



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:31 PM UTC

PDB ID : 2C2C / pdb_00002c2c
Title : REFINEMENT OF THE CRYSTAL STRUCTURE OF OXIDIZED RHO-
DOSPIRILLUM RUBRUM CYTOCHROME C2
Authors : Bhatia, G.; Finzel, B.C.; Kraut, J.
Deposited on : 1983-11-03
Resolution : 2.00 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)
Xtrriage (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

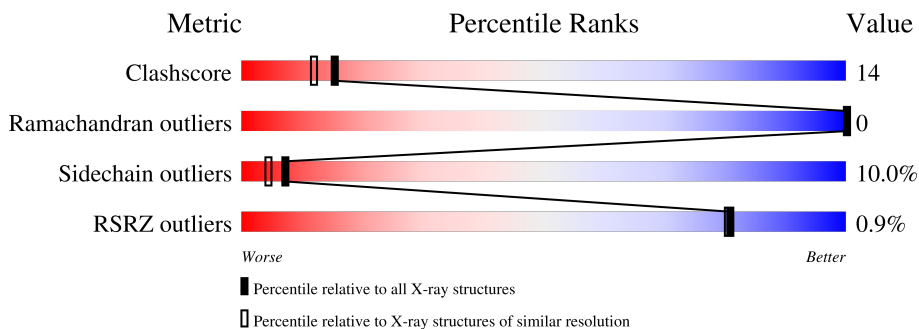
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	112	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 962 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.

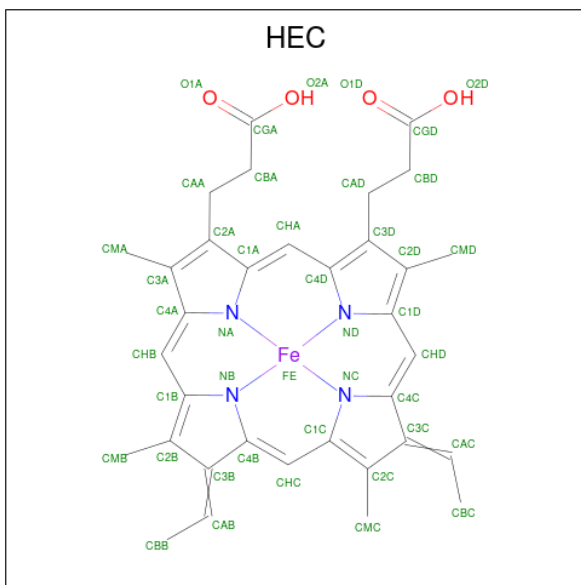
- Molecule 1 is a protein called CYTOCHROME C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	112	832	529	137	162	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASN	ASP	conflict	UNP P00092
A	73	ASN	ASP	conflict	UNP P00092

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

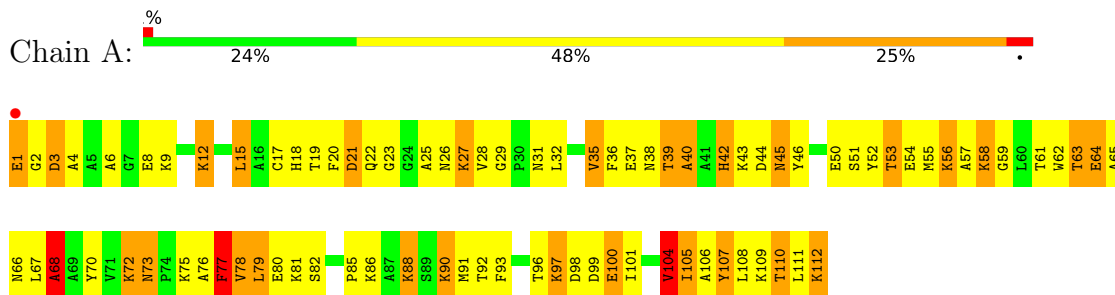
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	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: CYTOCHROME C2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	32.22Å 37.36Å 84.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 42.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 100.0 (42.31-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.68Å)	Xtrriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	962	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.54% 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: 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	2.98	72/848 (8.5%)	3.65	152/1144 (13.3%)

