



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:18 PM UTC

PDB ID : 2CCY / pdb_00002ccy
Title : STRUCTURE OF FERRICYTOCHROME C(PRIME) FROM RHO-DOSPIRILLUM MOLISCHIANUM AT 1.67 ANGSTROMS RESOLUTION
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Deposited on : 1985-08-27
Resolution : 1.67 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

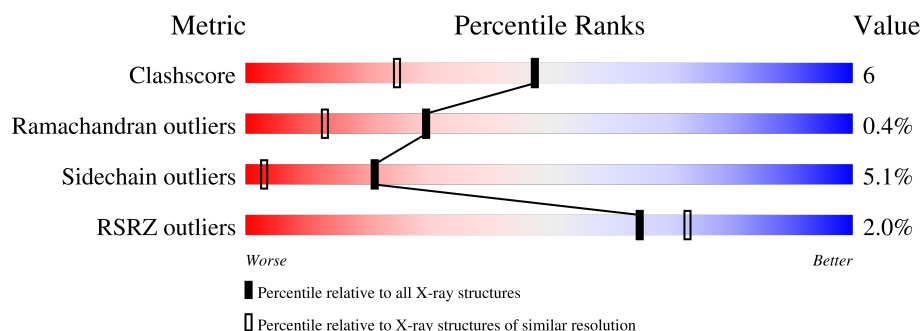
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	128	2% 40% 48% 9% ..
1	B	128	2% 34% 54% 11% ..

2 Entry composition [i](#)

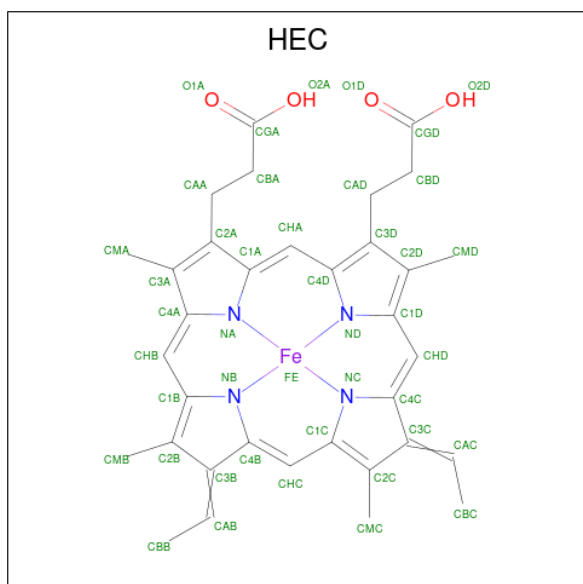
There are 3 unique types of molecules in this entry. The entry contains 2146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	1	0
			933	588	162	178	5			
1	B	127	Total	C	N	O	S	0	1	0
			933	588	162	178	5			

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



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

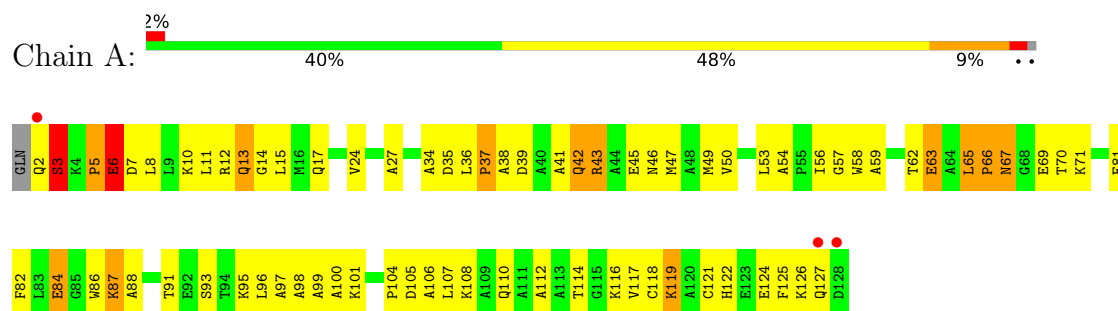
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total 96	O 96	0	0
3	B	98	Total 98	O 98	0	0

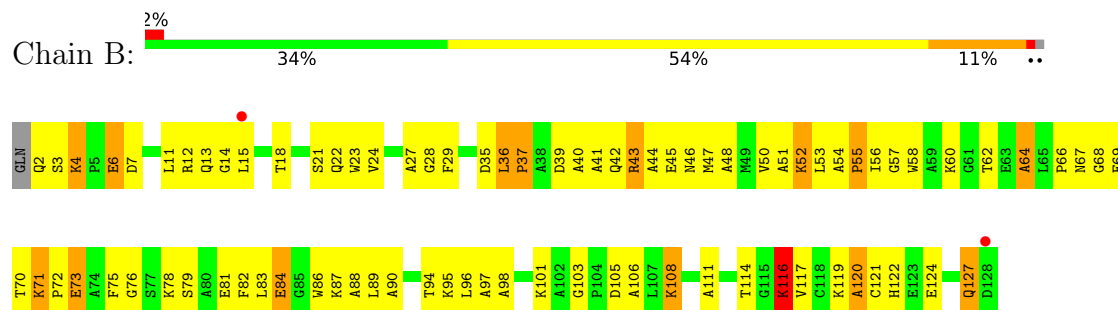
3 Residue-property plots [i](#)

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 C



• Molecule 1: CYTOCHROME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.58Å 72.33Å 75.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.67 52.21 – 1.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.67) 98.8 (52.21-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 1.50Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 119.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2146	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.96% 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	1.91	19/955 (2.0%)	3.01	117/1286 (9.1%)
1	B	2.16	29/955 (3.0%)	3.00	127/1286 (9.9%)
All	All	2.04	48/1910 (2.5%)	3.00	244/2572 (9.5%)

