



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:58 AM EDT

PDB ID : 1ARP / pdb_00001arp
Title : Crystal structure of the fungal peroxidase from *Arthromyces ramosus* at 1.9 angstroms resolution: structural comparisons with the lignin and cytochrome C peroxidases
Authors : Kunishima, N.; Fukuyama, K.
Deposited on : 1993-06-18
Resolution : 1.90 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

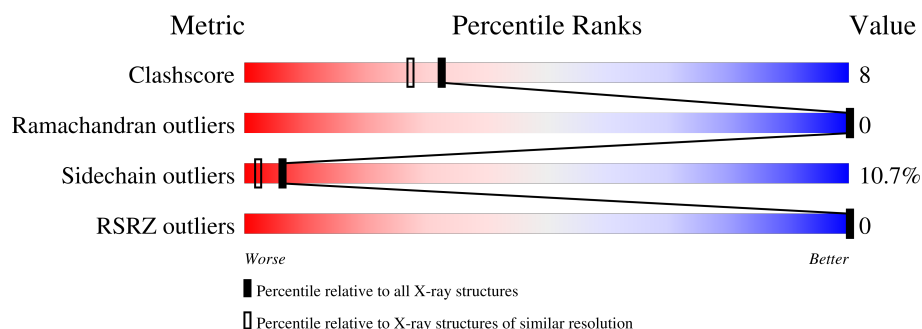
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	344	
2	B	2	

2 Entry composition [i](#)

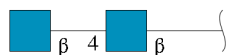
There are 5 unique types of molecules in this entry. The entry contains 2784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2465	1537	421	492	15			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

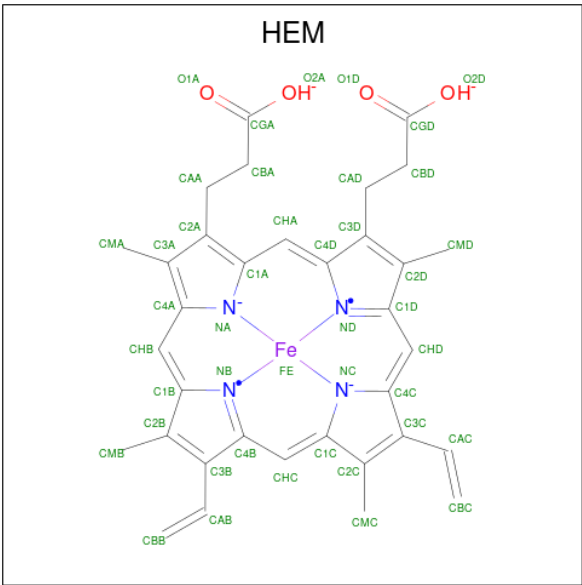


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is water.

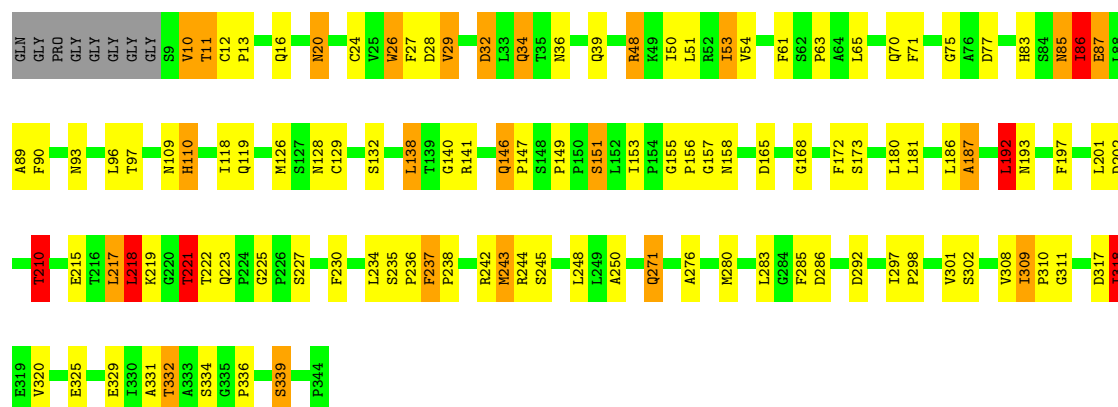
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	246	Total	O	0	0
			246	246		

