



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 AM UTC

PDB ID : 1A4E / pdb\_00001a4e  
Title : CATALASE A FROM SACCHAROMYCES CEREVISIAE  
Authors : Mate, M.J.  
Deposited on : 1998-01-29  
Resolution : 2.40 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](mailto: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>.

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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

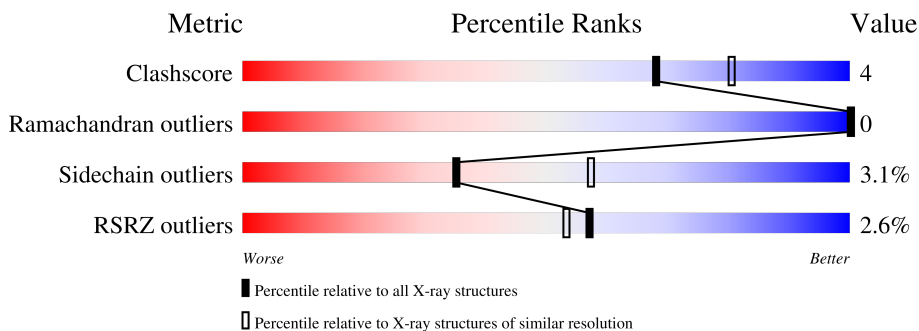
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

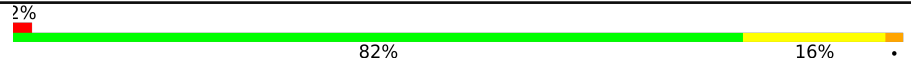

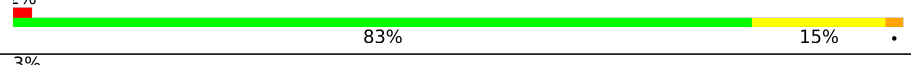

The reported resolution of this entry is 2.40 Å.

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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	488	 2% 82% 16%
1	B	488	 2% 84% 15%
1	C	488	 2% 83% 15%
1	D	488	 3% 79% 19%

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
2	AZI	A	504	-	X	-	-
2	AZI	B	504	-	X	-	-
2	AZI	C	504	-	X	-	-
2	AZI	D	504	-	X	-	-

## 2 Entry composition [i](#)

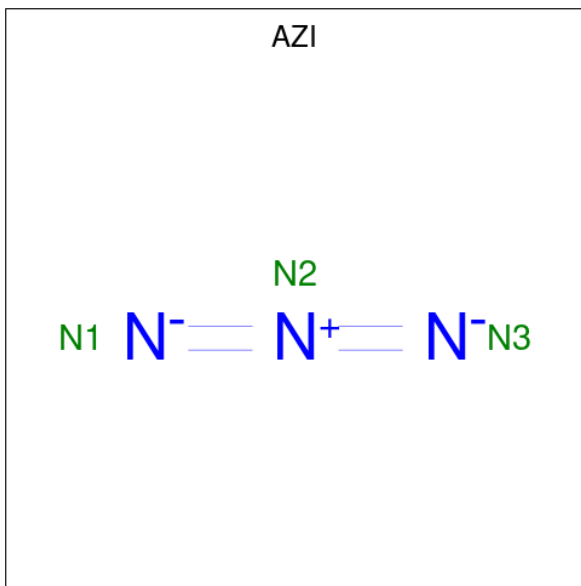
There are 5 unique types of molecules in this entry. The entry contains 16879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3932	2493	695	732	12	29	0	0
1	B	488	3932	2493	695	732	12	0	0	0
1	C	488	3932	2493	695	732	12	0	0	0
1	D	488	3932	2493	695	732	12	0	0	0

- Molecule 2 is AZIDE ION (CCD ID: AZI) (formula: N<sub>3</sub>).



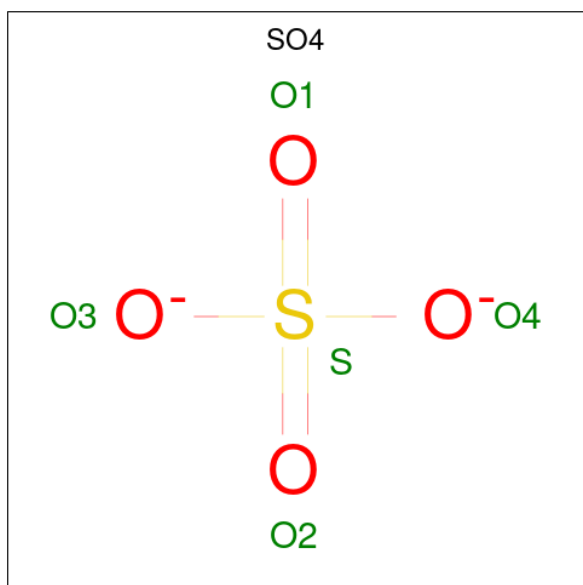
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 3	N 3	0	0
2	B	1	Total 3	N 3	0	0