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	3	3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	MET	C-O	16.22	1.44	1.24
1	A	63	THR	CA-CB	13.49	1.74	1.53
1	A	112	LYS	C-O	13.07	1.49	1.23
1	A	27	LYS	C-O	12.15	1.38	1.24
1	A	1	GLU	CA-CB	10.98	1.75	1.53
1	A	78	VAL	C-N	-10.41	1.20	1.33
1	A	21	ASP	CG-OD1	9.91	1.44	1.25
1	A	92	THR	N-CA	9.66	1.58	1.46
1	A	92	THR	CA-CB	9.31	1.69	1.53
1	A	105	ILE	CA-CB	9.14	1.66	1.54
1	A	99	ASP	C-O	-8.82	1.13	1.24
1	A	1	GLU	C-O	8.55	1.40	1.23
1	A	111	LEU	CA-CB	8.09	1.65	1.53
1	A	98	ASP	CA-CB	7.95	1.66	1.53
1	A	19	THR	CA-C	7.60	1.61	1.52
1	A	53	THR	CA-CB	7.57	1.65	1.53
1	A	1	GLU	C-N	-7.35	1.22	1.33
1	A	55	MET	C-O	7.35	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	LEU	CA-C	7.35	1.62	1.52
1	A	85	PRO	CA-C	7.29	1.65	1.52
1	A	99	ASP	CG-OD2	7.22	1.39	1.25
1	A	50	GLU	CD-OE1	7.07	1.38	1.25
1	A	29	GLY	CA-C	7.04	1.61	1.51
1	A	59	GLY	C-O	7.01	1.34	1.24
1	A	97	LYS	CA-C	-6.76	1.44	1.52
1	A	63	THR	CB-OG1	6.65	1.54	1.43
1	A	85	PRO	N-CA	6.38	1.55	1.47
1	A	86	LYS	N-CA	6.33	1.53	1.46
1	A	50	GLU	CA-C	-6.32	1.43	1.52
1	A	82	SER	CA-C	6.28	1.61	1.52
1	A	56	LYS	CA-C	6.27	1.60	1.52
1	A	42	HIS	ND1-CE1	6.21	1.38	1.32
1	A	35	VAL	C-O	-6.16	1.16	1.24
1	A	23	GLY	CA-C	-6.16	1.43	1.51
1	A	15	LEU	CB-CG	-6.12	1.41	1.53
1	A	28	VAL	CA-CB	-6.06	1.46	1.55
1	A	20	PHE	N-CA	-6.00	1.37	1.45
1	A	21	ASP	CG-OD2	5.98	1.36	1.25
1	A	107	TYR	N-CA	5.97	1.54	1.46
1	A	8	GLU	CA-C	5.95	1.60	1.52
1	A	6	ALA	N-CA	5.81	1.53	1.46
1	A	77	PHE	N-CA	-5.77	1.38	1.46
1	A	6	ALA	CA-CB	-5.71	1.44	1.53
1	A	72	LYS	CA-CB	5.67	1.62	1.53
1	A	27	LYS	C-N	-5.63	1.25	1.33
1	A	58	LYS	N-CA	-5.63	1.38	1.46
1	A	81	LYS	CE-NZ	5.61	1.66	1.49
1	A	37	GLU	CD-OE1	5.61	1.36	1.25
1	A	80	GLU	C-N	-5.57	1.25	1.33
1	A	37	GLU	CA-C	-5.57	1.45	1.52
1	A	101	ILE	N-CA	-5.56	1.40	1.46
1	A	98	ASP	CB-CG	5.54	1.66	1.52
1	A	56	LYS	C-N	-5.52	1.26	1.33
1	A	86	LYS	CA-C	5.45	1.60	1.52
1	A	82	SER	C-N	-5.41	1.26	1.33
1	A	91	MET	C-N	-5.38	1.26	1.33
1	A	9	LYS	CD-CE	5.33	1.68	1.52
1	A	67	LEU	C-O	-5.33	1.17	1.24
1	A	68	ALA	C-N	-5.28	1.27	1.33
1	A	97	LYS	C-N	-5.22	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	LYS	CA-C	-5.22	1.45	1.52
1	A	56	LYS	CA-CB	-5.21	1.45	1.53
1	A	52	TYR	C-N	-5.20	1.27	1.33
1	A	109	LYS	C-O	5.17	1.30	1.24
1	A	90	LYS	CE-NZ	5.15	1.64	1.49
1	A	104	VAL	N-CA	5.11	1.52	1.46
1	A	99	ASP	CG-OD1	5.11	1.35	1.25
1	A	99	ASP	C-N	5.06	1.40	1.33
1	A	85	PRO	CA-CB	5.04	1.61	1.53
1	A	63	THR	C-N	-5.01	1.27	1.33
1	A	9	LYS	CE-NZ	5.00	1.64	1.49
1	A	96	THR	C-N	-5.00	1.26	1.33