3 Residue-property plots

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: PEROXIDASE

Chain A: 



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	74.57Å 74.57Å 117.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90 7.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.90) 71.5 (7.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , (Not available) 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2784	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: CA, NAG, 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	1.03	3/2521 (0.1%)	1.96	83/3436 (2.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	ILE	CA-CB	7.42	1.62	1.55
1	A	318	ILE	CA-CB	6.69	1.63	1.54
1	A	149	PRO	CA-C	5.69	1.55	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASP	CA-CB-CG	12.42	125.02	112.60
1	A	39	GLN	OE1-CD-NE2	-10.95	111.65	122.60
1	A	271	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	A	271	GLN	CG-CD-NE2	9.57	130.75	116.40
1	A	48	ARG	NE-CZ-NH2	-9.29	110.84	119.20
1	A	210	THR	N-CA-CB	-9.13	95.24	110.39
1	A	187	ALA	N-CA-C	8.92	122.63	109.07
1	A	311	GLY	N-CA-C	7.96	125.11	113.48
1	A	336	PRO	N-CA-C	-7.95	99.48	111.57
1	A	149	PRO	O-C-N	-7.89	117.68	121.31
1	A	119	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	A	39	GLN	CG-CD-NE2	7.53	127.70	116.40
1	A	153	ILE	CA-C-O	-7.27	114.46	119.19
1	A	132	SER	N-CA-C	7.17	118.94	109.83
1	A	83	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	244	ARG	CA-C-O	-6.80	113.62	120.90
1	A	286	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	334	SER	N-CA-C	-6.74	101.31	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH1	6.57	128.06	121.50
1	A	155	GLY	CA-C-N	6.53	126.16	119.56
1	A	155	GLY	C-N-CA	6.53	126.16	119.56
1	A	16	GLN	N-CA-C	-6.53	101.73	110.55
1	A	11	THR	N-CA-C	-6.52	98.57	109.07
1	A	221	THR	N-CA-CB	-6.51	99.49	110.49
1	A	158	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	A	10	VAL	N-CA-C	6.49	116.58	107.37
1	A	165	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	151	SER	N-CA-C	6.44	120.71	112.86
1	A	339	SER	N-CA-C	-6.26	97.62	108.69
1	A	237	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	36	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	97	THR	N-CA-C	6.14	118.47	111.11
1	A	70	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	26	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	A	271	GLN	CB-CG-CD	5.99	122.78	112.60
1	A	83	HIS	CG-CD2-NE2	-5.87	101.33	107.20
1	A	192	LEU	N-CA-C	-5.86	105.22	112.90
1	A	89	ALA	N-CA-C	-5.85	106.18	113.38
1	A	110	HIS	CG-CD2-NE2	-5.84	101.36	107.20
1	A	141	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	A	93	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	126	MET	CA-CB-CG	-5.83	102.45	114.10
1	A	24	CYS	CA-C-O	-5.82	114.38	120.55
1	A	285	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	325	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	309	ILE	N-CA-C	-5.78	101.30	107.77
1	A	193	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	32	ASP	CA-CB-CG	5.75	118.34	112.60
1	A	77	ASP	N-CA-C	5.73	119.97	112.92
1	A	71	PHE	N-CA-C	-5.73	101.17	109.59
1	A	10	VAL	CB-CA-C	-5.72	105.73	111.80
1	A	158	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	153	ILE	CA-C-N	5.60	125.53	119.76
1	A	153	ILE	C-N-CA	5.60	125.53	119.76
1	A	90	PHE	CA-C-N	5.55	125.64	119.32
1	A	90	PHE	C-N-CA	5.55	125.64	119.32
1	A	20	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	243	MET	CG-SD-CE	-5.52	88.75	100.90
1	A	87	GLU	N-CA-C	5.45	118.14	111.82
1	A	128	ASN	OD1-CG-ND2	-5.43	117.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	HIS	ND1-CG-CD2	5.41	111.51	106.10
1	A	109	ASN	CA-C-O	-5.40	114.70	120.42
1	A	235	SER	CA-C-O	-5.37	116.30	121.08
1	A	27	PHE	N-CA-C	-5.37	105.46	112.23
1	A	218	LEU	CA-CB-CG	5.37	135.08	116.30
1	A	225	GLY	CA-C-N	5.35	125.67	119.47
1	A	225	GLY	C-N-CA	5.35	125.67	119.47
1	A	332	THR	CA-CB-OG1	-5.32	101.62	109.60
1	A	197	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	53	ILE	O-C-N	-5.26	116.77	121.87
1	A	28	ASP	CB-CA-C	-5.22	102.02	110.79
1	A	140	GLY	O-C-N	-5.16	115.99	122.70
1	A	223	GLN	N-CA-C	-5.16	99.41	108.69
1	A	34	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	157	GLY	N-CA-C	-5.13	106.69	115.61
1	A	129	CYS	CA-C-N	5.12	125.13	119.90
1	A	129	CYS	C-N-CA	5.12	125.13	119.90
1	A	309	ILE	CA-C-O	5.11	122.93	119.20
1	A	146	GLN	CA-C-N	5.02	124.78	119.76
1	A	146	GLN	C-N-CA	5.02	124.78	119.76
1	A	173	SER	CA-C-N	5.02	125.04	119.32
1	A	173	SER	C-N-CA	5.02	125.04	119.32
1	A	10	VAL	O-C-N	5.01	127.81	122.45