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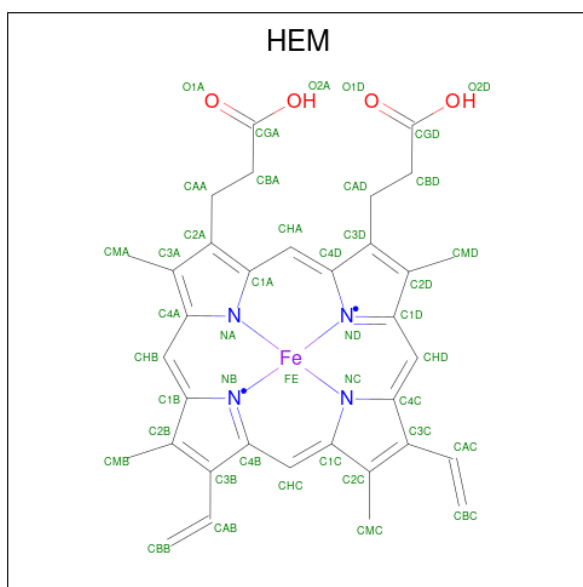
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total N 3 3	0	0
2	D	1	Total N 3 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

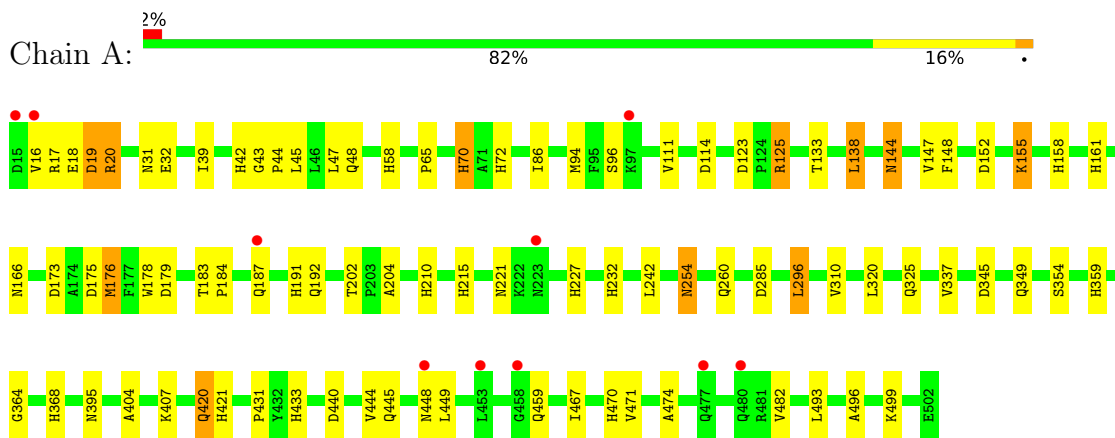
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	221	221	221	0	0
5	B	262	262	262	0	0
5	C	242	242	242	0	0
5	D	232	232	232	0	0

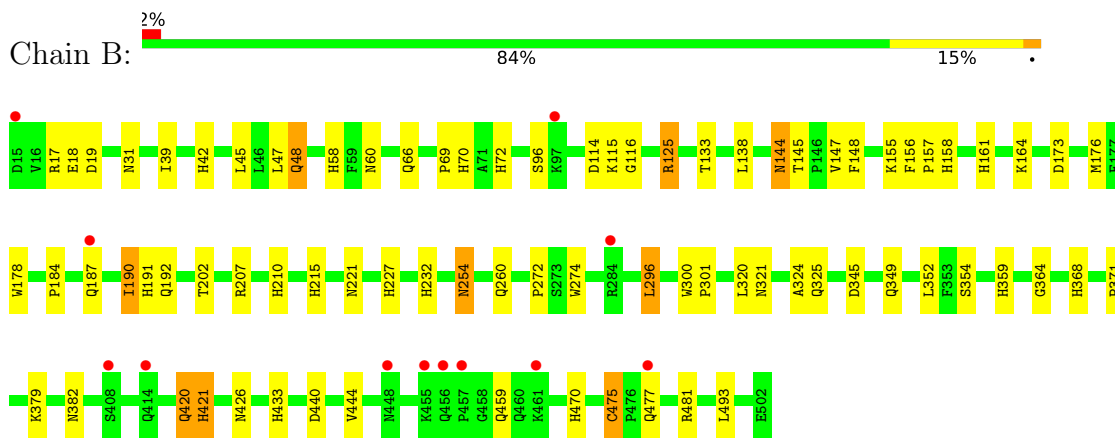
### 3 Residue-property plots [i](#)

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.