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	3
1	B	0	4
All	All	0	7

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ALA	N-CA	9.54	1.57	1.46
1	B	57	GLY	N-CA	9.02	1.59	1.45
1	A	62	THR	CA-CB	8.76	1.65	1.53
1	B	54	ALA	N-CA	8.48	1.55	1.46
1	A	50	VAL	N-CA	8.44	1.56	1.46
1	B	70	THR	CA-CB	8.25	1.66	1.53
1	B	12	ARG	C-O	8.07	1.33	1.24
1	B	94	THR	CA-CB	7.23	1.64	1.53
1	A	70	THR	N-CA	7.21	1.54	1.46
1	B	24	VAL	C-O	7.15	1.30	1.24
1	B	121	CYS	N-CA	-6.96	1.38	1.46
1	B	106	ALA	N-CA	6.82	1.55	1.46
1	B	84	GLU	N-CA	-6.74	1.37	1.46
1	B	28	GLY	N-CA	6.71	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	MET	C-N	-6.58	1.24	1.34
1	B	12	ARG	CZ-NH2	6.30	1.41	1.33
1	A	43	ARG	C-N	6.28	1.41	1.33
1	A	14	GLY	CA-C	6.15	1.59	1.52
1	B	24	VAL	CA-CB	6.14	1.57	1.54
1	A	49	MET	C-N	-6.14	1.26	1.33
1	A	107	LEU	N-CA	6.09	1.53	1.46
1	B	79	SER	CA-CB	6.09	1.62	1.53
1	A	122	HIS	C-O	6.02	1.31	1.24
1	B	15	LEU	CA-C	-5.94	1.45	1.52
1	B	108	LYS	CA-CB	5.89	1.62	1.53
1	B	87	LYS	C-N	-5.88	1.25	1.33
1	B	70	THR	N-CA	5.85	1.53	1.46
1	A	17	GLN	CA-C	5.82	1.60	1.52
1	B	12	ARG	CA-C	-5.69	1.45	1.52
1	A	42[A]	GLN	CA-C	5.68	1.59	1.52
1	A	42[B]	GLN	CA-C	5.68	1.59	1.52
1	A	87	LYS	C-O	5.67	1.30	1.24
1	B	55	PRO	N-CD	5.58	1.55	1.47
1	B	94	THR	N-CA	5.58	1.53	1.46
1	B	114	THR	CA-CB	5.58	1.62	1.53
1	A	50	VAL	C-O	5.54	1.30	1.24
1	A	7	ASP	C-O	5.42	1.30	1.24
1	A	10	LYS	N-CA	5.34	1.52	1.46
1	B	89	LEU	CA-CB	5.34	1.61	1.53
1	B	14	GLY	N-CA	-5.33	1.39	1.45
1	A	88	ALA	C-N	5.31	1.40	1.33
1	B	120	ALA	N-CA	-5.28	1.40	1.46
1	B	54	ALA	CA-CB	-5.25	1.47	1.53
1	B	122	HIS	N-CA	5.20	1.52	1.46
1	B	58	TRP	C-N	-5.15	1.26	1.33
1	A	107	LEU	C-O	5.13	1.30	1.24
1	A	97	ALA	C-N	-5.04	1.27	1.33
1	B	56	ILE	CB-CG1	5.00	1.63	1.53

