



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:44 AM EDT

PDB ID : 2B12 / pdb_00002b12
Title : Crystal structure of the protein-protein complex between F82Y cytochrome c and cytochrome c peroxidase
Authors : Kang, S.A.; Crane, B.R.
Deposited on : 2005-09-15
Resolution : 3.02 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

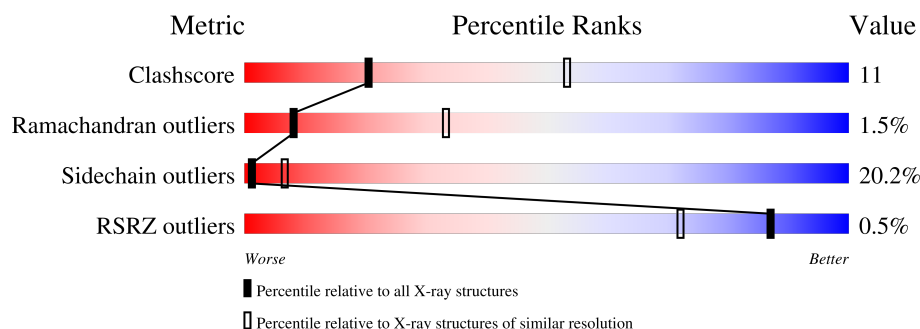
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	294	
2	B	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZNH	A	295	X	-	-	-
4	HEC	B	109	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3328 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 Cytochrome c peroxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2370	1512	395	457	6			

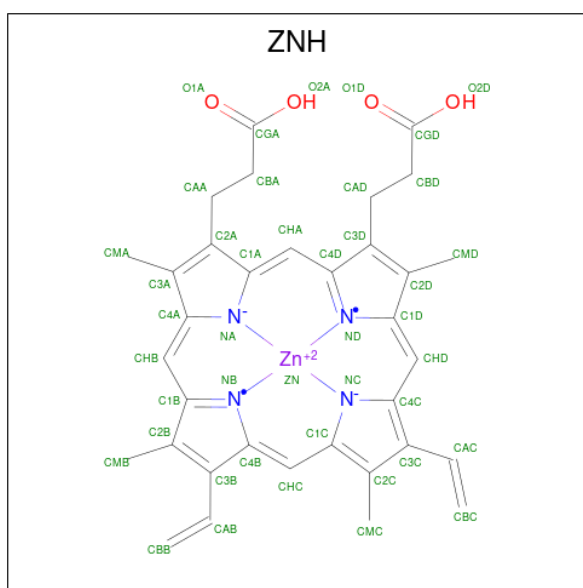
- Molecule 2 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			848	534	151	158	5			

There is a discrepancy between the modelled and reference sequences:

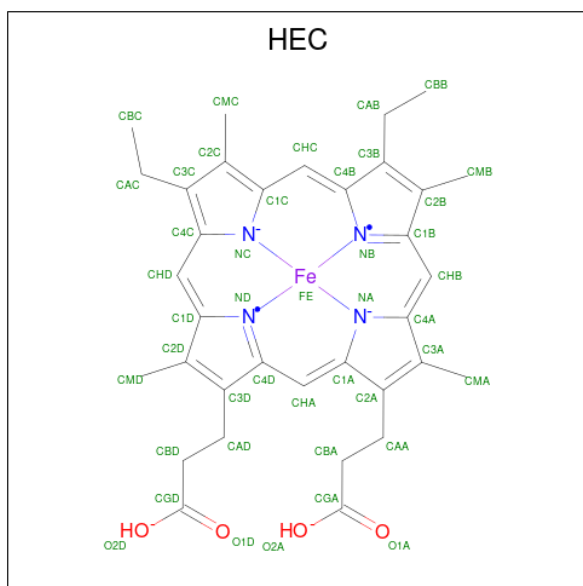
Chain	Residue	Modelled	Actual	Comment	Reference
B	82	TYR	PHE	engineered mutation	UNP P00044

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING ZN (CCD ID: ZNH) (formula: $C_{34}H_{32}N_4O_4Zn$).



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

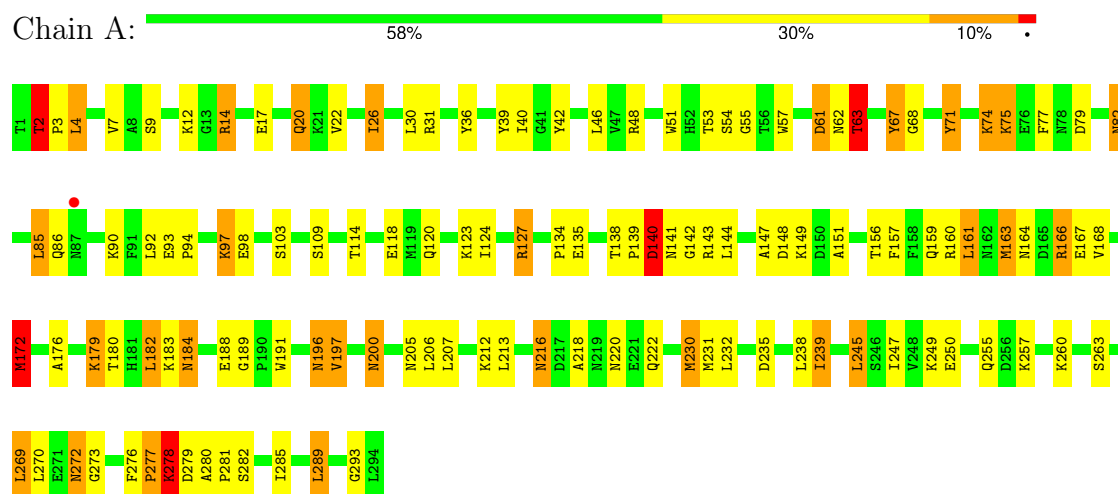
- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