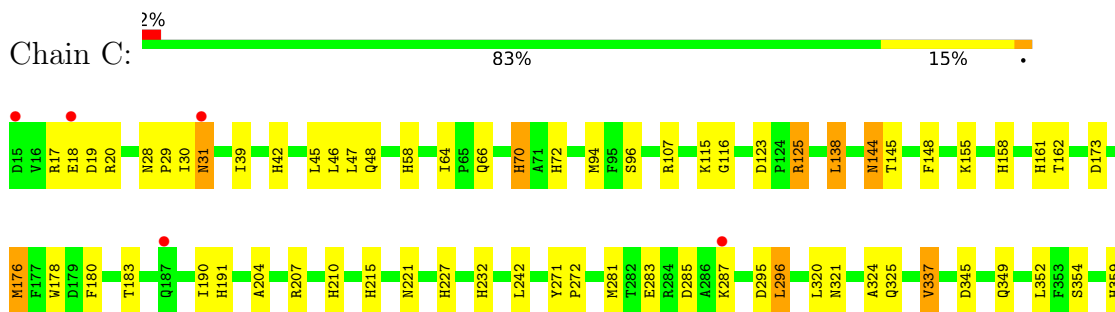
- Molecule 1: CATALASE A

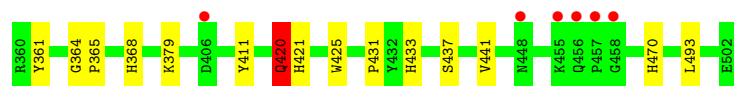


- Molecule 1: CATALASE A

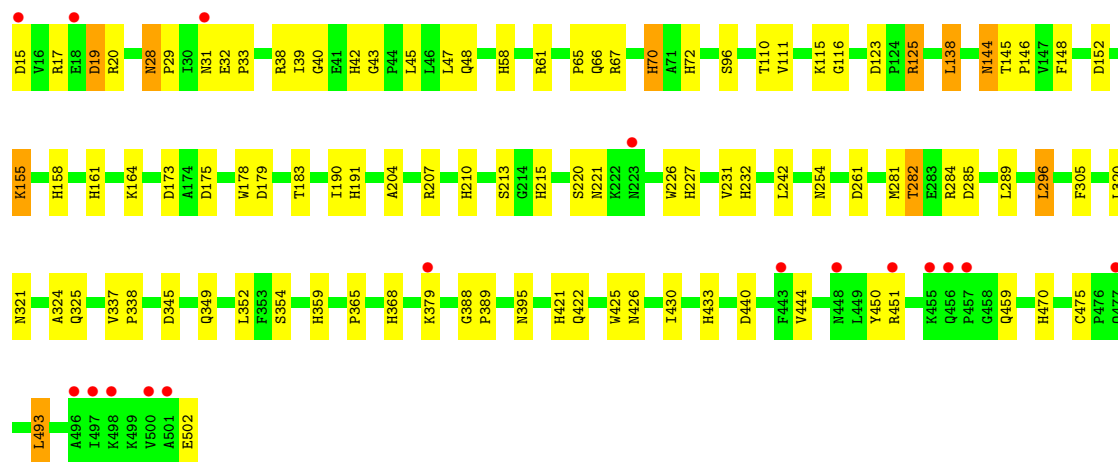
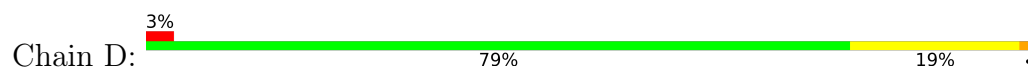


- Molecule 1: CATALASE A





● Molecule 1: CATALASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.17Å 184.17Å 304.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.40) 97.7 (20.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.84 (at 2.36Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.154 , 0.198 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, AZI, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.84	17/4047 (0.4%)	1.41	37/5505 (0.7%)
1	B	0.83	18/4047 (0.4%)	1.42	38/5505 (0.7%)
1	C	0.84	18/4047 (0.4%)	1.44	35/5505 (0.6%)
1	D	0.84	16/4047 (0.4%)	1.43	46/5505 (0.8%)
All	All	0.84	69/16188 (0.4%)	1.43	156/22020 (0.7%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	HIS	CD2-NE2	-7.04	1.30	1.37
1	D	158	HIS	CD2-NE2	-6.95	1.30	1.37
1	C	161	HIS	CD2-NE2	-6.91	1.30	1.37
1	C	158	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	215	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	161	HIS	CD2-NE2	-6.67	1.30	1.37
1	B	161	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	58	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	368	HIS	CD2-NE2	-6.57	1.30	1.37
1	C	421	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	72	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	368	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	421	HIS	CD2-NE2	-6.50	1.30	1.37
1	D	215	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	421	HIS	CD2-NE2	-6.45	1.30	1.37
1	C	227	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	359	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	215	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	210	HIS	CD2-NE2	-6.43	1.30	1.37
1	D	58	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	368	HIS	CD2-NE2	-6.41	1.30	1.37
1	D	433	HIS	CD2-NE2	-6.41	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	232	HIS	CD2-NE2	-6.38	1.30	1.37
1	D	210	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	359	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	470	HIS	CD2-NE2	-6.37	1.30	1.37
1	D	421	HIS	CD2-NE2	-6.36	1.30	1.37
1	D	232	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	433	HIS	CD2-NE2	-6.35	1.30	1.37
1	D	227	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	232	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	42	HIS	CD2-NE2	-6.33	1.30	1.37
1	D	70	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	470	HIS	CD2-NE2	-6.32	1.30	1.37
1	C	215	HIS	CD2-NE2	-6.32	1.30	1.37
1	C	42	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	158	HIS	CD2-NE2	-6.31	1.30	1.37
1	D	368	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	70	HIS	CD2-NE2	-6.27	1.30	1.37
1	C	70	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	72	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	191	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	42	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	42	HIS	CD2-NE2	-6.24	1.30	1.37
1	D	72	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.23	1.30	1.37
1	C	433	HIS	CD2-NE2	-6.22	1.31	1.37
1	D	359	HIS	CD2-NE2	-6.22	1.31	1.37
1	D	470	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	210	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	158	HIS	CD2-NE2	-6.19	1.31	1.37
1	C	191	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	58	HIS	CD2-NE2	-6.17	1.31	1.37
1	C	470	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	359	HIS	CD2-NE2	-6.16	1.31	1.37
1	B	433	HIS	CD2-NE2	-6.16	1.31	1.37
1	C	58	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	227	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	227	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	210	HIS	CD2-NE2	-6.09	1.31	1.37
1	C	72	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	191	HIS	CD2-NE2	-5.97	1.31	1.37
1	D	191	HIS	CD2-NE2	-5.87	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	HIS	CG-ND1	-5.24	1.32	1.38
1	A	72	HIS	CG-ND1	-5.21	1.32	1.38
1	B	72	HIS	CG-ND1	-5.15	1.32	1.38
1	C	359	HIS	CG-ND1	-5.08	1.32	1.38
1	C	210	HIS	CG-ND1	-5.02	1.32	1.38