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LYS	CA-CB-CG	18.62	151.35	114.10
1	A	97	LYS	CB-CG-CD	15.61	147.20	111.30
1	A	12	LYS	CB-CG-CD	13.98	143.45	111.30
1	A	54	GLU	CA-C-O	-13.75	104.98	120.24
1	A	85	PRO	O-C-N	13.32	141.00	122.35
1	A	63	THR	OG1-CB-CG2	-12.94	83.43	109.30
1	A	78	VAL	CA-C-O	-12.72	106.96	120.57
1	A	63	THR	CA-CB-CG2	-12.67	88.97	110.50
1	A	1	GLU	O-C-N	12.16	142.46	123.00
1	A	57	ALA	O-C-N	-12.10	109.29	122.12
1	A	99	ASP	CB-CG-OD2	11.77	145.47	118.40
1	A	112	LYS	CB-CA-C	11.50	131.94	110.10
1	A	3	ASP	CA-CB-CG	-11.29	101.31	112.60
1	A	1	GLU	CA-C-N	-11.14	99.58	121.41
1	A	1	GLU	C-N-CA	-11.14	99.58	121.41
1	A	78	VAL	CA-CB-CG1	10.91	128.95	110.40
1	A	1	GLU	CA-C-O	-10.71	102.59	120.80
1	A	82	SER	CA-C-O	-10.65	108.42	120.24
1	A	63	THR	CA-CB-OG1	-10.62	93.67	109.60
1	A	39	THR	CA-CB-CG2	10.55	128.44	110.50
1	A	92	THR	CA-C-O	-10.07	106.11	120.51
1	A	50	GLU	CB-CG-CD	10.02	129.64	112.60
1	A	38	ASN	OD1-CG-ND2	-9.67	112.93	122.60
1	A	98	ASP	CB-CG-OD2	-9.57	96.38	118.40
1	A	50	GLU	OE1-CD-OE2	9.44	145.56	122.90
1	A	68	ALA	CA-C-O	-9.08	111.54	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ALA	N-CA-C	-9.03	101.52	111.36
1	A	38	ASN	CB-CG-OD1	8.94	138.68	120.80
1	A	85	PRO	CA-C-N	-8.87	108.45	122.73
1	A	85	PRO	C-N-CA	-8.87	108.45	122.73
1	A	37	GLU	OE1-CD-OE2	8.85	144.15	122.90
1	A	27	LYS	CA-C-O	-8.72	111.92	120.90
1	A	98	ASP	CB-CG-OD1	8.68	138.36	118.40
1	A	18	HIS	ND1-CG-CD2	8.67	114.77	106.10
1	A	22	GLN	OE1-CD-NE2	-8.65	113.94	122.60
1	A	75	LYS	N-CA-CB	8.57	122.50	110.07
1	A	98	ASP	CA-CB-CG	-8.48	104.12	112.60
1	A	68	ALA	N-CA-C	-8.45	101.65	111.03
1	A	53	THR	CA-CB-OG1	-8.32	97.11	109.60
1	A	23	GLY	O-C-N	-8.14	112.93	122.45
1	A	99	ASP	OD1-CG-OD2	-8.10	103.47	122.90
1	A	28	VAL	N-CA-C	-8.06	105.25	111.62
1	A	88	LYS	O-C-N	-8.03	112.36	123.11
1	A	86	LYS	CB-CA-C	7.99	124.11	110.94
1	A	52	TYR	CA-C-O	-7.95	110.41	119.79
1	A	53	THR	N-CA-CB	-7.95	98.44	110.12
1	A	62	TRP	O-C-N	-7.88	113.08	122.46
1	A	55	MET	N-CA-C	-7.87	102.70	111.28
1	A	85	PRO	CA-C-O	-7.87	108.00	118.86
1	A	51	SER	O-C-N	-7.84	113.81	122.12
1	A	3	ASP	CA-C-O	-7.75	112.48	120.54
1	A	57	ALA	CA-C-N	7.73	136.65	121.58
1	A	57	ALA	C-N-CA	7.73	136.65	121.58
1	A	80	GLU	CA-CB-CG	7.45	129.00	114.10
1	A	43	LYS	O-C-N	-7.44	114.57	123.13
1	A	93	PHE	CA-C-O	-7.43	109.89	120.51
1	A	64	GLU	CA-CB-CG	7.42	128.93	114.10
1	A	44	ASP	CB-CG-OD1	7.41	135.43	118.40
1	A	72	LYS	N-CA-CB	7.38	121.66	110.30
1	A	40	ALA	N-CA-CB	-7.36	99.84	110.36
1	A	90	LYS	CB-CG-CD	7.29	128.06	111.30
1	A	12	LYS	CA-CB-CG	7.14	128.38	114.10
1	A	86	LYS	N-CA-C	-7.12	104.61	112.72
1	A	91	MET	CA-C-N	-7.03	108.11	121.54
1	A	91	MET	C-N-CA	-7.03	108.11	121.54
1	A	32	LEU	CA-C-N	-6.98	110.95	120.87
1	A	32	LEU	C-N-CA	-6.98	110.95	120.87
1	A	92	THR	N-CA-CB	6.89	122.14	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLU	O-C-N	-6.85	114.91	122.03
1	A	63	THR	N-CA-CB	-6.76	101.12	110.38
1	A	64	GLU	CA-C-O	-6.73	113.29	120.42
1	A	4	ALA	N-CA-C	-6.68	104.99	113.01
1	A	26	ASN	OD1-CG-ND2	6.67	129.27	122.60
1	A	79	LEU	CB-CG-CD2	6.56	130.37	110.70
1	A	18	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	A	99	ASP	N-CA-C	-6.48	104.14	111.14
1	A	31	ASN	CA-C-O	-6.44	114.72	121.55
1	A	67	LEU	O-C-N	-6.33	114.81	122.22