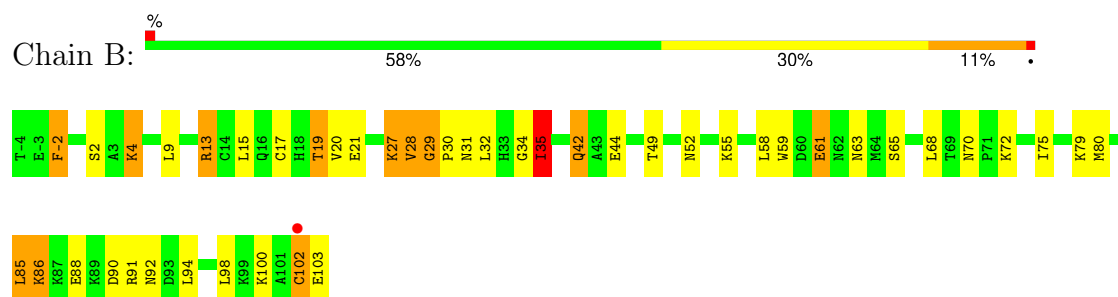
3 Residue-property plots [i](#)

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: Cytochrome c peroxidase, mitochondrial



- Molecule 2: Cytochrome c iso-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.79Å 51.83Å 183.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.02 20.00 – 3.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.02) 90.3 (20.00-3.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.277 , 0.268 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.5	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	0.84	EDS
Total number of atoms	3328	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: ZNH, HEC

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	15/2437 (0.6%)	1.52	38/3301 (1.2%)
2	B	1.02	1/866 (0.1%)	1.53	19/1158 (1.6%)
All	All	1.03	16/3303 (0.5%)	1.53	57/4459 (1.3%)

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	A	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	CYS	CB-SG	-11.78	1.42	1.81
1	A	163	MET	SD-CE	-9.45	1.55	1.79
1	A	2	THR	CA-C	9.00	1.64	1.52
1	A	278	LYS	CB-CG	8.61	1.78	1.52
1	A	230	MET	SD-CE	-6.84	1.62	1.79
1	A	140	ASP	C-O	-6.70	1.15	1.24
1	A	139	PRO	CA-CB	-6.25	1.46	1.53
1	A	276	PHE	CA-C	-6.20	1.46	1.53
1	A	172	MET	SD-CE	-6.10	1.64	1.79
1	A	53	THR	CB-OG1	5.67	1.52	1.43
1	A	197	VAL	CA-CB	5.59	1.61	1.54
1	A	141	ASN	N-CA	5.24	1.52	1.45
1	A	278	LYS	CG-CD	5.21	1.68	1.52
1	A	278	LYS	N-CA	-5.20	1.39	1.46
1	A	285	ILE	CA-CB	5.15	1.59	1.53
1	A	139	PRO	C-O	-5.04	1.18	1.23