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	2465	0	2375	39	0
2	B	28	0	25	0	0
3	A	2	0	0	0	0
4	A	43	0	30	3	0
5	A	246	0	0	5	0
All	All	2784	0	2430	39	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 8.

All (39) 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:217:LEU:HD13	1:A:250:ALA:HB1	1.82	0.61
1:A:156:PRO:HB3	1:A:243:MET:HE3	1.82	0.60
1:A:219:LYS:HG3	1:A:317:ASP:O	2.02	0.59
1:A:86:ILE:HG12	1:A:147:PRO:HB3	1.85	0.59
1:A:54:VAL:HG23	1:A:118:ILE:HG22	1.86	0.57
1:A:138:LEU:HD12	1:A:292:ASP:HA	1.87	0.57
1:A:243:MET:HE1	4:A:345:HEM:CHB	2.36	0.56
1:A:86:ILE:HG13	1:A:87:GLU:N	2.21	0.55
1:A:236:PRO:HD3	1:A:242:ARG:NH2	2.24	0.53
1:A:180:LEU:HD13	1:A:276:ALA:HB1	1.91	0.52
1:A:301:VAL:HG12	5:A:482:HOH:O	2.08	0.52
1:A:318:ILE:HD11	1:A:320:VAL:HG22	1.91	0.52
1:A:12:CYS:HB3	5:A:350:HOH:O	2.10	0.50
1:A:308:VAL:HG12	1:A:331:ALA:HB3	1.93	0.49
1:A:34:GLN:HE21	1:A:34:GLN:HA	1.78	0.49
1:A:48:ARG:HD3	1:A:187:ALA:HA	1.95	0.48
1:A:215:GLU:HA	1:A:218:LEU:CD2	2.43	0.48
1:A:243:MET:HE2	1:A:245:SER:OG	2.13	0.48
1:A:156:PRO:HB3	1:A:243:MET:CE	2.44	0.47
1:A:210:THR:HG22	5:A:530:HOH:O	2.14	0.46
1:A:26:TRP:HA	1:A:29:VAL:CG1	2.45	0.46
1:A:85:ASN:H	1:A:85:ASN:HD22	1.63	0.46
1:A:215:GLU:HA	1:A:218:LEU:HD22	1.97	0.46
1:A:156:PRO:CB	1:A:243:MET:HE3	2.46	0.45
1:A:221:THR:HG22	1:A:222:THR:OG1	2.17	0.44
1:A:48:ARG:HD2	4:A:345:HEM:O2D	2.19	0.43
1:A:51:LEU:HB2	4:A:345:HEM:HMD3	2.01	0.43
1:A:192:LEU:HG	1:A:230:PHE:O	2.19	0.43
1:A:297:ILE:HA	1:A:298:PRO:HD2	1.93	0.42
1:A:309:ILE:HA	1:A:310:PRO:HD3	1.79	0.42
1:A:280:MET:HA	1:A:283:LEU:HD13	2.02	0.42
1:A:221:THR:HG21	5:A:538:HOH:O	2.20	0.41
1:A:20:ASN:HB2	5:A:563:HOH:O	2.21	0.41
1:A:32:ASP:OD2	1:A:110:HIS:HE1	2.04	0.41
1:A:168:GLY:HA2	1:A:172:PHE:O	2.21	0.41
1:A:238:PRO:HB2	1:A:339:SER:HA	2.02	0.40
1:A:51:LEU:O	1:A:54:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HG13	1:A:96:LEU:HD22	2.04	0.40
1:A:61:PHE:HB2	1:A:75:GLY:HA2	2.02	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	334/344 (97%)	325 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/273 (99%)	242 (89%)	29 (11%)	6	2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	11	THR
1	A	13	PRO
1	A	29	VAL