1	A	96	THR	CA-C-O	-6.32	112.10	119.05
1	A	55	MET	CA-C-O	-6.32	113.86	120.55
1	A	85	PRO	CA-N-CD	-6.29	103.20	112.00
1	A	27	LYS	CA-C-N	6.28	129.82	123.16
1	A	27	LYS	C-N-CA	6.28	129.82	123.16
1	A	62	TRP	CA-C-N	6.21	132.74	121.06
1	A	62	TRP	C-N-CA	6.21	132.74	121.06
1	A	65	ALA	N-CA-CB	-6.21	100.97	110.16
1	A	105	ILE	O-C-N	6.20	128.21	121.83
1	A	9	LYS	CD-CE-NZ	-6.15	92.23	111.90
1	A	72	LYS	CB-CA-C	-6.11	97.91	110.38
1	A	57	ALA	N-CA-C	6.08	118.68	111.33
1	A	110	THR	OG1-CB-CG2	6.06	121.42	109.30
1	A	90	LYS	CG-CD-CE	6.04	125.18	111.30
1	A	37	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	54	GLU	N-CA-C	-6.01	104.30	111.69
1	A	4	ALA	CA-C-O	-6.00	111.25	119.05
1	A	40	ALA	N-CA-C	-5.98	102.64	110.53
1	A	82	SER	O-C-N	5.93	129.93	122.23
1	A	44	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	6	ALA	CA-C-N	5.91	126.54	119.98
1	A	6	ALA	C-N-CA	5.91	126.54	119.98
1	A	53	THR	O-C-N	-5.87	115.90	122.12
1	A	107	TYR	CA-C-O	-5.83	112.91	119.79
1	A	37	GLU	CG-CD-OE2	-5.80	105.06	118.40
1	A	15	LEU	CA-C-O	-5.79	112.49	119.49
1	A	28	VAL	O-C-N	5.76	126.42	121.98
1	A	42	HIS	CG-CD2-NE2	5.75	112.95	107.20
1	A	78	VAL	O-C-N	5.72	127.64	121.87
1	A	27	LYS	CB-CA-C	-5.70	102.12	110.95
1	A	3	ASP	CB-CG-OD2	-5.67	105.36	118.40
1	A	70	TYR	CG-CD1-CE1	5.66	129.69	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	THR	O-C-N	-5.60	114.73	122.46
1	A	36	PHE	N-CA-CB	5.58	118.23	109.69
1	A	61	THR	OG1-CB-CG2	5.55	120.40	109.30
1	A	1	GLU	CB-CA-C	-5.54	99.56	110.10
1	A	64	GLU	CG-CD-OE2	-5.54	105.66	118.40
1	A	18	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	A	112	LYS	CA-C-O	5.50	137.49	121.00
1	A	38	ASN	CB-CG-ND2	-5.47	108.20	116.40
1	A	8	GLU	O-C-N	5.43	128.34	122.15
1	A	67	LEU	N-CA-CB	-5.41	101.88	110.22
1	A	54	GLU	CG-CD-OE1	5.41	130.85	118.40
1	A	80	GLU	CA-C-N	5.40	129.86	120.68
1	A	80	GLU	C-N-CA	5.40	129.86	120.68
1	A	61	THR	O-C-N	-5.40	115.88	123.11
1	A	18	HIS	CG-CD2-NE2	-5.33	101.87	107.20
1	A	68	ALA	O-C-N	-5.32	116.28	122.03
1	A	9	LYS	CA-C-N	5.31	128.01	120.53
1	A	9	LYS	C-N-CA	5.31	128.01	120.53
1	A	73	ASN	O-C-N	-5.29	115.23	121.32
1	A	66	ASN	CA-C-N	-5.24	112.73	120.28
1	A	66	ASN	C-N-CA	-5.24	112.73	120.28
1	A	101	ILE	N-CA-CB	-5.23	104.43	110.55
1	A	96	THR	N-CA-C	-5.22	106.93	113.72
1	A	100	GLU	O-C-N	-5.22	116.58	122.12
1	A	93	PHE	CB-CG-CD2	-5.19	111.87	120.70
1	A	106	ALA	CA-C-O	-5.19	114.92	120.42
1	A	25	ALA	CA-C-O	5.19	127.93	121.81
1	A	36	PHE	CE1-CZ-CE2	5.16	129.28	120.00
1	A	58	LYS	N-CA-CB	5.15	119.07	110.41
1	A	97	LYS	CD-CE-NZ	-5.14	95.44	111.90
1	A	2	GLY	CA-C-O	-5.12	111.66	120.57
1	A	26	ASN	CB-CG-ND2	-5.10	108.75	116.40
1	A	44	ASP	CB-CG-OD2	-5.09	106.69	118.40
1	A	62	TRP	CD2-CE3-CZ3	-5.09	111.99	118.60
1	A	82	SER	N-CA-C	-5.08	105.44	111.69
1	A	46	TYR	O-C-N	-5.07	116.64	123.23
1	A	22	GLN	O-C-N	-5.07	116.66	122.95
1	A	104	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	A	50	GLU	CG-CD-OE2	-5.05	106.79	118.40
1	A	108	LEU	CA-C-O	-5.05	113.17	119.38
1	A	27	LYS	O-C-N	-5.05	116.58	122.03
1	A	8	GLU	CG-CD-OE2	-5.04	106.81	118.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	39	THR	CB
1	A	110	THR	CB
1	A	112	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LYS	Mainchain
1	A	68	ALA	Mainchain
1	A	77	PHE	Mainchain