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	VAL	N-CA-C	13.15	125.52	111.58
1	A	279	ASP	N-CA-C	-12.03	94.18	113.19
2	B	70	ASN	CA-C-N	10.20	129.85	119.24
2	B	70	ASN	C-N-CA	10.20	129.85	119.24
1	A	2	THR	N-CA-C	9.81	131.50	109.81
1	A	277	PRO	CB-CA-C	8.40	121.96	111.12
1	A	276	PHE	CA-C-N	-7.83	111.55	119.92
1	A	276	PHE	C-N-CA	-7.83	111.55	119.92
1	A	276	PHE	N-CA-C	7.78	119.57	109.93
1	A	278	LYS	N-CA-CB	-7.77	99.21	110.56
1	A	139	PRO	CB-CA-C	-7.25	104.80	111.40
2	B	42	GLN	N-CA-C	7.11	121.37	111.56
1	A	151	ALA	N-CA-C	6.91	119.40	111.11
2	B	65	SER	N-CA-C	-6.76	103.38	111.69
1	A	68	GLY	N-CA-C	6.74	121.88	114.40
1	A	61	ASP	N-CA-C	6.71	122.67	112.54
2	B	13	ARG	N-CA-C	6.43	121.29	113.38
1	A	269	LEU	CA-CB-CG	6.30	138.36	116.30
1	A	245	LEU	CA-CB-CG	6.25	138.16	116.30
1	A	3	PRO	N-CA-C	-6.22	101.85	111.13
1	A	142	GLY	N-CA-C	6.19	123.86	115.32
2	B	29	GLY	CA-C-N	6.16	127.01	120.11
2	B	29	GLY	C-N-CA	6.16	127.01	120.11
1	A	139	PRO	CA-C-O	6.12	128.44	120.85
1	A	74	LYS	N-CA-C	6.00	123.58	110.80
1	A	179	LYS	N-CA-C	5.95	118.00	109.14
1	A	148	ASP	N-CA-C	5.88	120.19	113.19
1	A	36	TYR	N-CA-C	5.88	119.00	110.42
1	A	98	GLU	N-CA-C	-5.79	106.35	113.41
2	B	35	ILE	N-CA-C	5.78	116.56	110.72
2	B	98	LEU	N-CA-C	5.74	118.48	111.82
1	A	138	THR	N-CA-C	-5.73	101.27	109.24
2	B	28	VAL	N-CA-C	-5.66	104.02	111.09
2	B	49	THR	N-CA-C	-5.62	102.20	110.52
1	A	39	TYR	N-CA-C	5.62	121.37	113.56
1	A	144	LEU	N-CA-C	-5.55	103.65	110.31
1	A	57	TRP	N-CA-C	5.54	117.89	110.35
2	B	94	LEU	N-CA-C	5.53	117.39	111.36
1	A	63	THR	CB-CA-C	5.50	119.23	109.72
1	A	147	ALA	N-CA-C	5.46	119.11	112.23
1	A	278	LYS	CB-CG-CD	5.41	123.74	111.30
1	A	272	ASN	N-CA-C	5.40	118.41	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	TYR	N-CA-C	-5.35	105.89	112.90
1	A	149	LYS	N-CA-C	5.33	118.13	109.86
1	A	139	PRO	N-CA-C	5.32	118.94	110.21
1	A	54	SER	N-CA-C	-5.30	107.47	114.31
1	A	184	ASN	N-CA-C	5.29	119.65	111.56
2	B	63	ASN	CA-C-N	5.27	128.32	120.31
2	B	63	ASN	C-N-CA	5.27	128.32	120.31
1	A	2	THR	CA-C-N	5.26	125.72	120.52
1	A	2	THR	C-N-CA	5.26	125.72	120.52
1	A	176	ALA	N-CA-C	-5.22	106.17	112.54
2	B	30	PRO	N-CA-C	5.18	118.74	111.33
2	B	59	TRP	N-CA-C	5.15	116.57	109.15
2	B	61	GLU	N-CA-C	5.15	121.76	110.80
1	A	196	ASN	N-CA-C	5.11	119.15	113.02
2	B	86	LYS	N-CA-C	5.06	118.61	112.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ASP	Mainchain
1	A	61	ASP	Mainchain
1	A	63	THR	Mainchain
1	A	71	TYR	Sidechain

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	2370	0	2246	56	1
2	B	848	0	849	17	1
3	A	43	0	30	0	0
4	B	43	0	30	6	0
5	A	19	0	0	2	0
5	B	5	0	0	0	0
All	All	3328	0	3155	72	1

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 11.