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Mol	Chain	Res	Type
1	A	50	ILE
1	A	63	PRO
1	A	65	LEU
1	A	85	ASN
1	A	86	ILE
1	A	138	LEU
1	A	146	GLN
1	A	151	SER
1	A	181	LEU
1	A	186	LEU
1	A	192	LEU
1	A	201	LEU
1	A	210	THR
1	A	217	LEU
1	A	218	LEU
1	A	221	THR
1	A	227	SER
1	A	234	LEU
1	A	237	PHE
1	A	248	LEU
1	A	271	GLN
1	A	302	SER
1	A	318	ILE
1	A	329	GLU
1	A	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	36	ASN
1	A	83	HIS
1	A	85	ASN
1	A	110	HIS
1	A	193	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.63	0	17,19,21	1.37	3 (17%)
2	NAG	B	2	2	14,14,15	0.61	0	17,19,21	0.98	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-C2-N2	3.35	115.71	110.43
2	B	1	NAG	O5-C1-C2	-2.42	107.55	111.29
2	B	1	NAG	C6-C5-C4	-2.34	107.26	113.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6

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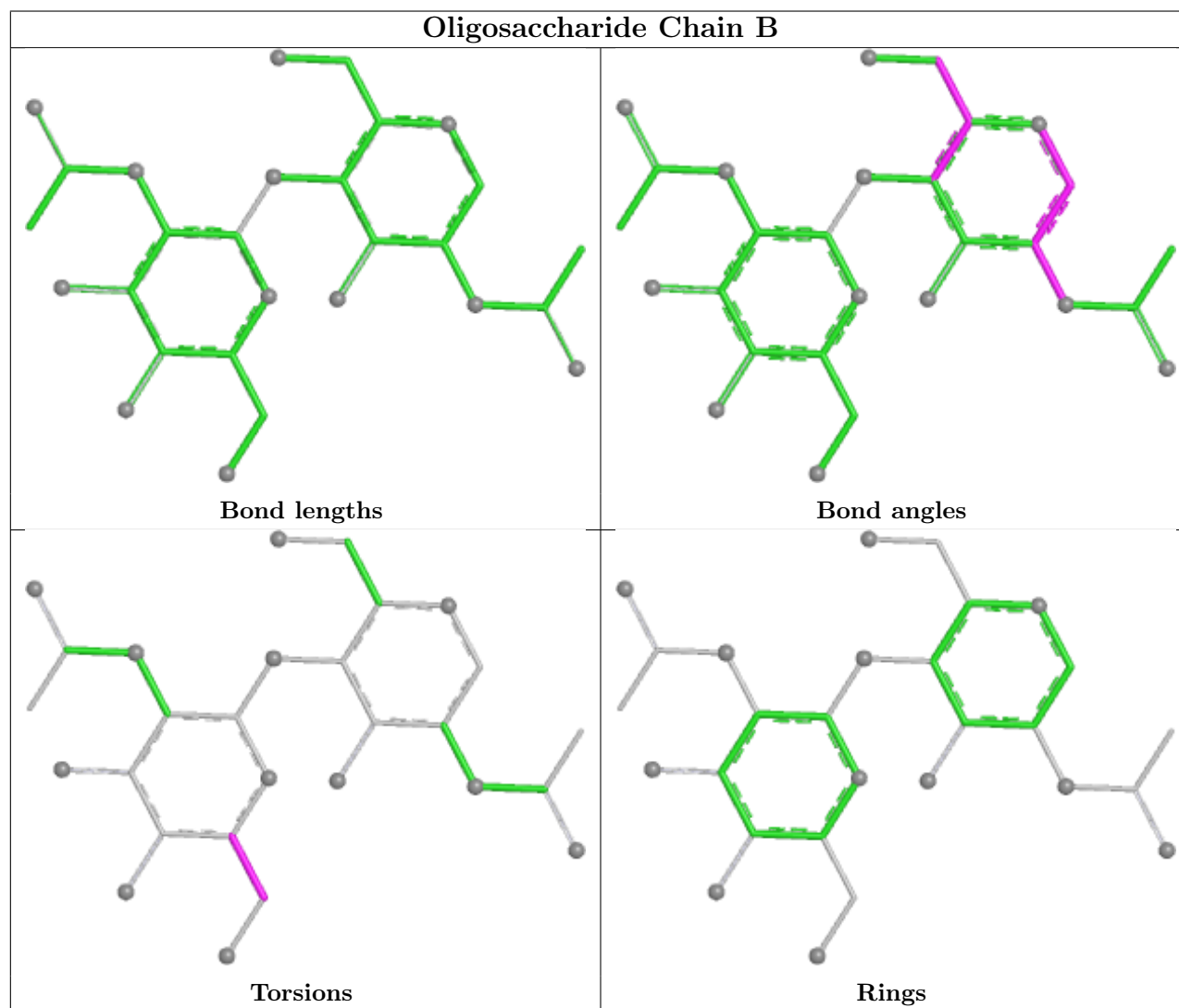
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Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	HEM	A	345	1	50,50,50	1.23	7 (14%)	67,82,82	0.86	2 (2%)

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
4	HEM	A	345	1	-	4/14/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	345	HEM	CAC-C3C	-3.05	1.39	1.47
4	A	345	HEM	O2D-CGD	-3.01	1.20	1.30
4	A	345	HEM	CBB-CAB	3.01	1.44	1.30
4	A	345	HEM	CBC-CAC	2.95	1.44	1.30
4	A	345	HEM	O2A-CGA	-2.54	1.22	1.30
4	A	345	HEM	CAB-C3B	-2.44	1.40	1.47
4	A	345	HEM	C4D-C3D	-2.17	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	345	HEM	C3B-C4B-NB	2.54	111.29	109.47
4	A	345	HEM	O2D-CGD-CBD	2.35	121.44	114.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