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	832	0	795	23	11
2	A	43	0	31	5	0
3	A	87	0	0	5	11
All	All	962	0	826	23	11

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 14.

All (23) 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:1:GLU:CA	1:A:1:GLU:CB	1.75	1.60
1:A:17:CYS:SG	2:A:113:HEC:CAC	2.13	1.35
1:A:88:LYS:CB	3:A:185:HOH:O	1.95	1.14
1:A:17:CYS:SG	2:A:113:HEC:HAC	2.00	0.97
1:A:100:GLU:O	1:A:104:VAL:HG23	1.71	0.88
1:A:73:ASN:OD1	3:A:201:HOH:O	2.00	0.79
1:A:1:GLU:CB	1:A:1:GLU:C	2.56	0.78
1:A:17:CYS:SG	2:A:113:HEC:CBC	2.73	0.76
1:A:17:CYS:SG	2:A:113:HEC:C3C	2.83	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:ND1	2:A:113:HEC:O2A	2.25	0.65
1:A:1:GLU:CB	1:A:1:GLU:N	2.61	0.62
1:A:63:THR:HG22	3:A:141:HOH:O	2.03	0.59
1:A:39:THR:HG21	1:A:56:LYS:HD2	1.85	0.58
1:A:39:THR:HG23	1:A:40:ALA:O	2.04	0.57
1:A:107:TYR:O	1:A:110:THR:HG22	2.05	0.56
1:A:64:GLU:HG3	1:A:105:ILE:HG21	1.88	0.56
1:A:63:THR:CG2	3:A:141:HOH:O	2.59	0.50
1:A:45:ASN:HD22	1:A:45:ASN:H	1.63	0.45
1:A:3:ASP:OD1	1:A:3:ASP:C	2.59	0.44
1:A:12:LYS:CD	3:A:205:HOH:O	2.66	0.43
1:A:35:VAL:HG23	1:A:42:HIS:CE1	2.54	0.43
1:A:76:ALA:O	1:A:77:PHE:C	2.60	0.42
1:A:68:ALA:O	1:A:72:LYS:HE2	2.20	0.40