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	SER	N-CA-C	9.62	122.97	111.33
1	C	354	SER	N-CA-C	8.98	121.88	111.11
1	B	354	SER	N-CA-C	8.78	121.95	111.33
1	A	354	SER	N-CA-C	8.53	121.65	111.33
1	B	96	SER	N-CA-C	8.29	121.25	111.71
1	A	31	ASN	CA-CB-CG	7.67	120.27	112.60
1	C	31	ASN	N-CA-C	7.64	119.25	111.07
1	A	96	SER	N-CA-C	7.18	120.94	111.75
1	A	58	HIS	CB-CG-CD2	-6.84	122.30	131.20
1	C	96	SER	N-CA-C	6.84	119.58	111.71
1	D	254	ASN	CA-C-N	6.56	126.25	119.56
1	D	254	ASN	C-N-CA	6.56	126.25	119.56
1	B	173	ASP	CA-CB-CG	6.51	119.11	112.60
1	B	164	LYS	N-CA-C	6.51	114.12	108.78
1	C	58	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	B	215	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	58	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	215	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	C	425	TRP	CE2-CD2-CG	-6.22	99.73	107.20
1	C	215	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	D	58	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	C	42	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	C	441	VAL	N-CA-C	6.09	117.56	110.62
1	D	388	GLY	CA-C-N	6.08	126.11	119.90
1	D	388	GLY	C-N-CA	6.08	126.11	119.90
1	C	364	GLY	CA-C-N	6.07	126.24	119.32
1	C	364	GLY	C-N-CA	6.07	126.24	119.32
1	C	425	TRP	CG-CD2-CE3	6.00	139.90	133.90
1	D	164	LYS	N-CA-C	6.00	113.70	108.78
1	D	345	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	420	GLN	CB-CA-C	-5.98	100.87	110.79
1	D	215	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	B	345	ASP	CA-CB-CG	5.91	118.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	SER	N-CA-C	5.90	117.38	111.07
1	C	345	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	379	LYS	N-CA-C	5.80	118.42	110.24
1	B	48	GLN	CA-CB-CG	5.77	125.65	114.10
1	A	459	GLN	N-CA-C	5.77	118.51	111.82
1	A	18	GLU	N-CA-C	5.75	118.29	111.33
1	B	42	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	A	254	ASN	CA-C-N	5.74	125.42	119.56
1	A	254	ASN	C-N-CA	5.74	125.42	119.56
1	A	364	GLY	CA-C-N	5.71	125.82	119.32
1	A	364	GLY	C-N-CA	5.71	125.82	119.32
1	A	285	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	227	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	C	161	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	D	183	THR	CA-C-N	5.64	125.11	119.24
1	D	183	THR	C-N-CA	5.64	125.11	119.24
1	B	221	ASN	CA-CB-CG	5.64	118.24	112.60
1	D	282	THR	CA-CB-OG1	-5.63	101.15	109.60
1	C	420	GLN	CB-CA-C	-5.63	101.44	110.79
1	C	221	ASN	CA-CB-CG	5.63	118.23	112.60
1	D	422	GLN	N-CA-C	5.62	114.15	108.75
1	C	20	ARG	N-CA-C	5.62	119.19	111.54
1	A	345	ASP	CA-C-N	5.62	125.29	119.05
1	A	345	ASP	C-N-CA	5.62	125.29	119.05
1	D	173	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	18	GLU	N-CA-C	5.57	119.34	112.54
1	D	28	ASN	CA-C-N	5.54	125.30	119.76
1	D	28	ASN	C-N-CA	5.54	125.30	119.76
1	A	166	ASN	CA-C-N	5.53	125.36	119.28
1	A	166	ASN	C-N-CA	5.53	125.36	119.28
1	B	145	THR	CA-C-N	5.53	125.36	119.28
1	B	145	THR	C-N-CA	5.53	125.36	119.28
1	A	43	GLY	CA-C-N	5.53	125.43	119.85
1	A	43	GLY	C-N-CA	5.53	125.43	119.85
1	D	221	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	178	TRP	CG-CD2-CE3	5.52	139.42	133.90
1	A	176	MET	CB-CA-C	-5.52	102.22	110.88
1	D	31	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	420	GLN	CB-CA-C	-5.49	101.68	110.79
1	C	145	THR	CA-C-N	5.48	125.00	119.19
1	C	145	THR	C-N-CA	5.48	125.00	119.19
1	D	345	ASP	CA-C-N	5.47	125.29	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	ASP	C-N-CA	5.47	125.29	119.28
1	A	161	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	D	111	VAL	N-CA-C	5.43	116.58	111.48
1	C	176	MET	CB-CA-C	-5.43	102.36	110.88
1	A	20	ARG	N-CA-C	5.42	118.92	111.54
1	A	183	THR	CA-C-N	5.42	124.88	119.24
1	A	183	THR	C-N-CA	5.42	124.88	119.24
1	D	459	GLN	N-CA-C	5.41	118.09	111.82
1	B	161	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	B	364	GLY	CA-C-N	5.40	125.73	119.47
1	B	364	GLY	C-N-CA	5.40	125.73	119.47
1	D	227	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	D	43	GLY	CA-C-N	5.38	125.28	119.85
1	D	43	GLY	C-N-CA	5.38	125.28	119.85
1	B	345	ASP	CA-C-N	5.37	125.19	119.28
1	B	345	ASP	C-N-CA	5.37	125.19	119.28
1	D	15	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	289	LEU	CA-C-N	5.35	125.17	119.28
1	D	289	LEU	C-N-CA	5.35	125.17	119.28
1	A	42	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	D	178	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	D	433	HIS	CA-CB-CG	5.33	119.13	113.80
1	D	451	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	32	GLU	CA-C-N	5.33	125.14	119.28
1	D	32	GLU	C-N-CA	5.33	125.14	119.28
1	B	176	MET	CB-CA-C	-5.32	102.53	110.88
1	B	368	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	337	VAL	CA-C-N	5.29	125.30	119.90
1	C	337	VAL	C-N-CA	5.29	125.30	119.90
1	D	31	ASN	N-CA-C	5.29	117.45	111.11
1	C	183	THR	CA-C-N	5.28	124.74	119.24
1	C	183	THR	C-N-CA	5.28	124.74	119.24
1	B	31	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	382	ASN	CA-C-N	5.26	125.07	119.28
1	B	382	ASN	C-N-CA	5.26	125.07	119.28
1	B	459	GLN	N-CA-C	5.25	117.91	111.82
1	A	221	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	178	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	C	379	LYS	N-CA-C	5.24	117.62	110.24
1	A	474	ALA	N-CA-C	5.23	117.43	110.53
1	D	161	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	B	190	ILE	N-CA-C	5.21	115.93	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	HIS	CB-CG-CD2	-5.20	124.45	131.20
1	C	437	SER	CA-C-N	5.19	125.13	119.78
1	C	437	SER	C-N-CA	5.19	125.13	119.78
1	C	178	TRP	CG-CD2-CE3	5.19	139.09	133.90
1	D	430	ILE	CA-C-N	5.18	126.32	119.84
1	D	430	ILE	C-N-CA	5.18	126.32	119.84
1	A	58	HIS	CB-CG-ND1	5.16	130.44	122.70
1	C	178	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	178	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	B	202	THR	CA-C-N	5.13	125.06	119.78
1	B	202	THR	C-N-CA	5.13	125.06	119.78
1	D	178	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	B	470	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	B	18	GLU	N-CA-C	5.11	116.85	111.28
1	B	232	HIS	CB-CG-CD2	-5.10	124.56	131.20
1	A	19	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	425	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	D	19	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	475	CYS	CA-C-N	5.08	125.11	119.32
1	B	475	CYS	C-N-CA	5.08	125.11	119.32
1	A	202	THR	CA-C-N	5.06	125.00	119.78
1	A	202	THR	C-N-CA	5.06	125.00	119.78
1	D	20	ARG	N-CA-C	5.06	118.58	111.90
1	D	475	CYS	CA-C-N	5.06	125.09	119.32
1	D	475	CYS	C-N-CA	5.06	125.09	119.32
1	B	274	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	178	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	368	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	C	361	TYR	CA-C-N	5.05	127.01	120.44
1	C	361	TYR	C-N-CA	5.05	127.01	120.44
1	B	254	ASN	CA-C-N	5.05	124.71	119.56
1	B	254	ASN	C-N-CA	5.05	124.71	119.56
1	C	30	ILE	CA-C-N	5.04	127.00	120.44
1	C	30	ILE	C-N-CA	5.04	127.00	120.44
1	A	32	GLU	CA-C-N	5.03	125.06	119.32
1	A	32	GLU	C-N-CA	5.03	125.06	119.32
1	C	295	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	42	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	227	HIS	CB-CG-CD2	-5.00	124.69	131.20