All (72) 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:278:LYS:CB	1:A:278:LYS:CG	1.78	1.60
2:B:17:CYS:SG	4:B:109:HEC:CAC	2.02	1.47
1:A:14:ARG:HG2	1:A:14:ARG:HH21	1.30	0.97
1:A:63:THR:HG23	1:A:143:ARG:HH12	1.30	0.96
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.40	0.87
1:A:48:ARG:HG3	1:A:85:LEU:HD11	1.58	0.82
1:A:278:LYS:CG	1:A:278:LYS:H	1.93	0.82
1:A:63:THR:HG23	1:A:143:ARG:NH1	1.96	0.80
2:B:55:LYS:HD3	2:B:75:ILE:HG12	1.65	0.78
1:A:278:LYS:H	1:A:278:LYS:HG2	1.48	0.78
2:B:17:CYS:CB	4:B:109:HEC:CAC	2.63	0.76
1:A:26:ILE:HG23	1:A:114:THR:HG21	1.70	0.74
1:A:278:LYS:CG	1:A:278:LYS:N	2.52	0.72
1:A:4:LEU:H	1:A:4:LEU:HD12	1.56	0.70
1:A:206:LEU:HG	1:A:239:ILE:HD12	1.76	0.68
1:A:182:LEU:HD21	1:A:218:ALA:HB2	1.76	0.67
2:B:17:CYS:SG	4:B:109:HEC:CBC	2.81	0.66
1:A:127:ARG:HG2	1:A:127:ARG:NH1	2.11	0.64
2:B:85:LEU:HD11	2:B:90:ASP:HB2	1.81	0.62
1:A:22:VAL:O	1:A:26:ILE:HG22	2.00	0.62
1:A:278:LYS:CG	1:A:278:LYS:CA	2.74	0.61
2:B:34:GLY:H	2:B:102:CYS:HB2	1.67	0.59
1:A:182:LEU:HD12	1:A:188:GLU:HB2	1.85	0.58
1:A:200:ASN:H	1:A:200:ASN:HD22	1.50	0.58
1:A:216:ASN:HD22	1:A:218:ALA:H	1.52	0.58
1:A:143:ARG:O	1:A:160:ARG:NH1	2.31	0.58
1:A:79:ASP:HB3	1:A:82:ASN:HB2	1.84	0.57
1:A:163:MET:HG3	1:A:167:GLU:HB3	1.85	0.57
1:A:77:PHE:CZ	1:A:86:GLN:HG3	2.41	0.55
2:B:2:SER:HB2	2:B:4:LYS:HE3	1.89	0.55
2:B:85:LEU:HD12	2:B:91:ARG:HG3	1.89	0.55
1:A:180:THR:HG22	1:A:189:GLY:O	2.07	0.54
1:A:196:ASN:ND2	5:A:516:HOH:O	2.40	0.53
1:A:42:TYR:O	1:A:46:LEU:HD13	2.11	0.50
1:A:55:GLY:HA2	1:A:161:LEU:HD21	1.94	0.50
1:A:182:LEU:CD2	1:A:218:ALA:HB2	2.42	0.49
1:A:26:ILE:HD11	1:A:46:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HG2	1:A:14:ARG:NH2	2.07	0.48
2:B:35:ILE:HG22	2:B:102:CYS:SG	2.53	0.48
2:B:17:CYS:HB2	4:B:109:HEC:C3C	2.43	0.48
1:A:191:TRP:NE1	1:A:235:ASP:OD1	2.44	0.47
1:A:62:ASN:HD21	1:A:273:GLY:HA2	1.80	0.47
2:B:17:CYS:CB	4:B:109:HEC:C3C	2.93	0.46
1:A:206:LEU:HD13	1:A:231:MET:SD	2.56	0.46
1:A:31:ARG:CZ	1:A:289:LEU:HD23	2.46	0.46
1:A:4:LEU:HD12	1:A:4:LEU:N	2.26	0.46
1:A:166:ARG:HH22	1:A:250:GLU:CD	2.23	0.45
1:A:124:ILE:HG12	1:A:263:SER:HA	1.97	0.45
2:B:27:LYS:HB3	2:B:28:VAL:H	1.42	0.45
1:A:109:SER:HB2	1:A:270:LEU:HD13	1.99	0.45
1:A:216:ASN:ND2	1:A:220:ASN:H	2.15	0.45
2:B:17:CYS:O	2:B:29:GLY:N	2.48	0.45
1:A:164:ASN:O	1:A:168:VAL:HG13	2.18	0.44
1:A:17:GLU:HA	1:A:20:GLN:HB2	1.97	0.44
1:A:157:PHE:HE2	1:A:160:ARG:HH11	1.65	0.44
2:B:19:THR:HG22	2:B:31:ASN:OD1	2.18	0.44
1:A:75:LYS:HE3	1:A:140:ASP:HA	2.00	0.43
2:B:-2:PHE:HD1	2:B:92:ASN:HD22	1.66	0.43
1:A:205:ASN:HD21	2:B:72:LYS:HE2	1.83	0.43
1:A:4:LEU:H	1:A:4:LEU:CD1	2.26	0.42
1:A:7:VAL:O	1:A:67:TYR:OH	2.32	0.41
1:A:280:ALA:HB1	1:A:281:PRO:HD2	2.02	0.41
1:A:172:MET:HG2	1:A:238:LEU:HD11	2.02	0.41
1:A:166:ARG:HH21	1:A:257:LYS:HE3	1.85	0.41
2:B:17:CYS:SG	4:B:109:HEC:HBC1	2.60	0.41
1:A:272:ASN:HB2	5:A:503:HOH:O	2.18	0.41
1:A:114:THR:O	1:A:118:GLU:HB2	2.20	0.41
1:A:166:ARG:HA	1:A:247:ILE:HD13	2.02	0.41
1:A:40:ILE:O	1:A:196:ASN:HB3	2.20	0.41
1:A:216:ASN:HD22	1:A:216:ASN:C	2.28	0.41
1:A:184:ASN:N	1:A:184:ASN:HD22	2.18	0.41
1:A:94:PRO:HA	1:A:97:LYS:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLY:O	2:B:42:GLN:NE2[3_555]	2.09	0.11

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	292/294 (99%)	276 (94%)	11 (4%)	5 (2%)	7	30
2	B	106/108 (98%)	96 (91%)	9 (8%)	1 (1%)	14	46
All	All	398/402 (99%)	372 (94%)	20 (5%)	6 (2%)	8	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	12	LYS
2	B	61	GLU
1	A	74	LYS
1	A	140	ASP
1	A	67	TYR

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	252/253 (100%)	204 (81%)	48 (19%)	1	8
2	B	89/89 (100%)	68 (76%)	21 (24%)	1	4
All	All	341/342 (100%)	272 (80%)	69 (20%)	1	7

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	LEU
1	A	9	SER
1	A	14	ARG
1	A	20	GLN
1	A	26	ILE
1	A	30	LEU
1	A	51	TRP
1	A	75	LYS
1	A	82	ASN
1	A	85	LEU
1	A	90	LYS
1	A	92	LEU
1	A	93	GLU
1	A	97	LYS
1	A	103	SER
1	A	120	GLN
1	A	123	LYS
1	A	127	ARG
1	A	134	PRO
1	A	135	GLU
1	A	156	THR
1	A	159	GLN
1	A	161	LEU
1	A	166	ARG
1	A	172	MET
1	A	179	LYS
1	A	182	LEU
1	A	183	LYS
1	A	197	VAL
1	A	200	ASN
1	A	207	LEU
1	A	212	LYS
1	A	213	LEU
1	A	216	ASN
1	A	222	GLN
1	A	230	MET
1	A	232	LEU
1	A	239	ILE
1	A	245	LEU
1	A	249	LYS
1	A	255	GLN
1	A	260	LYS