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	O-C-N	16.39	139.79	122.09
1	B	13	GLN	CA-C-N	16.34	138.08	119.94
1	B	13	GLN	C-N-CA	16.34	138.08	119.94
1	A	17	GLN	CA-C-O	-12.20	107.49	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42[A]	GLN	O-C-N	11.24	134.23	122.09
1	A	42[B]	GLN	O-C-N	11.24	134.23	122.09
1	A	42[A]	GLN	CA-C-O	-10.33	110.06	120.70
1	A	42[B]	GLN	CA-C-O	-10.33	110.06	120.70
1	A	97	ALA	CA-C-O	-10.26	110.14	120.70
1	A	63	GLU	CB-CG-CD	9.98	129.57	112.60
1	A	49	MET	CA-C-O	-9.97	109.85	120.42
1	A	45	GLU	O-C-N	9.89	133.79	122.22
1	B	96	LEU	CA-C-N	9.69	133.03	120.44
1	B	96	LEU	C-N-CA	9.69	133.03	120.44
1	B	86	TRP	CZ3-CH2-CZ2	9.66	134.06	121.50
1	B	69	GLU	CA-C-N	-9.66	109.67	123.00
1	B	69	GLU	C-N-CA	-9.66	109.67	123.00
1	A	124	GLU	CA-CB-CG	9.51	133.12	114.10
1	A	14	GLY	CA-C-O	-9.47	110.62	120.66
1	A	17	GLN	O-C-N	9.41	132.88	122.15
1	A	47	MET	CA-C-O	-9.16	111.10	120.90
1	A	59	ALA	O-C-N	8.89	133.50	122.65
1	B	24	VAL	N-CA-CB	-8.73	104.67	110.52
1	A	116	LYS	CA-CB-CG	8.68	131.47	114.10
1	A	117	VAL	CA-C-O	-8.63	111.47	120.71
1	B	120	ALA	CA-C-O	-8.62	111.59	121.07
1	B	35	ASP	CA-CB-CG	-8.44	104.16	112.60
1	A	106	ALA	O-C-N	8.33	133.06	122.23
1	B	103	GLY	O-C-N	8.32	130.09	121.77
1	B	94	THR	CA-CB-OG1	-8.29	97.17	109.60
1	B	46	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	B	86	TRP	CE2-CD2-CE3	8.28	127.08	118.80
1	A	38	ALA	CA-C-O	8.23	129.44	119.97
1	A	57	GLY	N-CA-C	-8.21	105.64	114.67
1	B	86	TRP	CG-CD2-CE3	-8.19	125.71	133.90
1	A	43	ARG	CA-C-O	8.15	129.62	120.90
1	A	46	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	B	15	LEU	O-C-N	-8.03	113.61	122.12
1	B	54	ALA	CA-C-N	8.02	127.74	119.56
1	B	54	ALA	C-N-CA	8.02	127.74	119.56
1	B	124	GLU	CA-CB-CG	7.94	129.99	114.10
1	A	96	LEU	O-C-N	-7.85	113.04	122.22
1	B	53	LEU	CA-C-O	-7.80	110.59	119.79
1	A	49	MET	O-C-N	7.76	131.00	122.15
1	A	56	ILE	CA-C-O	-7.73	113.01	121.05
1	B	106	ALA	N-CA-CB	-7.69	98.36	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	O-C-N	7.65	130.87	122.15
1	A	8	LEU	O-C-N	7.62	130.19	122.12
1	B	13	GLN	OE1-CD-NE2	7.56	130.16	122.60
1	A	50	VAL	O-C-N	-7.54	114.55	121.87
1	B	83	LEU	CA-C-N	7.54	131.13	120.28
1	B	83	LEU	C-N-CA	7.54	131.13	120.28
1	B	36	LEU	O-C-N	7.53	128.19	121.18
1	B	13	GLN	CG-CD-NE2	-7.51	105.14	116.40
1	B	27	ALA	O-C-N	7.44	130.00	122.12
1	A	39	ASP	CA-C-O	-7.40	111.60	120.55
1	B	83	LEU	CB-CA-C	7.35	123.00	110.79
1	B	44	ALA	CA-C-O	-7.34	112.64	120.42
1	B	98	ALA	CA-C-O	-7.33	112.78	120.55
1	B	86	TRP	N-CA-CB	7.32	120.62	110.01
1	A	96	LEU	CA-C-N	7.30	130.37	120.44
1	A	96	LEU	C-N-CA	7.30	130.37	120.44
1	B	111	ALA	O-C-N	-7.28	113.70	122.22
1	A	67	ASN	CA-C-N	7.25	127.23	120.34
1	A	67	ASN	C-N-CA	7.25	127.23	120.34
1	B	13	GLN	O-C-N	-7.24	113.36	122.27
1	B	73	GLU	CA-CB-CG	7.20	128.50	114.10
1	B	70	THR	N-CA-CB	-7.18	99.30	110.57
1	A	10	LYS	CG-CD-CE	7.12	127.68	111.30
1	B	50	VAL	CA-C-N	7.11	130.14	120.54
1	B	50	VAL	C-N-CA	7.11	130.14	120.54
1	A	35	ASP	O-C-N	7.09	131.37	122.65
1	B	90	ALA	CA-C-O	-7.03	113.43	120.82
1	A	11	LEU	CA-C-O	7.02	129.23	121.02
1	B	22	GLN	OE1-CD-NE2	-7.01	115.59	122.60
1	B	79	SER	N-CA-CB	-7.00	99.83	110.12
1	B	95	LYS	O-C-N	6.99	129.53	122.12
1	B	106	ALA	N-CA-C	-6.98	103.72	111.82
1	A	14	GLY	O-C-N	6.87	128.85	122.19
1	A	58	TRP	CE3-CZ3-CH2	6.82	129.97	121.10
1	A	45	GLU	CA-C-O	-6.81	112.40	120.10
1	A	13	GLN	OE1-CD-NE2	6.70	129.30	122.60
1	B	83	LEU	O-C-N	-6.69	115.03	122.12
1	B	52	LYS	CA-CB-CG	-6.68	100.73	114.10
1	B	43	ARG	CA-CB-CG	-6.64	100.81	114.10
1	B	127	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	B	94	THR	CA-CB-CG2	-6.60	99.28	110.50
1	A	63	GLU	N-CA-CB	6.55	120.44	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ALA	CA-C-O	-6.55	112.43	119.97
1	A	46	ASN	CB-CG-ND2	6.55	126.22	116.40
1	A	56	ILE	O-C-N	6.50	128.26	121.89
1	B	67	ASN	O-C-N	6.45	128.79	121.88
1	A	69	GLU	CA-C-N	-6.45	113.27	122.94
1	A	69	GLU	C-N-CA	-6.45	113.27	122.94
1	A	118	CYS	O-C-N	6.40	128.66	122.07
1	B	45	GLU	CA-CB-CG	-6.39	101.31	114.10
1	A	97	ALA	CA-C-N	-6.37	112.16	120.44
1	A	97	ALA	C-N-CA	-6.37	112.16	120.44
1	A	122	HIS	N-CA-CB	6.34	119.20	110.01
1	A	84	GLU	N-CA-CB	6.33	119.54	110.16
1	A	8	LEU	CA-C-O	-6.33	113.84	120.55
1	B	51	ALA	CB-CA-C	6.30	120.89	110.81
1	B	71	LYS	CA-CB-CG	-6.29	101.52	114.10
1	B	86	TRP	CA-C-O	6.28	127.42	120.82
1	A	86	TRP	CA-C-O	6.28	127.21	120.55
1	A	46	ASN	CA-C-O	-6.26	114.25	120.70
1	A	11	LEU	CA-C-N	6.25	128.56	120.44
1	A	11	LEU	C-N-CA	6.25	128.56	120.44
1	A	6	GLU	N-CA-CB	6.19	119.88	110.28
1	B	39	ASP	CA-C-O	-6.18	112.17	120.15
1	B	37	PRO	CB-CA-C	6.17	118.93	111.46
1	A	34	ALA	CA-C-O	-6.17	114.84	121.38
1	B	54	ALA	O-C-N	-6.16	114.60	120.70
1	A	99	ALA	O-C-N	-6.13	115.62	122.12
1	A	58	TRP	CD2-CE3-CZ3	-6.12	110.65	118.60
1	B	57	GLY	N-CA-C	-6.11	107.31	115.32
1	B	86	TRP	CH2-CZ2-CE2	-6.07	109.61	117.50
1	A	37	PRO	CB-CA-C	6.05	118.78	111.46
1	B	124	GLU	CA-C-O	-6.04	112.64	120.00
1	B	124	GLU	N-CA-CB	6.01	119.22	110.26
1	A	91	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	93	SER	N-CA-C	-5.99	104.68	112.23