There are no chirality outliers.

There are no planarity outliers.

## 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	3932	0	3749	34	0
1	B	3932	0	3749	28	0
1	C	3932	0	3749	33	0
1	D	3932	0	3749	39	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
4	C	43	0	30	0	0
4	D	43	0	30	0	0
5	A	221	0	0	0	0
5	B	262	0	0	0	0
5	C	242	0	0	1	0
5	D	232	0	0	0	0
All	All	16879	0	15116	112	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 4.

All (112) 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:39:ILE:HG13	1:C:39:ILE:HG13	1.68	0.74
1:A:444:VAL:HG12	1:A:448:ASN:HD21	1.52	0.73
1:B:39:ILE:HG13	1:D:39:ILE:HG13	1.73	0.71
1:B:321:ASN:HD22	1:B:324:ALA:H	1.41	0.68
1:A:320:LEU:H	1:A:325:GLN:HE22	1.41	0.68
1:B:320:LEU:H	1:B:325:GLN:HE22	1.45	0.64
1:C:148:PHE:HB3	1:C:296:LEU:HD13	1.79	0.62
1:A:445:GLN:HA	1:A:448:ASN:HD22	1.66	0.61
1:C:320:LEU:H	1:C:325:GLN:HE22	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG23	1:B:192:GLN:HE21	1.66	0.61
1:D:320:LEU:H	1:D:325:GLN:HE22	1.48	0.60
1:D:321:ASN:HD22	1:D:324:ALA:H	1.48	0.59
1:A:349:GLN:HE22	1:B:48:GLN:HE21	1.50	0.59
1:B:148:PHE:HB3	1:B:296:LEU:HD13	1.86	0.58
1:C:321:ASN:HD22	1:C:324:ALA:H	1.51	0.58
1:D:148:PHE:HB3	1:D:296:LEU:HD13	1.85	0.57
1:A:148:PHE:HB3	1:A:296:LEU:HD13	1.86	0.57
1:A:173:ASP:HB3	1:A:176:MET:HE2	1.87	0.57
1:C:48:GLN:HE21	1:D:349:GLN:HE22	1.53	0.56
1:A:48:GLN:HE21	1:B:349:GLN:HE22	1.54	0.56
1:D:17:ARG:HD3	1:D:19:ASP:OD1	2.06	0.55
1:C:66:GLN:NE2	1:C:115:LYS:H	2.04	0.55
1:C:349:GLN:HE22	1:D:48:GLN:HE21	1.55	0.55
1:B:17:ARG:HD3	1:B:19:ASP:OD1	2.07	0.55
1:D:125:ARG:H	1:D:144:ASN:ND2	2.06	0.54
1:B:207:ARG:HG2	1:B:272:PRO:HB3	1.90	0.53
1:C:94:MET:SD	1:C:138:LEU:HD12	2.49	0.52
1:C:125:ARG:H	1:C:144:ASN:ND2	2.07	0.52
1:A:431:PRO:HD2	1:C:420:GLN:HG3	1.91	0.52
1:D:282:THR:HG22	1:D:284:ARG:H	1.74	0.52
1:B:66:GLN:NE2	1:B:115:LYS:H	2.07	0.51
1:B:426:ASN:HD22	1:D:426:ASN:HD22	1.58	0.51
1:A:125:ARG:H	1:A:144:ASN:ND2	2.08	0.51
1:D:138:LEU:HG	1:D:337:VAL:HG22	1.92	0.51
1:D:152:ASP:HB2	1:D:155:LYS:HE2	1.93	0.50
1:D:204:ALA:HA	1:D:242:LEU:HG	1.93	0.50
1:A:440:ASP:O	1:A:444:VAL:HG23	2.12	0.50
1:B:66:GLN:HE22	1:B:115:LYS:H	1.60	0.50
1:B:125:ARG:H	1:B:144:ASN:ND2	2.10	0.50
1:D:213:SER:HB2	1:D:231:VAL:H	1.77	0.50
1:C:173:ASP:HB3	1:C:176:MET:HE2	1.93	0.49
1:C:17:ARG:HB3	1:D:379:LYS:HE2	1.93	0.49
1:A:114:ASP:HB2	1:D:116:GLY:HA3	1.93	0.49
1:D:66:GLN:NE2	1:D:115:LYS:H	2.10	0.49
1:C:138:LEU:HG	1:C:337:VAL:HG22	1.93	0.49
1:C:66:GLN:HE22	1:C:115:LYS:H	1.59	0.49
1:D:320:LEU:N	1:D:325:GLN:HE22	2.10	0.49
1:B:321:ASN:ND2	1:B:324:ALA:H	2.10	0.48
1:C:204:ALA:HA	1:C:242:LEU:HG	1.94	0.48
1:A:404:ALA:HB3	1:A:407:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLN:HG3	1:C:431:PRO:HD2	1.95	0.48
1:D:281:MET:HG2	1:D:285:ASP:HB2	1.96	0.47
1:A:16:VAL:HG11	1:A:20:ARG:NH1	2.29	0.47
1:D:321:ASN:H	1:D:325:GLN:NE2	2.12	0.47
1:C:281:MET:HG2	1:C:285:ASP:HB2	1.98	0.46
1:A:444:VAL:HG12	1:A:448:ASN:ND2	2.23	0.46