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	277	PRO
1	A	278	LYS
1	A	282	SER
1	A	289	LEU
2	B	-2	PHE
2	B	4	LYS
2	B	9	LEU
2	B	13	ARG
2	B	15	LEU
2	B	19	THR
2	B	21	GLU
2	B	27	LYS
2	B	32	LEU
2	B	35	ILE
2	B	44	GLU
2	B	52	ASN
2	B	58	LEU
2	B	68	LEU
2	B	79	LYS
2	B	80	MET
2	B	85	LEU
2	B	86	LYS
2	B	88	GLU
2	B	100	LYS
2	B	103	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	62	ASN
1	A	82	ASN
1	A	181	HIS
1	A	184	ASN
1	A	195	ASN
1	A	196	ASN
1	A	200	ASN
1	A	205	ASN
1	A	208	ASN
1	A	216	ASN
1	A	292	GLN

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Mol	Chain	Res	Type
2	B	39	HIS
2	B	56	ASN
2	B	92	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
4	HEC	B	109	2	50,50,50	2.14	15 (30%)	68,82,82	1.45	9 (13%)
3	ZNH	A	295	1	50,50,50	1.22	5 (10%)	65,82,82	1.65	15 (23%)

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	HEC	B	109	2	1/1/3/7	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZNH	A	295	1	1/1/3/9	2/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	109	HEC	FE-NB	5.77	2.12	1.94
4	B	109	HEC	FE-ND	5.74	2.12	1.94
4	B	109	HEC	FE-NC	4.17	2.08	1.95
4	B	109	HEC	CAB-C3B	-4.09	1.40	1.51
4	B	109	HEC	FE-NA	3.92	2.08	1.95
4	B	109	HEC	CAC-C3C	-3.78	1.41	1.51
4	B	109	HEC	CHA-C1A	3.38	1.45	1.38
4	B	109	HEC	C1A-C2A	-3.34	1.39	1.45
4	B	109	HEC	C4A-C3A	-2.95	1.39	1.45
4	B	109	HEC	CHA-C4D	2.90	1.45	1.39
4	B	109	HEC	CBB-CAB	-2.89	1.39	1.51
4	B	109	HEC	CBC-CAC	-2.63	1.40	1.51
3	A	295	ZNH	CAB-C3B	-2.54	1.40	1.47
3	A	295	ZNH	ZN-NB	2.44	2.11	2.03
4	B	109	HEC	CHC-C4B	2.40	1.43	1.38
4	B	109	HEC	CMB-C2B	2.32	1.55	1.50
3	A	295	ZNH	ZN-NA	2.05	2.10	2.03
4	B	109	HEC	C4A-NA	-2.05	1.35	1.39
3	A	295	ZNH	CMD-C2D	-2.02	1.46	1.50
3	A	295	ZNH	CMB-C2B	2.01	1.54	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	109	HEC	CBC-CAC-C3C	4.71	125.19	112.42
4	B	109	HEC	CBB-CAB-C3B	4.28	124.01	112.42
3	A	295	ZNH	C1D-C2D-C3D	4.08	111.27	106.98
3	A	295	ZNH	CHC-C4B-NB	-3.86	119.77	124.75
3	A	295	ZNH	C4D-C3D-C2D	-3.66	101.56	106.89
4	B	109	HEC	C1D-ND-C4D	3.31	109.12	105.21
4	B	109	HEC	CHA-C4D-C3D	3.18	129.41	124.77
3	A	295	ZNH	C4B-NB-C1B	-2.97	102.53	106.47
4	B	109	HEC	C3D-C4D-ND	-2.71	107.73	110.35
3	A	295	ZNH	CAD-C3D-C4D	2.63	129.27	124.70
3	A	295	ZNH	C3B-C2B-C1B	-2.59	104.47	106.41
3	A	295	ZNH	C1C-CHC-C4B	2.56	132.28	126.25
4	B	109	HEC	CMD-C2D-C1D	-2.56	121.04	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	295	ZNH	C2B-C1B-NB	2.55	114.83	110.18
3	A	295	ZNH	C4A-NA-C1A	-2.55	102.72	106.52
3	A	295	ZNH	C3A-C4A-NA	2.49	114.15	110.35
4	B	109	HEC	C2D-C1D-ND	-2.43	107.04	109.84
3	A	295	ZNH	C4C-C3C-C2C	-2.40	104.31	107.30
3	A	295	ZNH	C4B-C3B-C2B	-2.37	105.11	107.28
4	B	109	HEC	C1D-C2D-C3D	2.36	109.47	106.98
3	A	295	ZNH	C2C-C1C-NC	2.35	111.98	109.02
3	A	295	ZNH	C4A-C3A-C2A	-2.27	103.60	106.97
4	B	109	HEC	CHA-C4D-ND	-2.16	122.09	124.42
3	A	295	ZNH	CHB-C1B-C2B	-2.05	121.79	125.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	295	ZNH	NA
4	B	109	HEC	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	295	ZNH	CAA-CBA-CGA-O2A
3	A	295	ZNH	CAA-CBA-CGA-O1A
4	B	109	HEC	CAA-CBA-CGA-O1A