1	A	110	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	B	56	ILE	O-C-N	5.98	128.56	121.80
1	A	112	ALA	CA-C-N	5.97	128.28	120.28
1	A	112	ALA	C-N-CA	5.97	128.28	120.28
1	A	81	GLU	N-CA-CB	5.97	118.89	110.12
1	B	114	THR	CA-C-N	-5.95	112.66	120.22
1	B	114	THR	C-N-CA	-5.95	112.66	120.22
1	B	47	MET	N-CA-C	-5.95	104.70	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PRO	N-CA-C	-5.92	101.90	111.19
1	B	11	LEU	N-CA-CB	-5.90	101.45	110.01
1	A	67	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	125	PHE	CA-CB-CG	5.85	119.65	113.80
1	B	44	ALA	N-CA-C	-5.84	105.00	111.36
1	A	41	ALA	CA-C-N	5.82	128.35	120.44
1	A	41	ALA	C-N-CA	5.82	128.35	120.44
1	B	98	ALA	N-CA-C	-5.79	104.97	111.28
1	A	124	GLU	N-CA-C	5.78	118.46	111.40
1	B	56	ILE	CA-CB-CG1	-5.78	100.58	110.40
1	B	84	GLU	CA-C-O	-5.76	113.59	120.10
1	A	5	PRO	N-CA-CB	5.76	109.04	103.51
1	B	73	GLU	N-CA-C	-5.74	105.53	112.54
1	B	69	GLU	O-C-N	5.72	129.66	122.22
1	B	105	ASP	CA-C-N	-5.72	111.62	120.31
1	B	105	ASP	C-N-CA	-5.72	111.62	120.31
1	A	99	ALA	CA-C-O	5.70	126.59	120.55
1	B	4	LYS	N-CA-CB	5.69	118.42	110.11
1	A	118	CYS	N-CA-C	-5.69	104.98	111.07
1	B	48	ALA	CA-C-O	-5.67	113.45	119.97
1	B	94	THR	N-CA-CB	-5.66	101.78	110.16
1	B	111	ALA	CA-C-N	5.66	127.80	120.44
1	B	111	ALA	C-N-CA	5.66	127.80	120.44
1	B	18	THR	N-CA-C	-5.64	105.21	111.36
1	B	64	ALA	CA-C-O	-5.63	113.82	122.32
1	A	107	LEU	N-CA-CB	-5.62	101.84	110.16
1	B	67	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	63	GLU	CA-CB-CG	5.60	125.30	114.10
1	B	21	SER	N-CA-CB	5.59	118.34	110.12
1	A	82	PHE	CA-C-O	-5.58	114.96	120.70
1	B	119	LYS	O-C-N	-5.57	116.33	122.07
1	B	68	GLY	N-CA-C	-5.57	105.53	111.93
1	A	95	LYS	CA-C-O	-5.56	113.57	119.97
1	A	100	ALA	CA-C-N	5.56	128.76	120.31
1	A	100	ALA	C-N-CA	5.56	128.76	120.31
1	A	114	THR	O-C-N	5.56	129.46	122.23
1	B	23	TRP	N-CA-C	5.54	118.51	111.69
1	A	63	GLU	CA-C-N	-5.54	114.90	122.87
1	A	63	GLU	C-N-CA	-5.54	114.90	122.87
1	A	8	LEU	N-CA-CB	5.53	118.25	110.12
1	A	39	ASP	CB-CG-OD1	5.49	131.02	118.40
1	B	56	ILE	N-CA-C	-5.47	104.26	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	LYS	CG-CD-CE	5.46	123.86	111.30
1	B	87	LYS	O-C-N	5.45	128.97	122.27
1	B	14	GLY	CA-C-O	-5.44	115.12	121.00
1	A	95	LYS	O-C-N	5.43	128.96	122.27
1	B	56	ILE	CB-CA-C	-5.43	103.46	112.26
1	B	57	GLY	O-C-N	-5.43	115.03	122.68
1	B	117	VAL	CA-CB-CG1	-5.42	101.18	110.40
1	A	5	PRO	CB-CA-C	5.41	119.58	111.68
1	A	96	LEU	CA-C-O	5.41	126.21	120.10
1	A	17	GLN	N-CA-C	-5.41	105.47	111.36
1	B	87	LYS	CA-C-O	-5.38	113.78	119.97
1	B	14	GLY	O-C-N	5.38	127.34	122.18
1	A	11	LEU	O-C-N	-5.37	115.71	122.20
1	A	41	ALA	N-CA-CB	5.36	117.85	110.07
1	A	63	GLU	CA-C-O	-5.34	113.82	119.97
1	B	44	ALA	O-C-N	5.33	128.23	122.15
1	B	73	GLU	CB-CA-C	-5.33	99.17	110.31
1	B	41	ALA	O-C-N	-5.32	116.48	122.12
1	B	76	GLY	CA-C-O	-5.31	111.33	120.57
1	B	47	MET	CA-C-O	-5.30	115.25	120.82
1	B	43	ARG	O-C-N	-5.30	116.50	122.12
1	B	116	LYS	CA-CB-CG	5.29	124.69	114.10
1	A	54	ALA	CA-C-N	5.29	125.61	119.47
1	A	54	ALA	C-N-CA	5.29	125.61	119.47
1	B	97	ALA	N-CA-CB	5.29	117.68	110.01
1	B	75	PHE	O-C-N	5.28	129.70	122.46
1	B	43	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	105	ASP	O-C-N	5.27	128.75	122.27
1	A	95	LYS	CB-CG-CD	-5.23	99.27	111.30
1	A	53	LEU	CA-C-O	-5.22	113.49	119.60
1	B	86	TRP	CE3-CZ3-CH2	-5.22	114.32	121.10
1	A	126	LYS	O-C-N	-5.21	117.10	123.10
1	B	72	PRO	CA-C-O	-5.21	111.73	119.18
1	B	35	ASP	CB-CG-OD2	-5.21	106.42	118.40
1	A	38	ALA	N-CA-CB	-5.20	102.21	110.28
1	A	107	LEU	CB-CA-C	5.20	119.69	110.85
1	A	27	ALA	N-CA-C	-5.20	105.61	111.28
1	B	62	THR	CA-CB-CG2	5.20	119.34	110.50
1	B	6	GLU	CA-C-O	-5.20	114.91	120.42
1	A	13	GLN	CA-C-O	-5.19	114.92	120.42
1	A	65	LEU	N-CA-C	-5.19	103.50	109.93
1	A	117	VAL	O-C-N	5.18	128.68	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	CYS	N-CA-CB	5.18	117.83	110.16
1	B	4	LYS	CA-C-O	5.17	126.34	120.70
1	B	14	GLY	N-CA-C	-5.16	106.52	112.50
1	B	84	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	34	ALA	O-C-N	5.13	128.65	123.26
1	B	78	LYS	CA-C-O	5.13	126.00	119.95
1	B	68	GLY	CA-C-O	5.11	127.54	121.71
1	A	8	LEU	CA-C-N	-5.11	111.84	120.58
1	A	8	LEU	C-N-CA	-5.11	111.84	120.58
1	B	82	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	87	LYS	N-CA-C	-5.09	105.63	111.07
1	B	45	GLU	CG-CD-OE2	-5.09	106.70	118.40
1	B	40	ALA	CA-C-O	-5.08	115.46	120.90
1	A	17	GLN	N-CA-CB	5.08	117.68	110.16
1	A	119	LYS	N-CA-C	5.08	116.50	111.07
1	A	71	LYS	CA-C-O	5.07	125.45	120.17
1	B	53	LEU	O-C-N	5.07	129.13	122.33
1	A	127	GLN	CA-C-O	5.07	126.75	120.92
1	B	56	ILE	CA-C-N	-5.06	109.60	121.34
1	B	56	ILE	C-N-CA	-5.06	109.60	121.34
1	B	88	ALA	N-CA-C	-5.06	105.84	111.36
1	A	38	ALA	O-C-N	-5.05	116.05	122.27
1	B	60	LYS	N-CA-CB	5.05	117.73	109.69
1	B	58	TRP	CA-C-O	-5.05	114.44	120.65
1	B	35	ASP	OD1-CG-OD2	5.04	135.00	122.90
1	A	24	VAL	CA-C-N	5.02	124.63	119.05
1	A	24	VAL	C-N-CA	5.02	124.63	119.05
1	A	15	LEU	O-C-N	-5.02	116.80	122.12
1	B	81	GLU	CA-C-O	-5.01	115.11	120.42
1	B	75	PHE	CA-C-O	-5.00	113.42	119.27