1:C:321:ASN:ND2	1:D:395:ASN:HD22	2.14	0.46
1:B:116:GLY:H	1:C:116:GLY:H	1.64	0.45
1:C:365:PRO:HG3	1:D:61:ARG:HD3	1.97	0.45
1:A:395:ASN:HD22	1:B:321:ASN:HD21	1.64	0.45
1:D:365:PRO:HG2	1:D:389:PRO:HD2	1.99	0.45
1:A:204:ALA:HA	1:A:242:LEU:HG	1.99	0.45
1:D:365:PRO:CG	1:D:389:PRO:HD2	2.46	0.45
1:D:281:MET:HE2	1:D:305:PHE:CZ	2.52	0.44
1:D:440:ASP:O	1:D:444:VAL:HG23	2.17	0.44
1:C:207:ARG:HG2	1:C:272:PRO:HB3	1.99	0.44
1:B:321:ASN:H	1:B:325:GLN:HE21	1.66	0.44
1:A:44:PRO:HB2	1:C:46:LEU:HD22	2.00	0.44
1:A:467:ILE:O	1:A:471:VAL:HG23	2.18	0.44
1:C:17:ARG:HD3	1:C:19:ASP:OD1	2.17	0.44
1:A:65:PRO:HG3	1:D:65:PRO:HD3	2.00	0.43
1:A:94:MET:SD	1:A:138:LEU:HD12	2.58	0.43
1:B:477:GLN:O	1:B:481:ARG:HG3	2.18	0.43
1:C:28:ASN:HA	1:C:29:PRO:HD3	1.91	0.43
1:C:64:ILE:HG22	1:D:389:PRO:HG3	1.99	0.43
1:A:17:ARG:HD3	1:A:19:ASP:OD1	2.18	0.43
1:D:220:SER:HB3	1:D:226:TRP:HB3	2.01	0.43
1:A:496:ALA:HA	1:A:499:LYS:HD2	2.01	0.43
1:B:184:PRO:HA	1:B:187:GLN:NE2	2.34	0.42
1:C:162:THR:HG21	1:C:180:PHE:HB2	2.01	0.42
1:C:411:TYR:CZ	1:D:33:PRO:HB3	2.55	0.42
1:D:145:THR:HA	1:D:146:PRO:HD3	1.94	0.42
1:A:175:ASP:O	1:A:179:ASP:HB2	2.20	0.42
1:D:175:ASP:O	1:D:179:ASP:HB2	2.20	0.42
1:B:254:ASN:HD21	1:B:260:GLN:NE2	2.17	0.41
1:C:321:ASN:HD21	1:D:395:ASN:HD22	1.67	0.41
1:A:320:LEU:N	1:A:325:GLN:HE22	2.12	0.41
1:B:321:ASN:H	1:B:325:GLN:NE2	2.17	0.41
1:C:271:TYR:HA	1:C:272:PRO:HD2	1.94	0.41
1:C:320:LEU:N	1:C:325:GLN:HE22	2.17	0.41
1:D:207:ARG:HD3	1:D:261:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:TYR:CE1	1:D:493:LEU:HG	2.55	0.41
1:B:421:HIS:H	1:B:421:HIS:CD2	2.37	0.41
1:C:283:GLU:HG2	1:C:287:LYS:HE3	2.02	0.41
1:A:147:VAL:HG23	1:A:192:GLN:HE21	1.85	0.41
1:D:28:ASN:HA	1:D:29:PRO:HD3	1.91	0.41
1:B:114:ASP:HB2	1:C:116:GLY:CA	2.51	0.41
1:A:86:ILE:HG21	1:A:310:VAL:HG22	2.03	0.41
1:B:426:ASN:HD22	1:D:426:ASN:ND2	2.18	0.41
1:A:70:HIS:CE1	1:A:111:VAL:HG22	2.56	0.41
1:A:138:LEU:HG	1:A:337:VAL:HG22	2.02	0.41
1:B:60:ASN:HA	5:C:568:HOH:O	2.21	0.41
1:B:440:ASP:O	1:B:444:VAL:HG23	2.21	0.41
1:C:70:HIS:O	1:C:107:ARG:NH2	2.54	0.41
1:D:38:ARG:HG3	1:D:40:GLY:O	2.21	0.41
1:B:156:PHE:HB3	1:B:157:PRO:HD3	2.03	0.41
1:A:152:ASP:HB2	1:A:155:LYS:HE2	2.02	0.40
1:B:300:TRP:HA	1:B:301:PRO:HD3	1.92	0.40
1:D:70:HIS:HA	1:D:110:THR:O	2.22	0.40
1:A:184:PRO:HA	1:A:187:GLN:NE2	2.37	0.40
1:A:254:ASN:HD21	1:A:260:GLN:NE2	2.19	0.40
1:A:471:VAL:HG21	1:A:482:VAL:HG11	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	486/488 (100%)	471 (97%)	15 (3%)	0	100	100
1	B	486/488 (100%)	472 (97%)	14 (3%)	0	100	100
1	C	486/488 (100%)	472 (97%)	14 (3%)	0	100	100
1	D	486/488 (100%)	470 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1944/1952 (100%)	1885 (97%)	59 (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	422/422 (100%)	411 (97%)	11 (3%)	40	63
1	B	422/422 (100%)	407 (96%)	15 (4%)	31	52
1	C	422/422 (100%)	409 (97%)	13 (3%)	35	57
1	D	422/422 (100%)	408 (97%)	14 (3%)	33	55
All	All	1688/1688 (100%)	1635 (97%)	53 (3%)	35	57