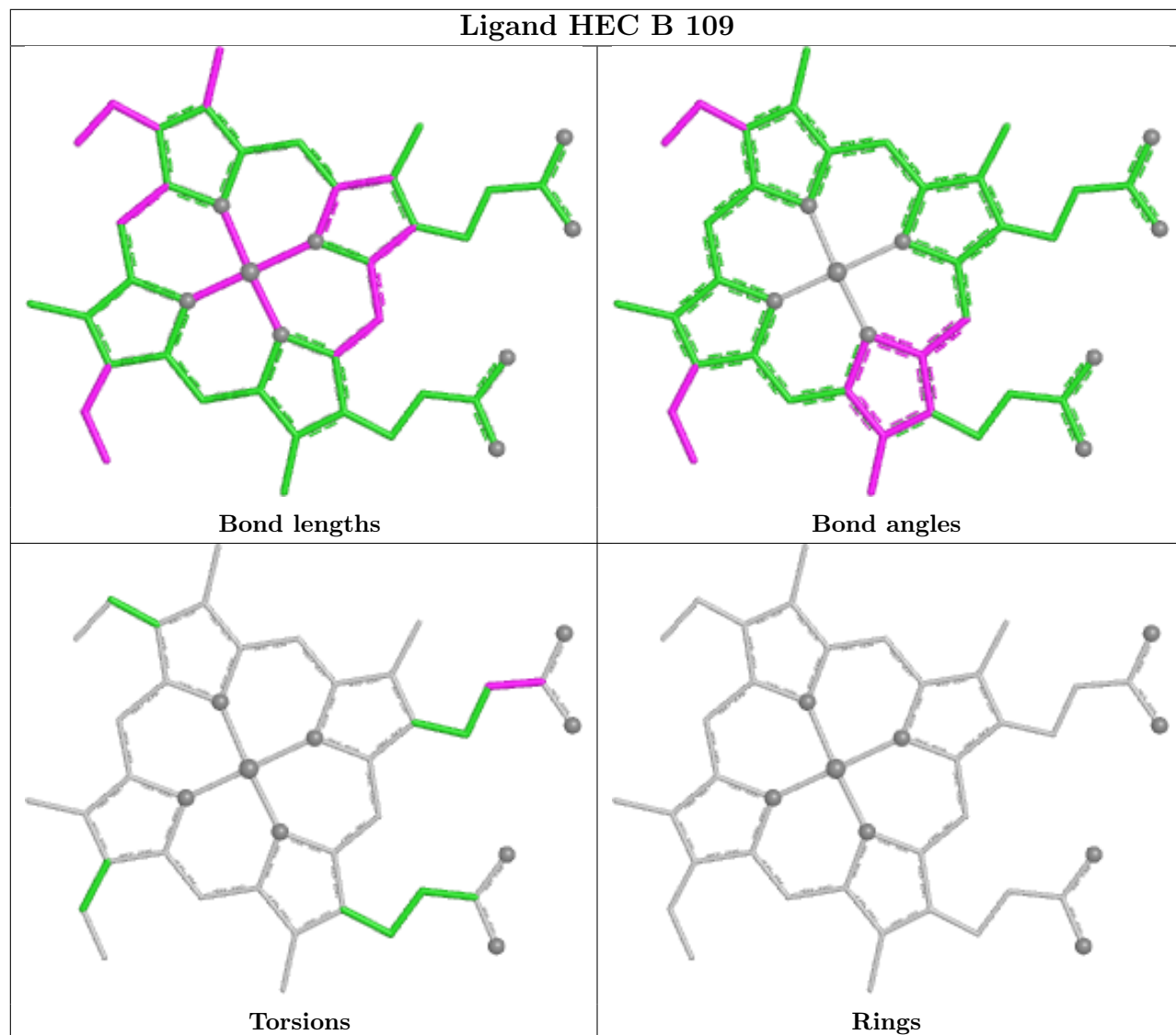
There are no ring outliers.