All (11) 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:90:LYS:CE	3:A:134:HOH:O[4_556]	1.20	1.00
1:A:63:THR:CB	3:A:203:HOH:O[3_745]	1.29	0.91
1:A:90:LYS:NZ	3:A:134:HOH:O[4_556]	1.32	0.88
1:A:112:LYS:CB	3:A:181:HOH:O[4_456]	1.43	0.77
1:A:64:GLU:OE2	3:A:200:HOH:O[3_745]	1.47	0.73
1:A:112:LYS:CB	3:A:182:HOH:O[4_456]	1.50	0.70
1:A:64:GLU:CB	3:A:200:HOH:O[3_745]	1.67	0.53
1:A:64:GLU:CG	3:A:200:HOH:O[3_745]	1.87	0.33
1:A:64:GLU:CD	3:A:200:HOH:O[3_745]	2.00	0.20
1:A:21:ASP:CB	3:A:183:HOH:O[4_456]	2.05	0.15
1:A:21:ASP:CB	3:A:194:HOH:O[4_456]	2.08	0.12

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	110/112 (98%)	103 (94%)	7 (6%)	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	80/89 (90%)	72 (90%)	8 (10%)	7	4

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	45	ASN
1	A	53	THR
1	A	58	LYS
1	A	78	VAL
1	A	79	LEU
1	A	97	LYS
1	A	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	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](#)

1 ligand is 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	HEC	A	113	1	46,50,50	2.27	15 (32%)	58,82,82	1.98	22 (37%)

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	HEC	A	113	1	-	4/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	113	HEC	CAB-C3B	5.34	1.52	1.35
2	A	113	HEC	CAC-C3C	4.80	1.50	1.35
2	A	113	HEC	CAA-C2A	4.78	1.63	1.51
2	A	113	HEC	C1C-C2C	4.69	1.54	1.43
2	A	113	HEC	CMA-C3A	4.03	1.59	1.50
2	A	113	HEC	C3B-C4B	-3.70	1.39	1.46
2	A	113	HEC	CBC-CAC	-3.58	1.36	1.49
2	A	113	HEC	CMD-C2D	3.30	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	113	HEC	CMB-C2B	3.22	1.57	1.50
2	A	113	HEC	C2A-C3A	-2.95	1.30	1.36
2	A	113	HEC	C3C-C2C	-2.31	1.33	1.41
2	A	113	HEC	C1C-NC	-2.27	1.35	1.39
2	A	113	HEC	O1D-CGD	2.23	1.29	1.22
2	A	113	HEC	C1A-C2A	-2.17	1.41	1.45
2	A	113	HEC	C1A-NA	-2.05	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	113	HEC	CBB-CAB-C3B	-4.35	118.73	127.43
2	A	113	HEC	CBC-CAC-C3C	-4.05	119.34	127.43
2	A	113	HEC	CHC-C1C-NC	3.75	130.66	123.86
2	A	113	HEC	C4D-ND-C1D	-3.44	100.22	105.82
2	A	113	HEC	C4C-NC-C1C	3.26	111.13	105.82
2	A	113	HEC	CHA-C1A-NA	3.18	127.92	124.45
2	A	113	HEC	C4B-NB-C1B	-3.14	100.70	105.82
2	A	113	HEC	CMD-C2D-C1D	-3.14	120.64	125.42
2	A	113	HEC	CHC-C4B-C3B	-3.12	119.95	125.21
2	A	113	HEC	CAD-CBD-CGD	2.97	121.54	113.67
2	A	113	HEC	O1D-CGD-CBD	-2.75	114.36	123.09
2	A	113	HEC	C3D-C4D-ND	2.65	113.09	110.15
2	A	113	HEC	CHB-C4A-NA	2.64	127.33	124.45
2	A	113	HEC	O2A-CGA-O1A	2.54	129.87	123.33
2	A	113	HEC	CMC-C2C-C1C	-2.42	121.74	125.42
2	A	113	HEC	C2C-C1C-NC	-2.33	106.40	110.14
2	A	113	HEC	CHD-C4C-NC	2.32	126.98	124.45
2	A	113	HEC	C2D-C1D-ND	2.28	113.80	110.14
2	A	113	HEC	C2A-C1A-NA	-2.25	108.16	110.32
2	A	113	HEC	CMC-C2C-C3C	2.23	131.80	126.55
2	A	113	HEC	CHD-C1D-ND	-2.16	119.94	123.86
2	A	113	HEC	O2D-CGD-CBD	2.11	120.66	114.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

