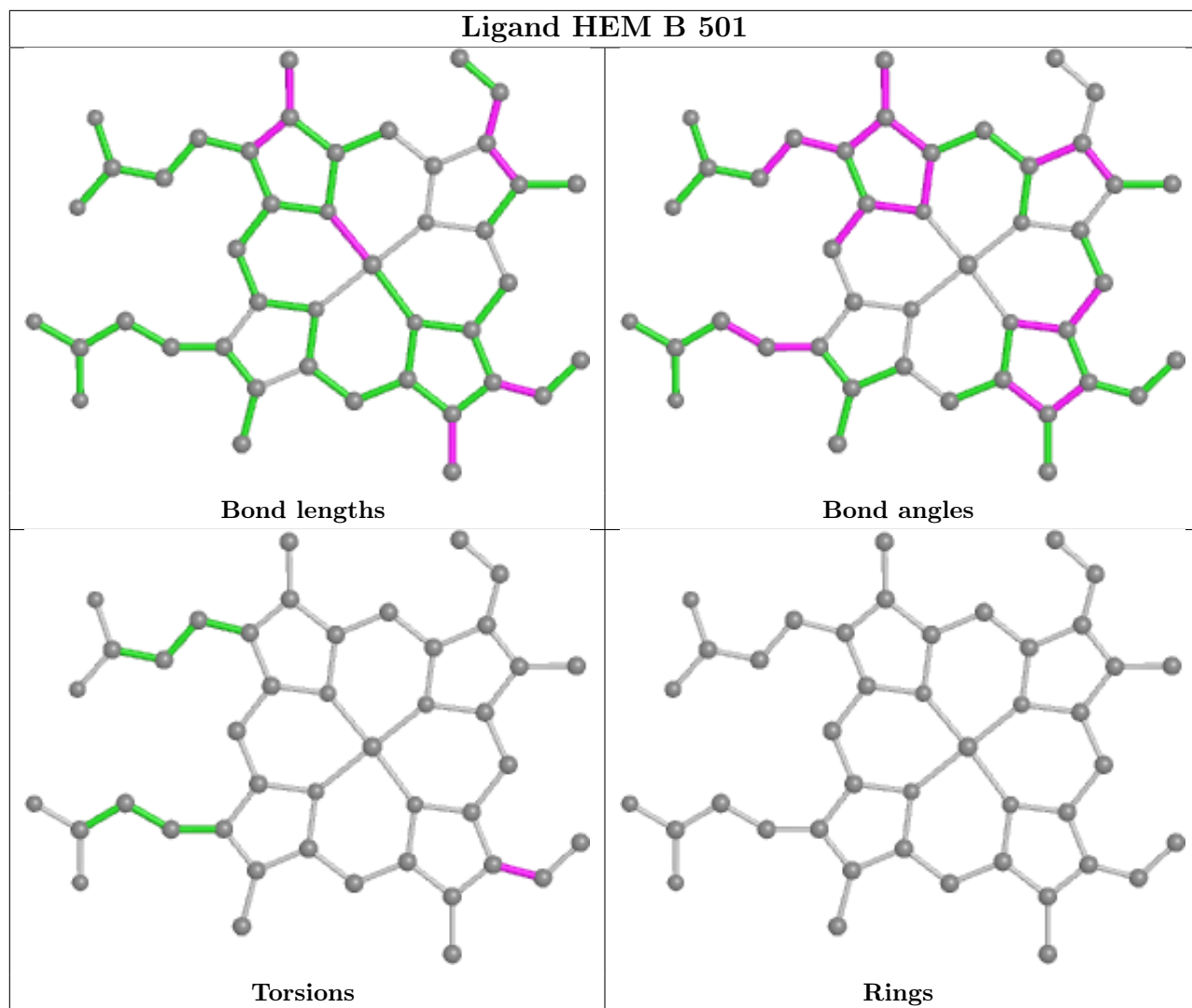
There are no ring outliers.