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	13	GLN	Mainchain
1	A	43	ARG	Sidechain
1	B	116	LYS	Mainchain
1	B	120	ALA	Mainchain
1	B	43	ARG	Sidechain
1	B	55	PRO	Mainchain

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	933	0	941	9	0
1	B	933	0	941	10	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	96	0	0	2	0
3	B	98	0	0	3	0
All	All	2146	0	1942	22	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 (22) 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:2:GLN:O	1:A:3:SER:HB2	1.82	0.78
1:A:66:PRO:O	1:A:67:ASN:HB2	1.98	0.63
2:B:129:HEC:HBC3	2:B:129:HEC:HMC1	1.84	0.59
1:B:71:LYS:HB3	1:B:73:GLU:OE2	2.05	0.57
1:A:5:PRO:HD2	1:A:6:GLU:OE1	2.09	0.52
1:B:52:LYS:NZ	3:B:519:HOH:O	2.40	0.51
1:B:64:ALA:N	3:B:317:HOH:O	2.44	0.49
1:B:29:PHE:CE2	1:B:108:LYS:HG3	2.50	0.47
1:B:2:GLN:O	1:B:3:SER:HB2	2.16	0.45
2:B:129:HEC:HMC1	2:B:129:HEC:CBC	2.47	0.44
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.87	0.44
2:A:129:HEC:HMC1	2:A:129:HEC:HBC3	2.00	0.43
1:B:36:LEU:HA	1:B:37:PRO:HD3	1.89	0.43
1:B:6:GLU:CD	1:B:6:GLU:H	2.27	0.42
1:A:84:GLU:HG2	3:A:208:HOH:O	2.19	0.42
1:A:101:LYS:NZ	3:A:227:HOH:O	2.50	0.41
1:A:5:PRO:HB3	1:A:65:LEU:HD22	2.03	0.41
1:B:4:LYS:O	1:B:7:ASP:HB2	2.21	0.40
1:B:64:ALA:HB3	3:B:317:HOH:O	2.21	0.40
1:A:104:PRO:O	1:A:108:LYS:HG3	2.22	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	126/128 (98%)	122 (97%)	3 (2%)	1 (1%)	16	4
1	B	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
All	All	252/256 (98%)	245 (97%)	6 (2%)	1 (0%)	30	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER

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	89/90 (99%)	84 (94%)	5 (6%)	19	2
1	B	89/90 (99%)	85 (96%)	4 (4%)	24	4
All	All	178/180 (99%)	169 (95%)	9 (5%)	21	3

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	63	GLU
1	A	87	LYS
1	A	119	LYS
1	B	66	PRO
1	B	84	GLU
1	B	116	LYS
1	B	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	B	46	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
2	HEC	B	129	1	46,50,50	2.54	17 (36%)	58,82,82	2.76	29 (50%)
2	HEC	A	129	1	46,50,50	2.36	20 (43%)	58,82,82	2.36	25 (43%)

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	B	129	1	-	8/14/54/54	-
2	HEC	A	129	1	-	8/14/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	129	HEC	CAB-C3B	7.81	1.60	1.35
2	B	129	HEC	CAC-C3C	7.76	1.60	1.35
2	B	129	HEC	CAB-C3B	6.35	1.55	1.35
2	A	129	HEC	CAC-C3C	6.20	1.55	1.35
2	B	129	HEC	CMC-C2C	4.87	1.60	1.50
2	B	129	HEC	C4D-C3D	-4.69	1.35	1.44
2	B	129	HEC	C3B-C4B	-4.43	1.38	1.46
2	A	129	HEC	C4B-NB	-3.79	1.32	1.39
2	B	129	HEC	C4B-NB	3.77	1.46	1.39
2	B	129	HEC	C3C-C2C	-3.39	1.29	1.41
2	B	129	HEC	CMA-C3A	3.25	1.57	1.50
2	A	129	HEC	C1D-C2D	3.20	1.50	1.43
2	B	129	HEC	C4D-ND	3.19	1.45	1.39
2	B	129	HEC	C2A-C3A	-3.05	1.30	1.36
2	B	129	HEC	C1D-ND	3.03	1.45	1.39
2	A	129	HEC	C3D-C2D	-3.02	1.31	1.38
2	A	129	HEC	C1A-NA	3.00	1.45	1.39
2	A	129	HEC	CMA-C3A	2.83	1.56	1.50
2	A	129	HEC	CMD-C2D	2.80	1.56	1.50
2	A	129	HEC	CHD-C4C	2.75	1.43	1.38
2	A	129	HEC	CMB-C2B	2.65	1.56	1.50
2	A	129	HEC	O1A-CGA	2.62	1.30	1.22
2	A	129	HEC	C1A-C2A	-2.60	1.40	1.45
2	B	129	HEC	O2A-CGA	-2.56	1.22	1.30
2	B	129	HEC	CMD-C2D	2.42	1.55	1.50
2	A	129	HEC	CAD-C3D	2.41	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	129	HEC	CAA-C2A	2.41	1.57	1.51
2	A	129	HEC	O2A-CGA	-2.29	1.23	1.30
2	B	129	HEC	C4A-NA	-2.25	1.35	1.39
2	A	129	HEC	C3B-C2B	-2.21	1.33	1.41
2	B	129	HEC	C1C-NC	-2.21	1.35	1.39
2	A	129	HEC	CBB-CAB	-2.12	1.41	1.49
2	A	129	HEC	CBC-CAC	-2.07	1.41	1.49
2	B	129	HEC	C1A-C2A	2.06	1.48	1.45
2	B	129	HEC	C1C-C2C	2.04	1.47	1.43
2	A	129	HEC	O2D-CGD	-2.04	1.24	1.30
2	A	129	HEC	CHB-C4A	2.02	1.42	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	HEC	CHD-C4C-NC	6.75	131.81	124.45
2	B	129	HEC	CHA-C1A-NA	6.07	131.06	124.45
2	B	129	HEC	CBC-CAC-C3C	-5.78	115.89	127.43
2	B	129	HEC	CBB-CAB-C3B	-5.70	116.05	127.43
2	A	129	HEC	CHC-C4B-NB	5.67	130.62	124.45
2	A	129	HEC	CBB-CAB-C3B	-5.41	116.62	127.43
2	B	129	HEC	C2A-C1A-NA	-5.18	105.33	110.32
2	B	129	HEC	CHC-C1C-NC	5.16	133.22	123.86
2	B	129	HEC	C4D-ND-C1D	-4.85	97.91	105.82
2	A	129	HEC	CMD-C2D-C1D	-4.19	119.03	125.42
2	B	129	HEC	CAD-CBD-CGD	4.06	124.44	113.67
2	B	129	HEC	C2C-C1C-NC	-4.04	103.66	110.14
2	A	129	HEC	CHA-C4D-ND	4.00	131.11	123.86
2	B	129	HEC	C3D-C4D-ND	3.88	114.45	110.15
2	A	129	HEC	O1A-CGA-CBA	-3.86	110.86	123.09
2	A	129	HEC	O2A-CGA-CBA	3.79	125.97	114.00
2	A	129	HEC	C2D-C1D-ND	-3.75	104.13	110.14
2	A	129	HEC	CHD-C1D-ND	3.75	130.65	123.86
2	A	129	HEC	C4D-ND-C1D	3.74	111.92	105.82
2	B	129	HEC	C4B-NB-C1B	-3.68	99.82	105.82
2	A	129	HEC	C3D-C4D-ND	-3.62	106.14	110.15
2	B	129	HEC	C4C-NC-C1C	3.47	111.48	105.82
2	A	129	HEC	CHA-C1A-NA	-3.38	120.77	124.45
2	A	129	HEC	CHB-C1B-NB	3.36	129.95	123.86
2	B	129	HEC	C4A-NA-C1A	3.27	111.15	105.82
2	B	129	HEC	CMA-C3A-C4A	-3.15	119.18	124.73
2	A	129	HEC	CMD-C2D-C3D	3.12	132.23	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	129	HEC	C4A-NA-C1A	-3.05	100.86	105.82
2	B	129	HEC	CHB-C4A-NA	3.00	127.72	124.45
2	B	129	HEC	O1A-CGA-CBA	-2.83	114.13	123.09
2	A	129	HEC	CHD-C4C-C3C	-2.80	120.50	125.21
2	B	129	HEC	CAD-C3D-C2D	-2.76	120.89	127.07
2	B	129	HEC	CAD-C3D-C4D	2.67	130.16	124.94
2	A	129	HEC	CHC-C4B-C3B	-2.65	120.75	125.21
2	B	129	HEC	CHB-C1B-NB	-2.54	119.25	123.86
2	B	129	HEC	CHD-C1D-C2D	-2.45	120.31	127.43
2	B	129	HEC	C2B-C1B-NB	2.38	113.95	110.14
2	A	129	HEC	CHC-C1C-C2C	-2.37	120.56	127.43
2	A	129	HEC	CMB-C2B-C1B	-2.26	121.98	125.42
2	A	129	HEC	C1D-CHD-C4C	-2.20	117.86	124.66
2	B	129	HEC	CMC-C2C-C1C	-2.20	122.07	125.42
2	B	129	HEC	O1D-CGD-CBD	2.19	130.03	123.09
2	A	129	HEC	CHD-C4C-NC	2.15	126.80	124.45
2	A	129	HEC	CAA-C2A-C3A	-2.13	123.89	127.87
2	A	129	HEC	CMB-C2B-C3B	2.11	131.52	126.55
2	A	129	HEC	C1B-CHB-C4A	-2.10	118.19	124.66
2	B	129	HEC	CHC-C1C-C2C	-2.10	121.34	127.43
2	A	129	HEC	CHB-C4A-C3A	-2.09	121.15	125.49
2	B	129	HEC	CAA-C2A-C1A	-2.07	120.65	124.85
2	B	129	HEC	C2D-C1D-ND	2.06	113.45	110.14
2	B	129	HEC	CHA-C4D-ND	-2.06	120.13	123.86
2	B	129	HEC	C1C-CHC-C4B	-2.03	118.39	124.66
2	A	129	HEC	CHB-C1B-C2B	-2.03	121.55	127.43
2	B	129	HEC	CAA-CBA-CGA	-2.00	108.35	113.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	129	HEC	C2B-C3B-CAB-CBB
2	A	129	HEC	C4B-C3B-CAB-CBB
2	A	129	HEC	C2C-C3C-CAC-CBC
2	A	129	HEC	C4C-C3C-CAC-CBC
2	B	129	HEC	C2B-C3B-CAB-CBB
2	B	129	HEC	C4B-C3B-CAB-CBB
2	B	129	HEC	C2C-C3C-CAC-CBC
2	B	129	HEC	C4C-C3C-CAC-CBC
2	A	129	HEC	CAA-CBA-CGA-O2A
2	A	129	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	A	129	HEC	CAD-CBD-CGD-O2D
2	B	129	HEC	CAA-CBA-CGA-O2A
2	B	129	HEC	CAD-CBD-CGD-O2D
2	B	129	HEC	CAA-CBA-CGA-O1A
2	B	129	HEC	CAD-CBD-CGD-O1D
2	A	129	HEC	CAA-CBA-CGA-O1A