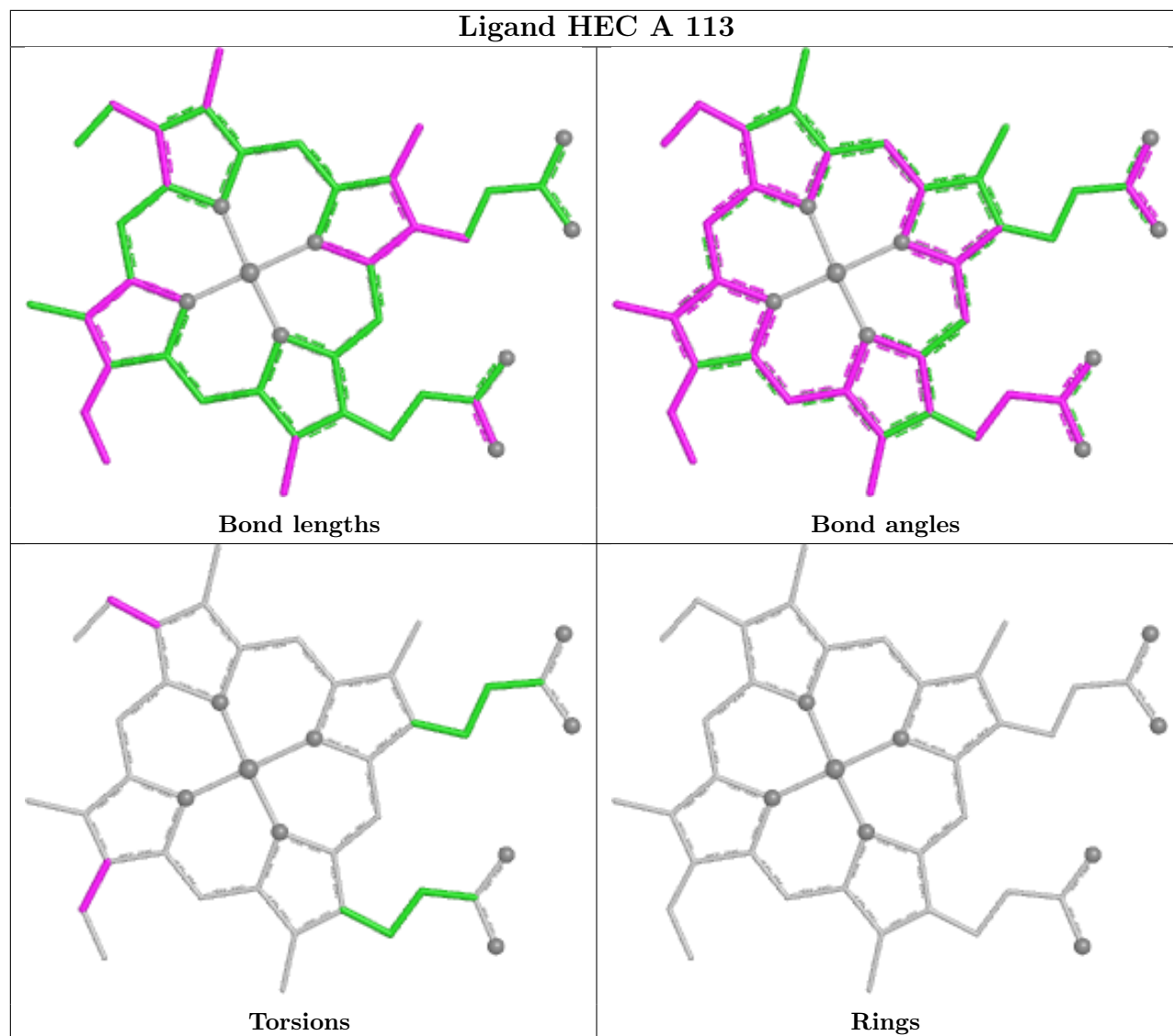
Mol	Chain	Res	Type	Atoms
2	A	113	HEC	C2B-C3B-CAB-CBB
2	A	113	HEC	C4B-C3B-CAB-CBB
2	A	113	HEC	C2C-C3C-CAC-CBC
2	A	113	HEC	C4C-C3C-CAC-CBC

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	113	HEC	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.