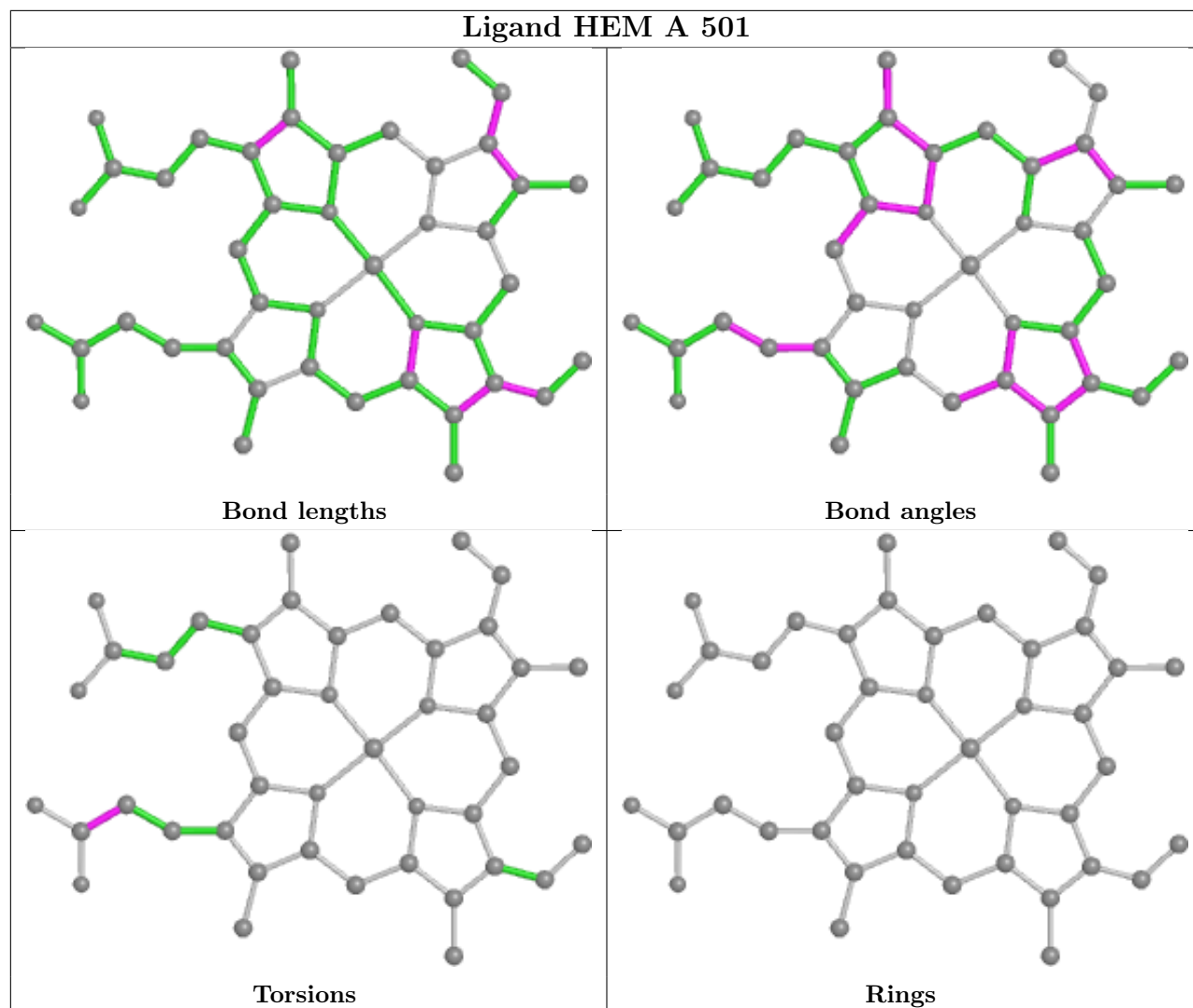
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	H4B	1	0
3	B	502	H4B	1	0
4	B	505	QJ7	1	0
4	A	503	QJ7	2	0
2	B	501	HEM	3	0
6	B	504	GOL	1	0
2	A	501	HEM	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