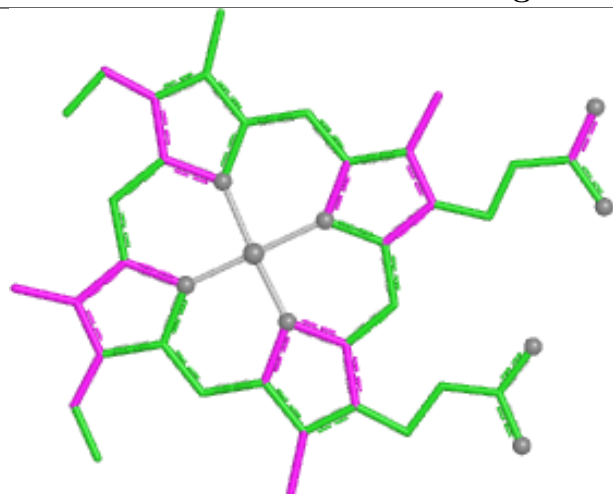
There are no ring outliers.

2 monomers are involved in 3 short contacts:

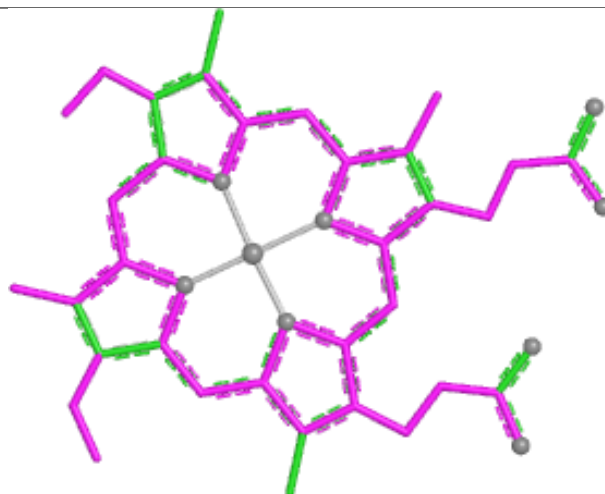
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	129	HEC	2	0
2	A	129	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