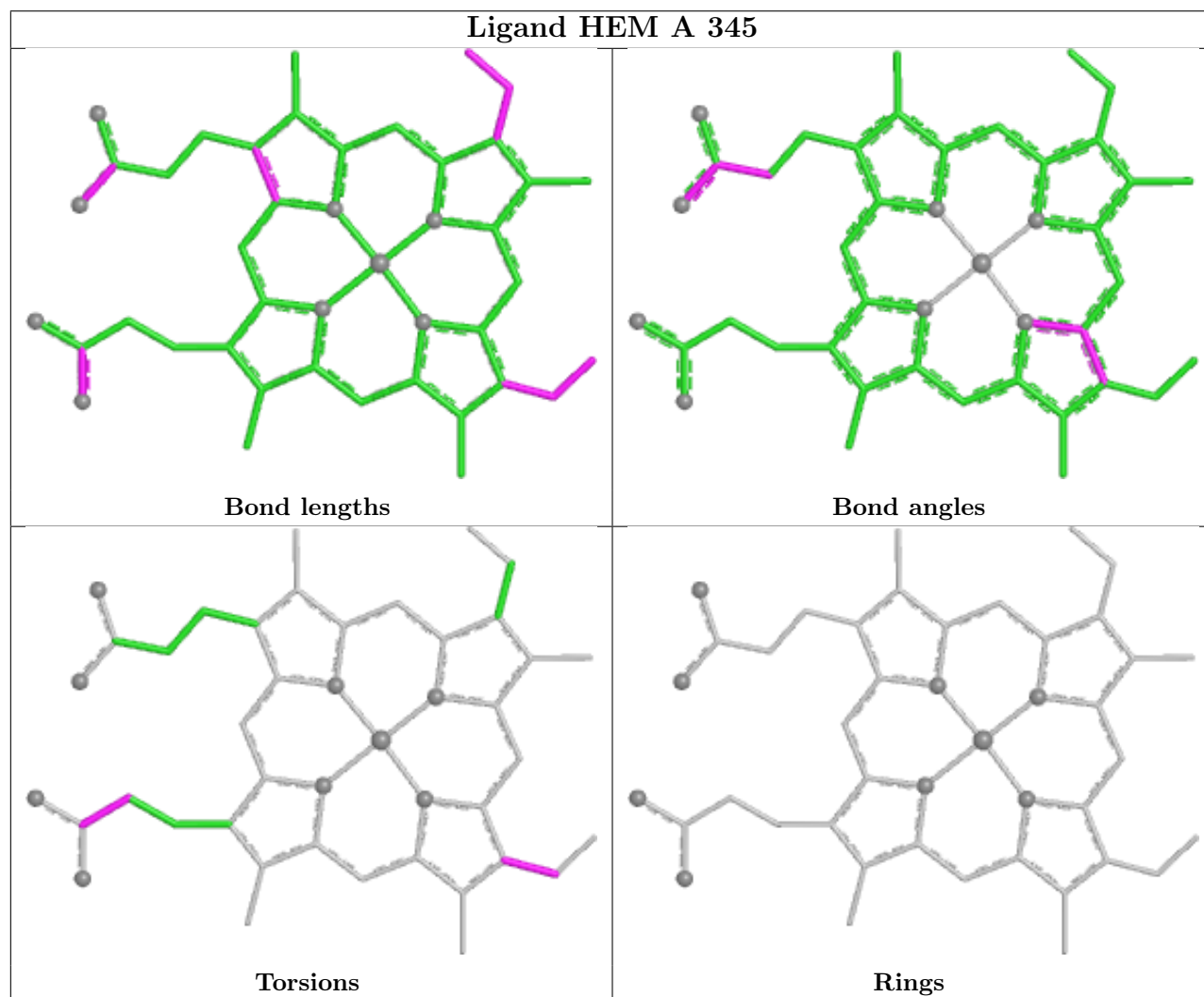
Mol	Chain	Res	Type	Atoms
4	A	345	HEM	C2B-C3B-CAB-CBB
4	A	345	HEM	C4B-C3B-CAB-CBB
4	A	345	HEM	CAA-CBA-CGA-O1A
4	A	345	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	345	HEM	3	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	336/344 (97%)	-0.74	0 100 100	7, 14, 25, 31	0

There are no RSRZ outliers to report.