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	405/443 (91%)	0.05	21 (5%) 27 30	26, 43, 68, 83	0
1	B	404/443 (91%)	-0.00	13 (3%) 47 50	29, 45, 71, 89	0
All	All	809/886 (91%)	0.03	34 (4%) 36 38	26, 44, 70, 89	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	5.0
1	A	239	GLY	4.7
1	A	259	GLN	4.1
1	B	111	LEU	3.9
1	B	110	LYS	3.8
1	A	123	GLU	3.8
1	A	160	ALA	3.6
1	A	126	LEU	3.4
1	A	91	GLN	3.1
1	B	144	GLY	3.1
1	B	260	ASP	3.0
1	B	122	ALA	2.9
1	B	121	PRO	2.9
1	A	109	ARG	2.9
1	A	153	GLN	2.7
1	B	123	GLU	2.6
1	A	338	VAL	2.6
1	A	238	PRO	2.6
1	B	108	PRO	2.5
1	A	124	GLN	2.5
1	B	141	LYS	2.5
1	A	122	ALA	2.5
1	B	142	ARG	2.5
1	A	121	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	LYS	2.4
1	A	156	GLU	2.4
1	A	127	SER	2.4
1	A	130	ARG	2.3
1	A	67	GLY	2.2
1	A	257	ARG	2.1
1	A	223	ARG	2.1
1	B	449	TRP	2.1
1	A	354	PRO	2.1
1	B	337	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	A	384	9/10	0.96	0.09	43,45,73,74	0
1	CAS	B	384	9/10	0.98	0.09	52,53,75,77	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

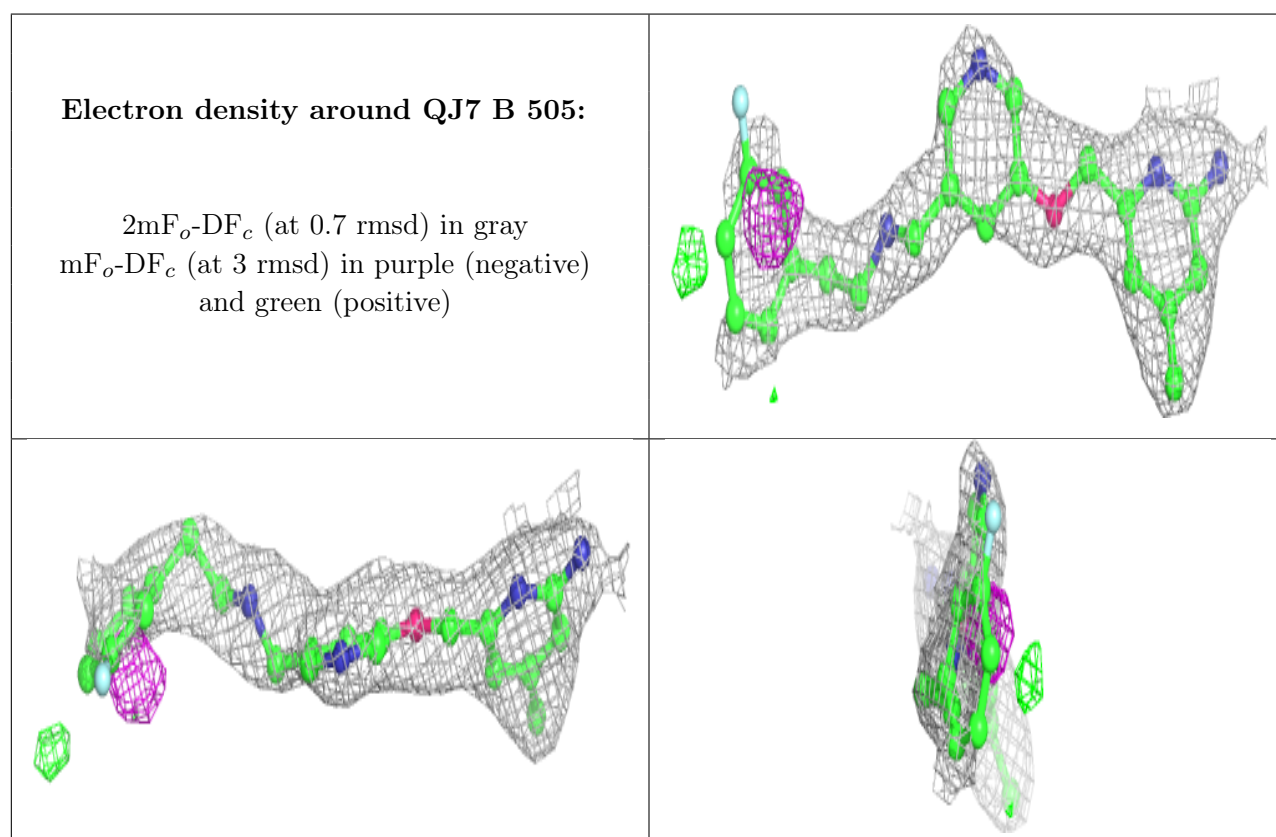
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QJ7	B	505	27/27	0.89	0.23	35,58,79,81	0
6	GOL	A	505	6/6	0.90	0.35	62,62,64,69	0
6	GOL	B	504	6/6	0.93	0.26	50,50,52,53	0
4	QJ7	A	503	27/27	0.94	0.24	29,49,72,75	0
5	ACT	B	503	4/4	0.94	0.23	51,51,52,54	0
5	ACT	A	504	4/4	0.96	0.14	47,47,49,49	0