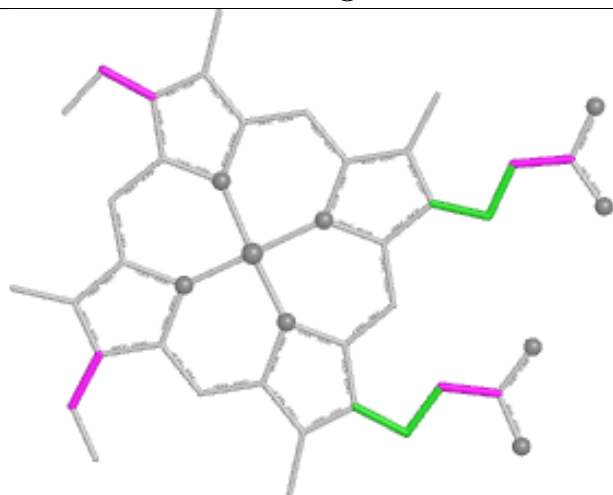
Ligand HEC B 129



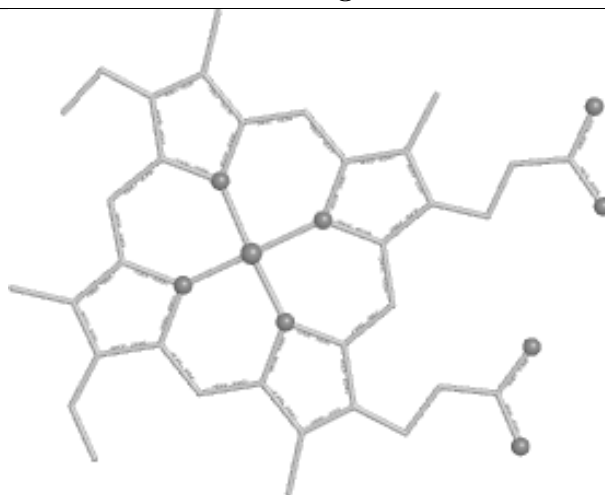
Bond lengths



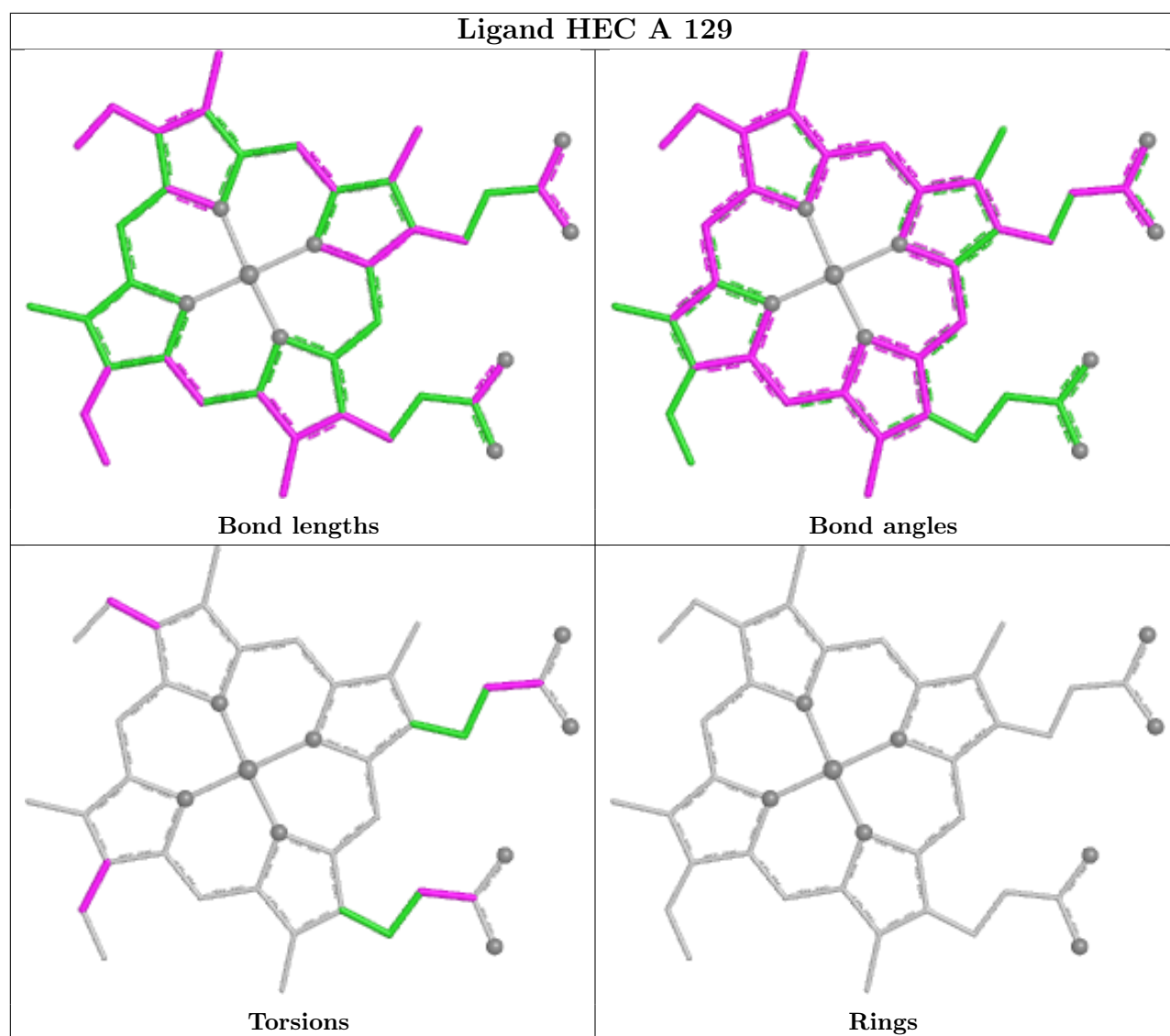
Bond angles



Torsions



Rings



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	127/128 (99%)	0.07	3 (2%) 59 67	15, 27, 47, 69	10 (7%)
1	B	127/128 (99%)	-0.21	2 (1%) 70 79	9, 21, 39, 74	9 (7%)
All	All	254/256 (99%)	-0.07	5 (1%) 65 73	9, 23, 46, 74	19 (7%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	ASP	3.7
1	B	15	LEU	3.0
1	B	128	ASP	2.5
1	A	127	GLN	2.4
1	A	2	GLN	2.1

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](#)