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	112/112 (100%)	-0.67	1 (0%) 81 80	7, 14, 25, 51	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLU	2.8

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](#)

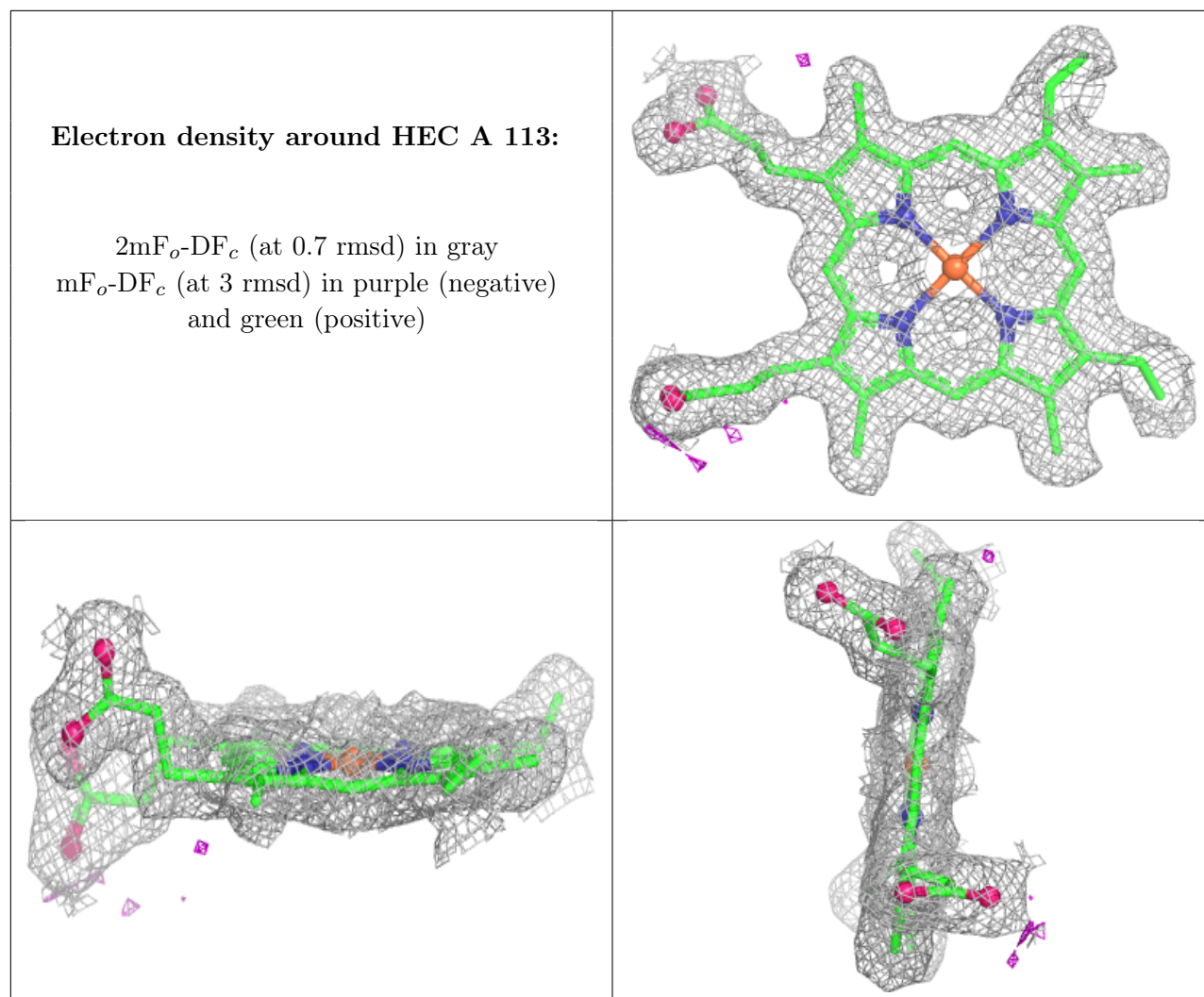
There are no oligosaccharides in this entry.

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
2	HEC	A	113	43/43	0.99	0.05	3,6,12,17	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.