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	LEU
1	A	123	ASP
1	A	125	ARG
1	A	133	THR
1	A	138	LEU
1	A	144	ASN
1	A	155	LYS
1	A	296	LEU
1	A	449	LEU
1	A	493	LEU
1	B	45	LEU
1	B	47	LEU
1	B	69	PRO
1	B	125	ARG
1	B	133	THR
1	B	138	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	144	ASN
1	B	155	LYS
1	B	190	ILE
1	B	296	LEU
1	B	352	LEU
1	B	371	PRO
1	B	420	GLN
1	B	475	CYS
1	B	493	LEU
1	C	31	ASN
1	C	45	LEU
1	C	47	LEU
1	C	123	ASP
1	C	125	ARG
1	C	138	LEU
1	C	144	ASN
1	C	155	LYS
1	C	190	ILE
1	C	296	LEU
1	C	352	LEU
1	C	420	GLN
1	C	493	LEU
1	D	45	LEU
1	D	47	LEU
1	D	67	ARG
1	D	123	ASP
1	D	125	ARG
1	D	138	LEU
1	D	144	ASN
1	D	155	LYS
1	D	190	ILE
1	D	296	LEU
1	D	338	PRO
1	D	352	LEU
1	D	493	LEU
1	D	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	37	GLN
1	A	48	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	63	ASN
1	A	144	ASN
1	A	158	HIS
1	A	187	GLN
1	A	192	GLN
1	A	223	ASN
1	A	241	ASN
1	A	260	GLN
1	A	270	ASN
1	A	304	GLN
1	A	325	GLN
1	A	421	HIS
1	A	426	ASN
1	A	448	ASN
1	B	37	GLN
1	B	48	GLN
1	B	66	GLN
1	B	144	ASN
1	B	163	GLN
1	B	170	ASN
1	B	192	GLN
1	B	260	GLN
1	B	321	ASN
1	B	325	GLN
1	B	421	HIS
1	B	426	ASN
1	B	459	GLN
1	C	31	ASN
1	C	66	GLN
1	C	144	ASN
1	C	170	ASN
1	C	192	GLN
1	C	227	HIS
1	C	260	GLN
1	C	321	ASN
1	C	325	GLN
1	C	421	HIS
1	C	480	GLN
1	D	31	ASN
1	D	37	GLN
1	D	48	GLN
1	D	66	GLN