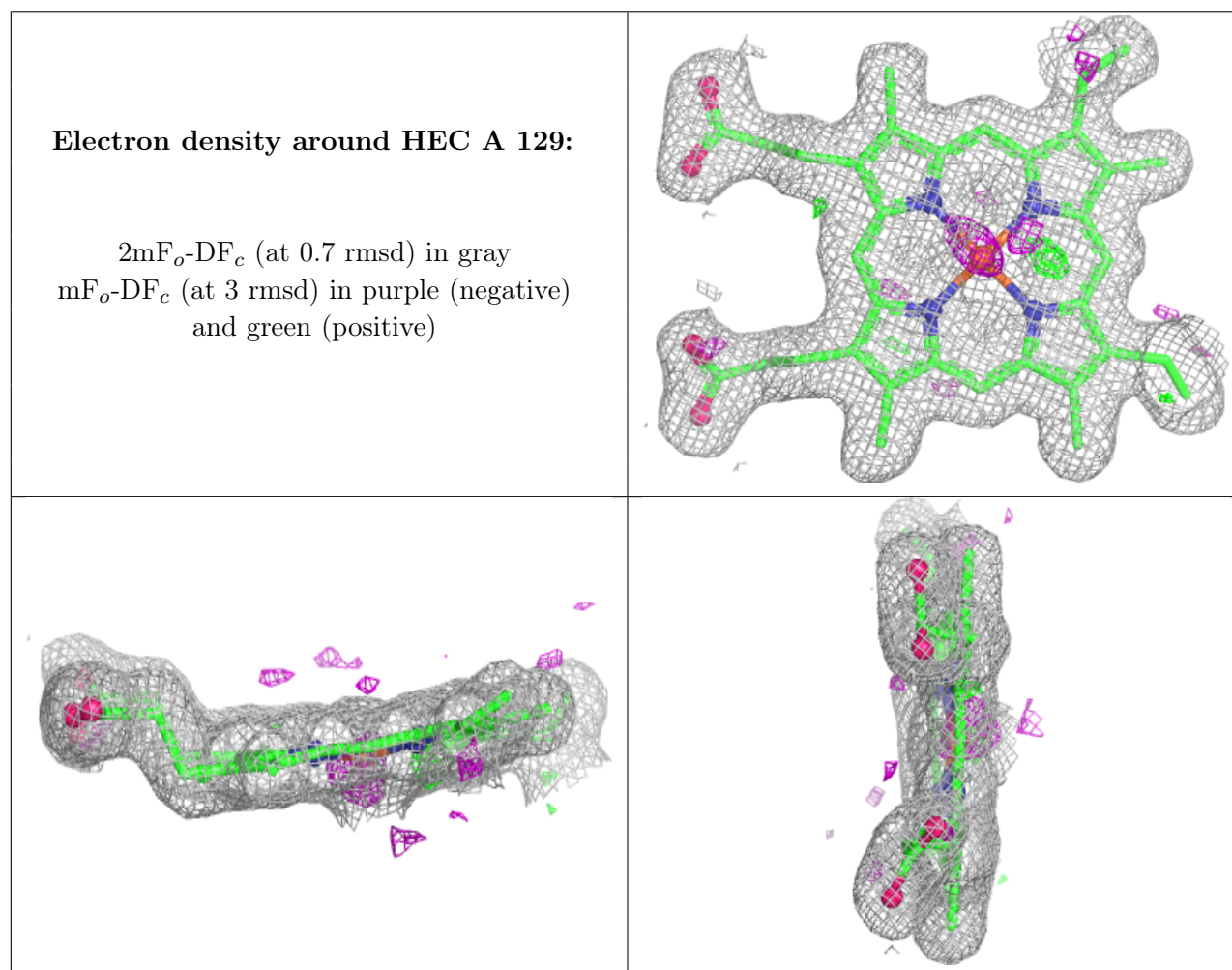
There are no oligosaccharides in this entry.

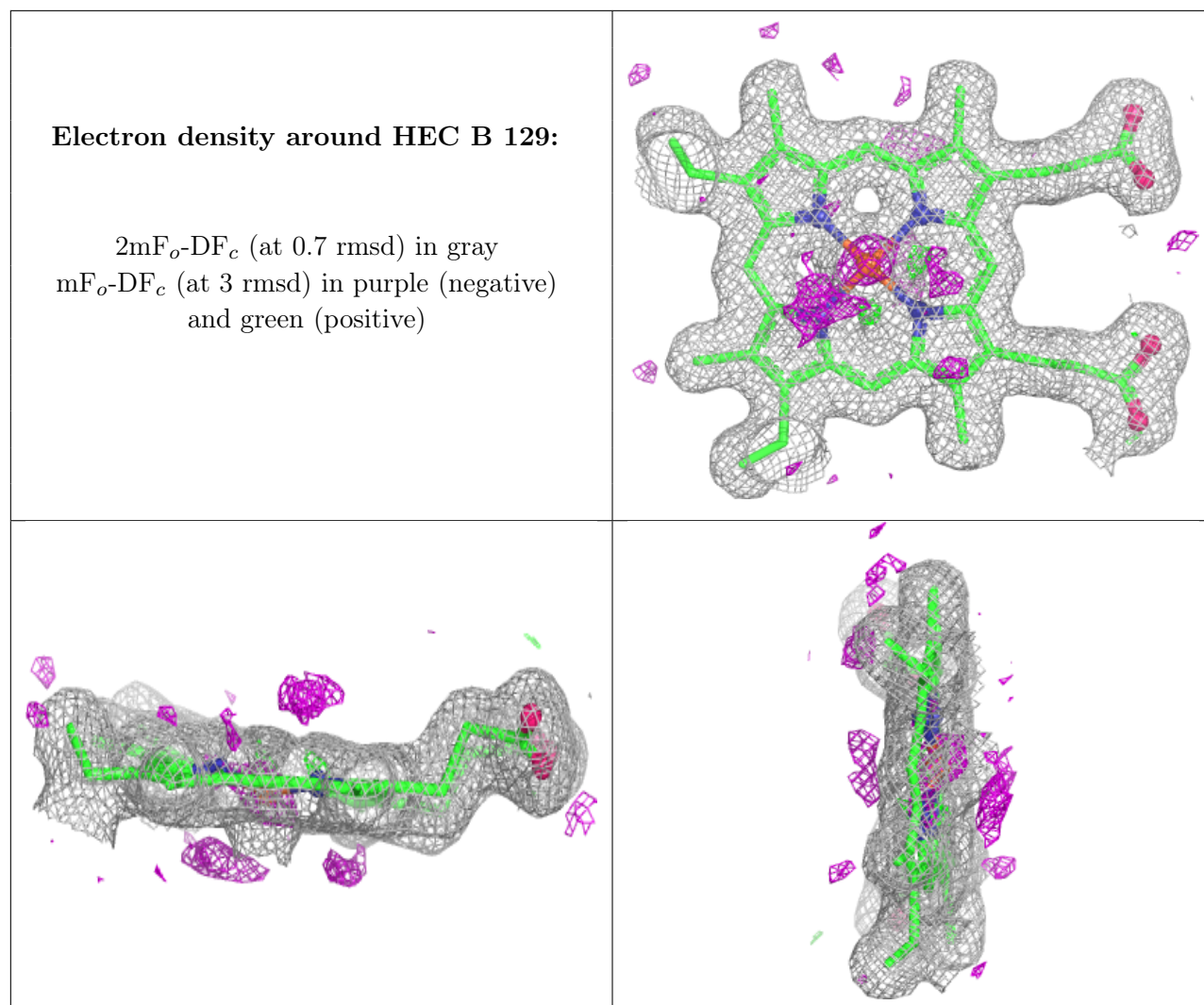
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	HEC	A	129	43/43	0.98	0.06	16,19,24,27	0
2	HEC	B	129	43/43	0.98	0.06	11,14,22,27	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.