Continued on next page...

Continued from previous page...

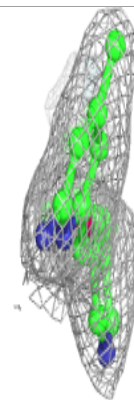
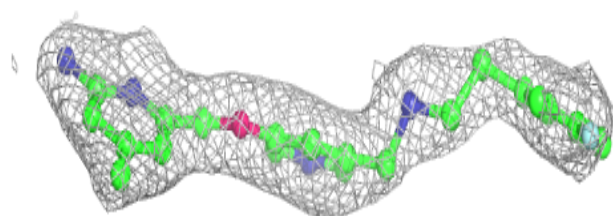
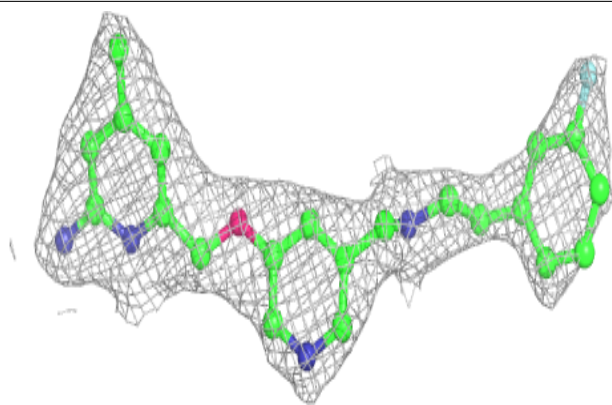
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	501	43/43	0.98	0.18	24,30,40,44	0
2	HEM	B	501	43/43	0.98	0.16	30,34,39,44	0
3	H4B	B	502	17/17	0.98	0.19	27,31,35,36	0
3	H4B	A	502	17/17	0.99	0.21	29,33,37,38	0
7	ZN	A	506	1/1	1.00	0.10	37,37,37,37	0

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.



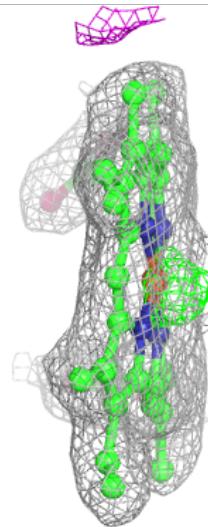
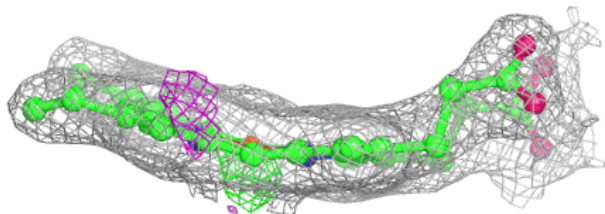
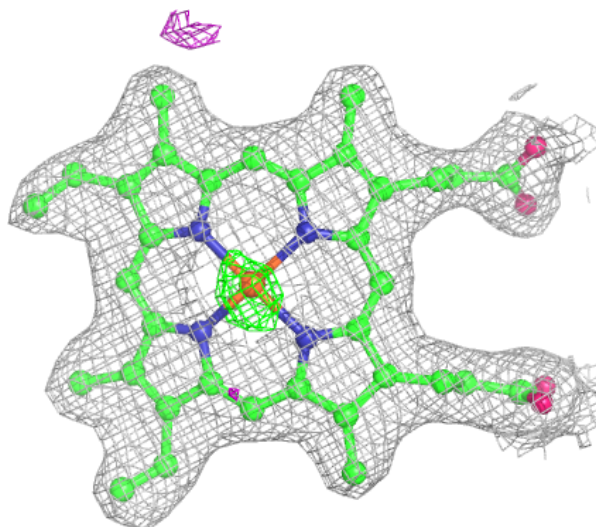
Electron density around QJ7 A 503:

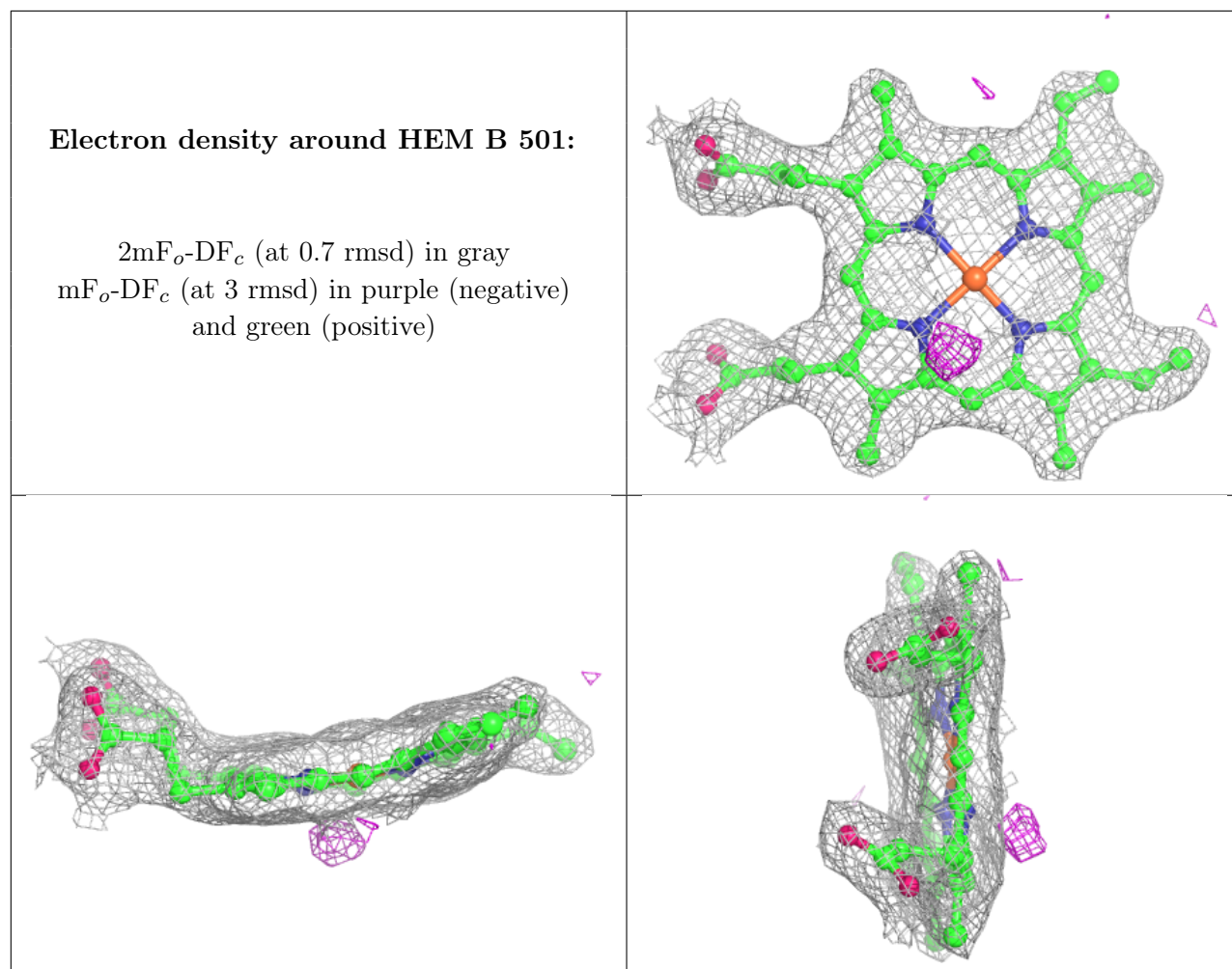
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.