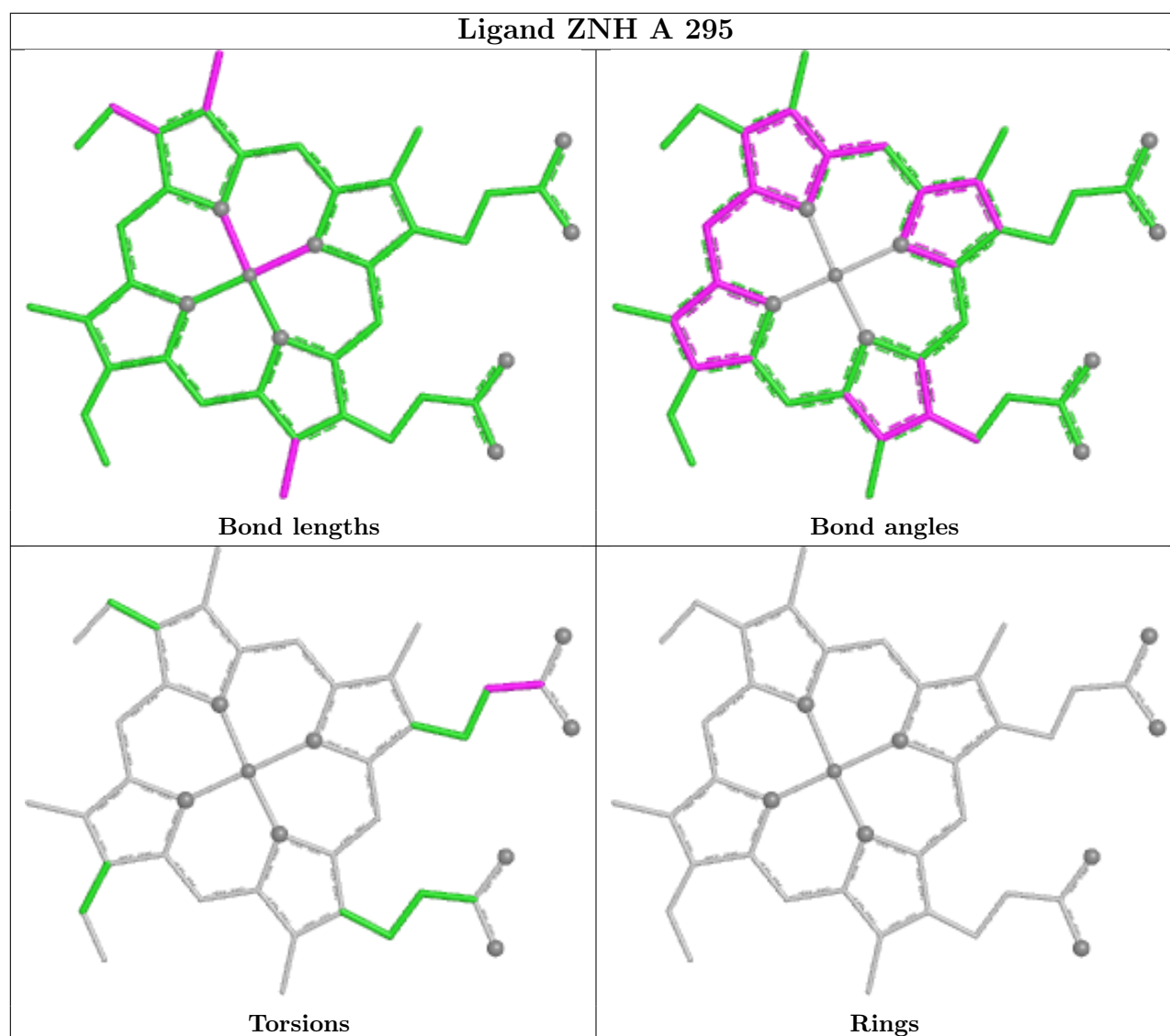
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	109	HEC	6	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	294/294 (100%)	0.37	1 (0%) 90 79	2, 3, 16, 28	0
2	B	108/108 (100%)	0.07	1 (0%) 81 61	2, 3, 15, 36	0
All	All	402/402 (100%)	0.29	2 (0%) 87 72	2, 3, 16, 36	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	102	CYS	2.4
1	A	87	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

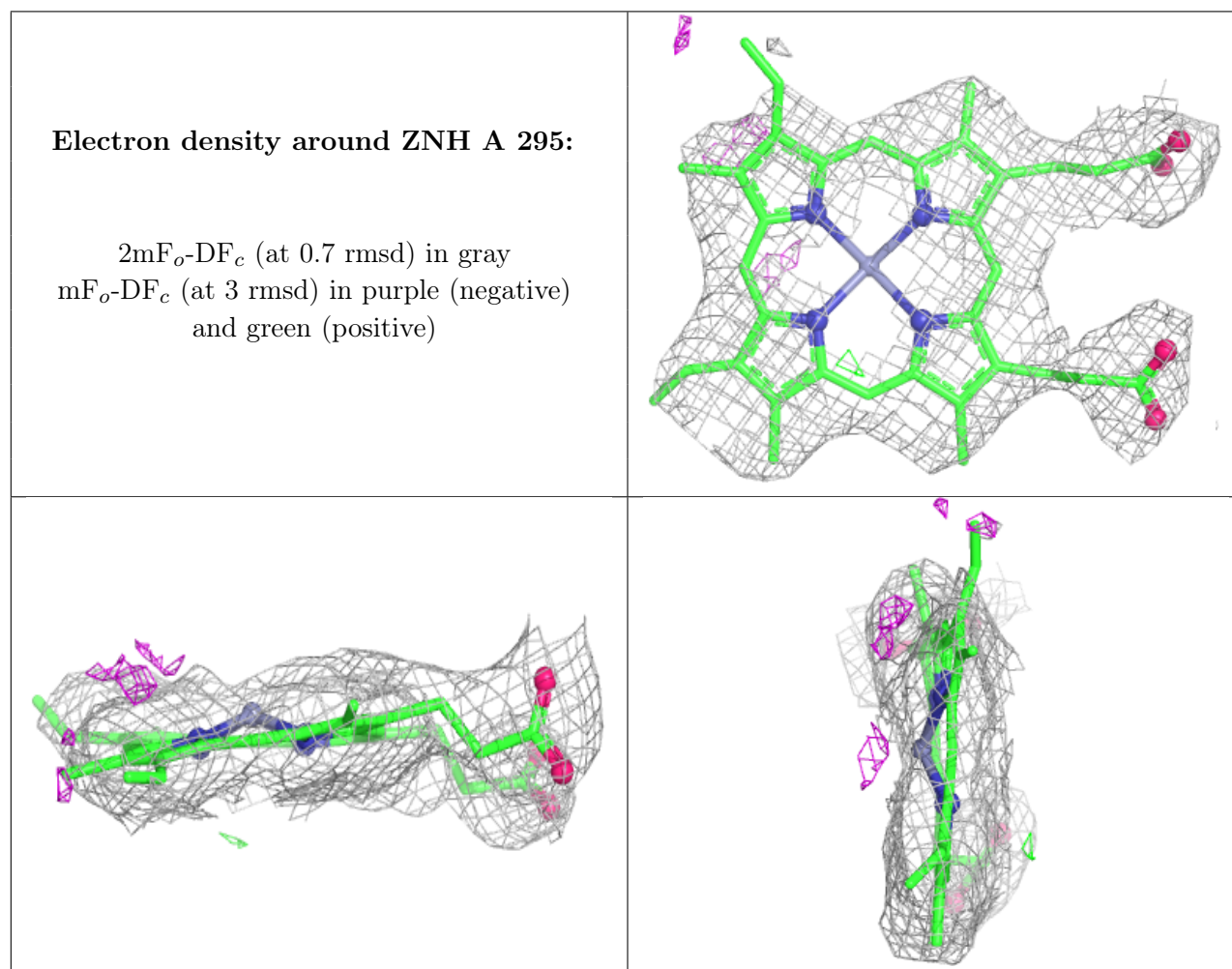
There are no oligosaccharides in this entry.