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

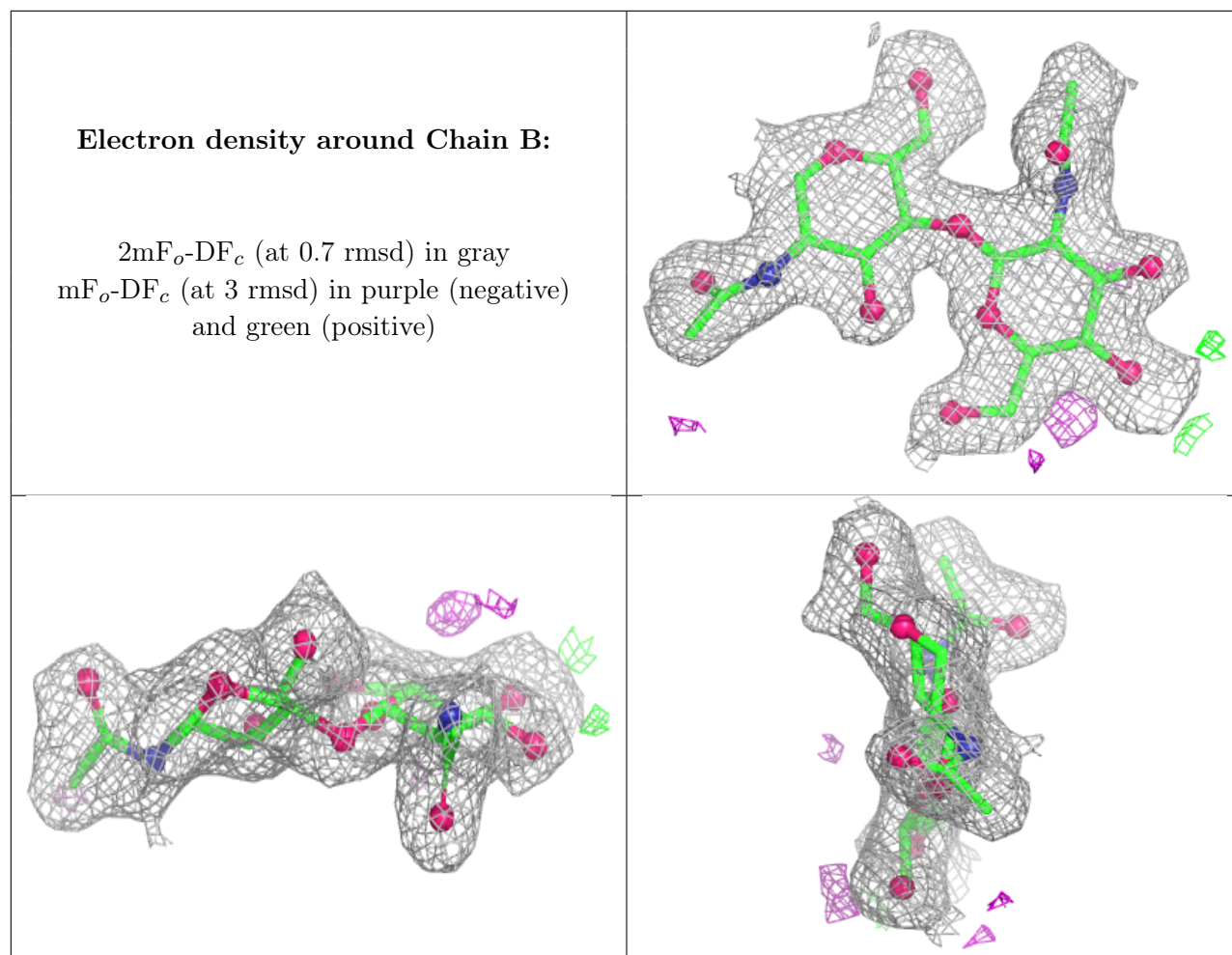
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	NAG	B	2	14/15	0.92	0.05	13,18,21,21	0
2	NAG	B	1	14/15	0.94	0.05	15,17,22,22	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

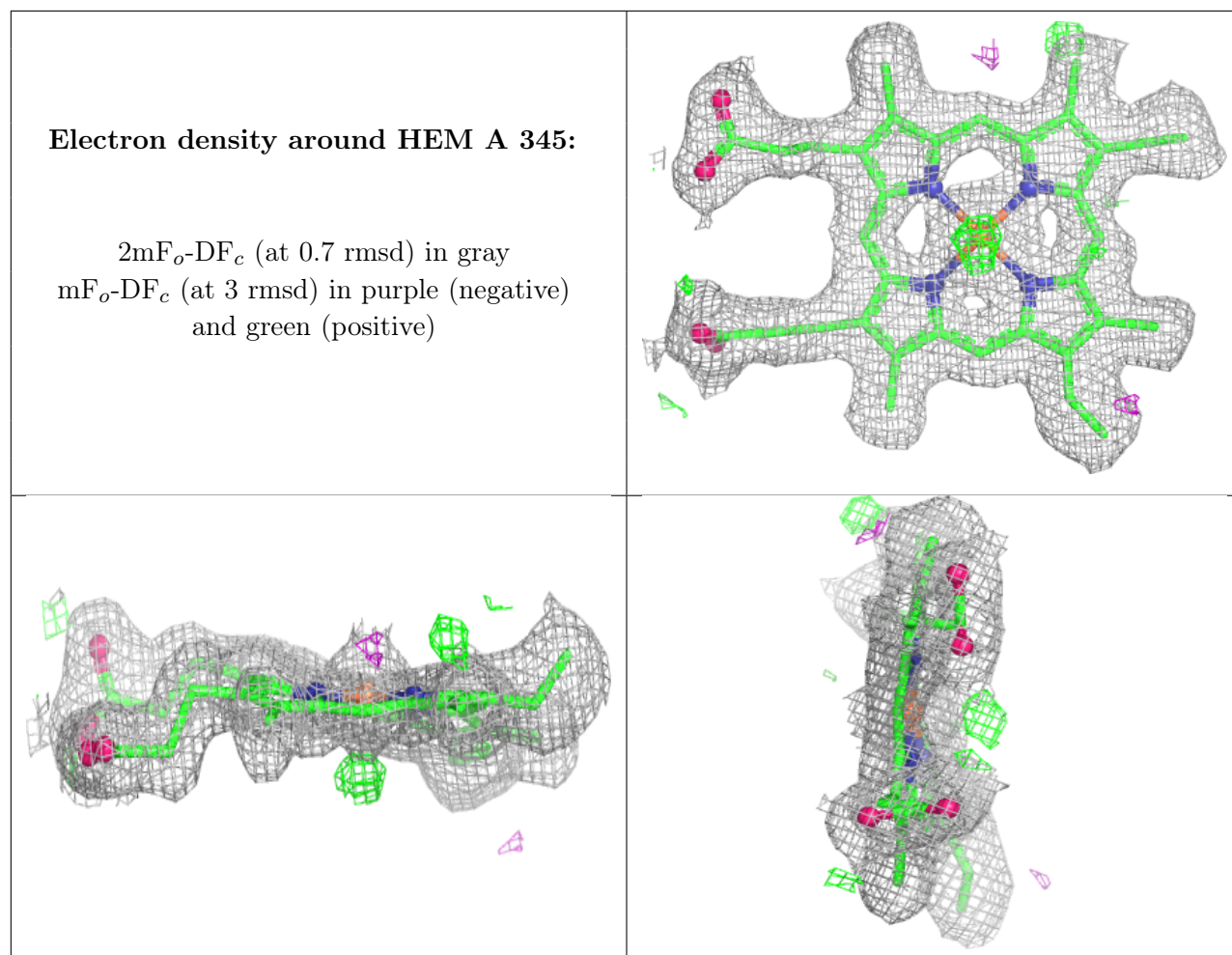


6.4 Ligands [i](#)

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
3	CA	A	346	1/1	0.98	0.02	12,12,12,12	0
4	HEM	A	345	43/43	0.98	0.04	8,11,14,19	0
3	CA	A	347	1/1	0.99	0.05	14,14,14,14	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.