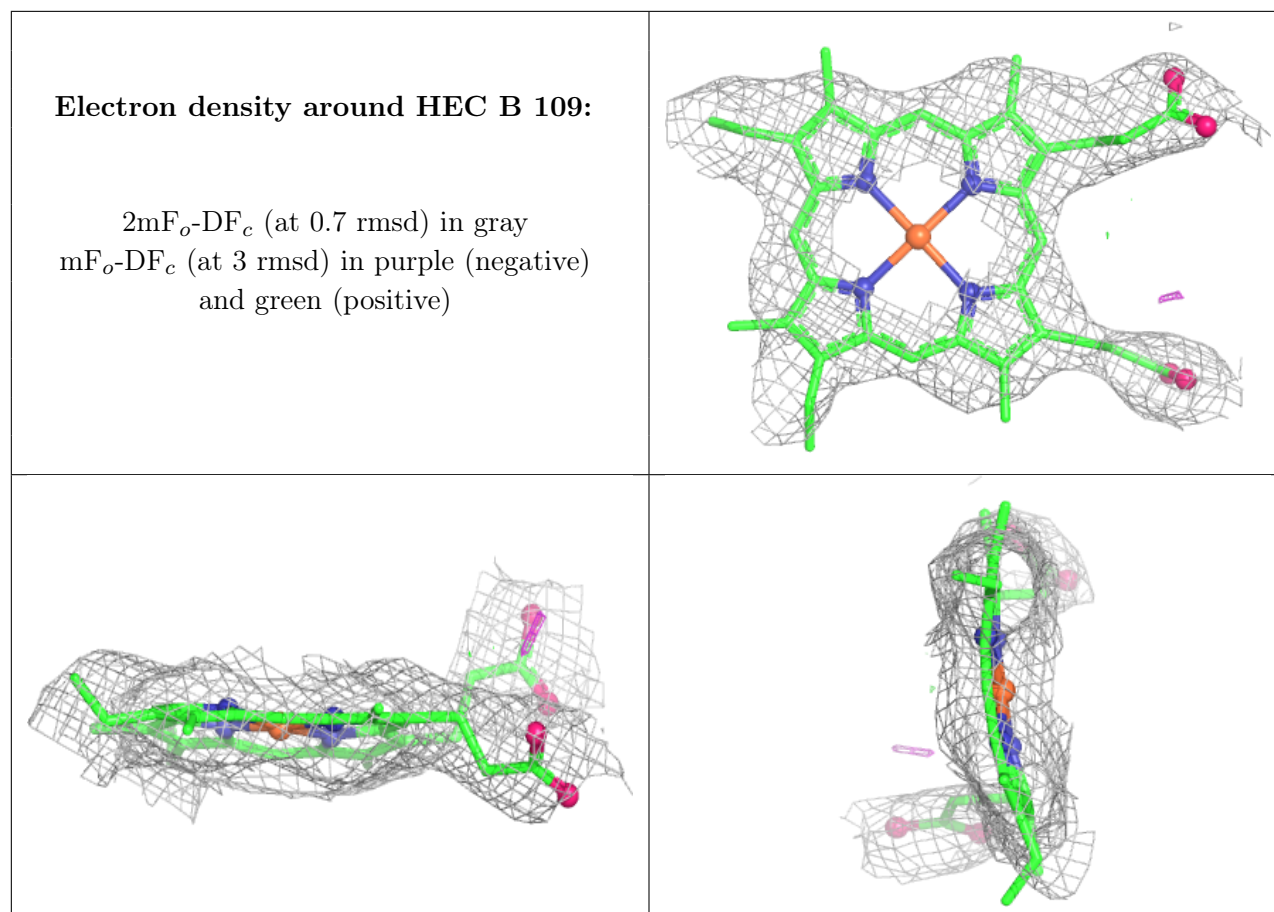
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZNH	A	295	43/43	0.93	0.11	2,2,3,15	0
4	HEC	B	109	43/43	0.95	0.09	2,2,8,21	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 [i](#)

There are no such residues in this entry.