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Mol	Chain	Res	Type
1	D	144	ASN
1	D	223	ASN
1	D	254	ASN
1	D	302	GLN
1	D	321	ASN
1	D	325	GLN
1	D	349	GLN
1	D	391	ASN
1	D	421	HIS
1	D	456	GLN

### 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](#)

10 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	$\# Z  > 2$
3	SO4	A	1	-	4,4,4	0.65	0	6,6,6	0.36	0
3	SO4	D	2	-	4,4,4	0.68	0	6,6,6	0.24	0
2	AZI	D	504	4	2,2,2	8.28	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AZI	A	504	4	2,2,2	8.30	2 (100%)	0,1,1	-	-
2	AZI	C	504	4	2,2,2	8.48	2 (100%)	0,1,1	-	-
4	HEM	B	503	1,2	50,50,50	1.15	6 (12%)	67,82,82	0.89	2 (2%)
4	HEM	C	503	1,2	50,50,50	1.14	6 (12%)	67,82,82	0.86	1 (1%)
4	HEM	D	503	1,2	50,50,50	1.12	6 (12%)	67,82,82	0.86	1 (1%)
2	AZI	B	504	4	2,2,2	8.28	2 (100%)	0,1,1	-	-
4	HEM	A	503	1,2	50,50,50	1.11	6 (12%)	67,82,82	0.87	1 (1%)

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	C	503	1,2	-	4/14/54/54	-
4	HEM	A	503	1,2	-	5/14/54/54	-
4	HEM	B	503	1,2	-	6/14/54/54	-
4	HEM	D	503	1,2	-	6/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	504	AZI	N3-N2	8.50	1.40	1.23
2	C	504	AZI	N1-N2	8.46	1.40	1.23
2	D	504	AZI	N3-N2	8.37	1.40	1.23
2	A	504	AZI	N3-N2	8.34	1.40	1.23
2	B	504	AZI	N3-N2	8.29	1.40	1.23
2	B	504	AZI	N1-N2	8.27	1.40	1.23
2	A	504	AZI	N1-N2	8.25	1.40	1.23
2	D	504	AZI	N1-N2	8.19	1.39	1.23
4	B	503	HEM	CBB-CAB	3.58	1.47	1.30
4	D	503	HEM	CBB-CAB	3.27	1.46	1.30
4	C	503	HEM	CBC-CAC	3.24	1.45	1.30
4	A	503	HEM	CBC-CAC	3.24	1.45	1.30
4	A	503	HEM	CBB-CAB	3.21	1.45	1.30
4	C	503	HEM	CBB-CAB	3.18	1.45	1.30
4	D	503	HEM	CBC-CAC	3.11	1.45	1.30
4	B	503	HEM	CAC-C3C	-3.09	1.39	1.47
4	B	503	HEM	CBC-CAC	3.07	1.45	1.30
4	D	503	HEM	CAC-C3C	-2.86	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	HEM	CAC-C3C	-2.85	1.39	1.47
4	A	503	HEM	CAC-C3C	-2.81	1.39	1.47
4	A	503	HEM	CAB-C3B	-2.67	1.40	1.47
4	D	503	HEM	CAB-C3B	-2.66	1.40	1.47
4	C	503	HEM	O2A-CGA	-2.66	1.22	1.30
4	C	503	HEM	CAB-C3B	-2.65	1.40	1.47
4	D	503	HEM	O2A-CGA	-2.59	1.22	1.30
4	B	503	HEM	CAB-C3B	-2.59	1.40	1.47
4	D	503	HEM	O2D-CGD	-2.56	1.22	1.30
4	B	503	HEM	O2A-CGA	-2.51	1.22	1.30
4	C	503	HEM	O2D-CGD	-2.46	1.22	1.30
4	A	503	HEM	O2D-CGD	-2.41	1.22	1.30
4	B	503	HEM	O2D-CGD	-2.38	1.22	1.30
4	A	503	HEM	O2A-CGA	-2.36	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	HEM	C3B-C4B-NB	3.46	111.96	109.47
4	C	503	HEM	C3B-C4B-NB	3.24	111.79	109.47
4	A	503	HEM	C3B-C4B-NB	3.19	111.76	109.47
4	D	503	HEM	C3B-C4B-NB	2.88	111.54	109.47
4	B	503	HEM	C4B-C3B-C2B	-2.23	105.23	107.28

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	HEM	C2C-C3C-CAC-CBC
4	D	503	HEM	C2C-C3C-CAC-CBC
4	B	503	HEM	C4C-C3C-CAC-CBC
4	A	503	HEM	CAD-CBD-CGD-O2D
4	C	503	HEM	CAD-CBD-CGD-O1D
4	C	503	HEM	CAD-CBD-CGD-O2D
4	A	503	HEM	CAD-CBD-CGD-O1D
4	D	503	HEM	CAD-CBD-CGD-O2D
4	B	503	HEM	CAD-CBD-CGD-O2D
4	C	503	HEM	C2C-C3C-CAC-CBC
4	D	503	HEM	CAA-CBA-CGA-O2A
4	B	503	HEM	CAA-CBA-CGA-O2A
4	B	503	HEM	CAD-CBD-CGD-O1D
4	A	503	HEM	C4C-C3C-CAC-CBC

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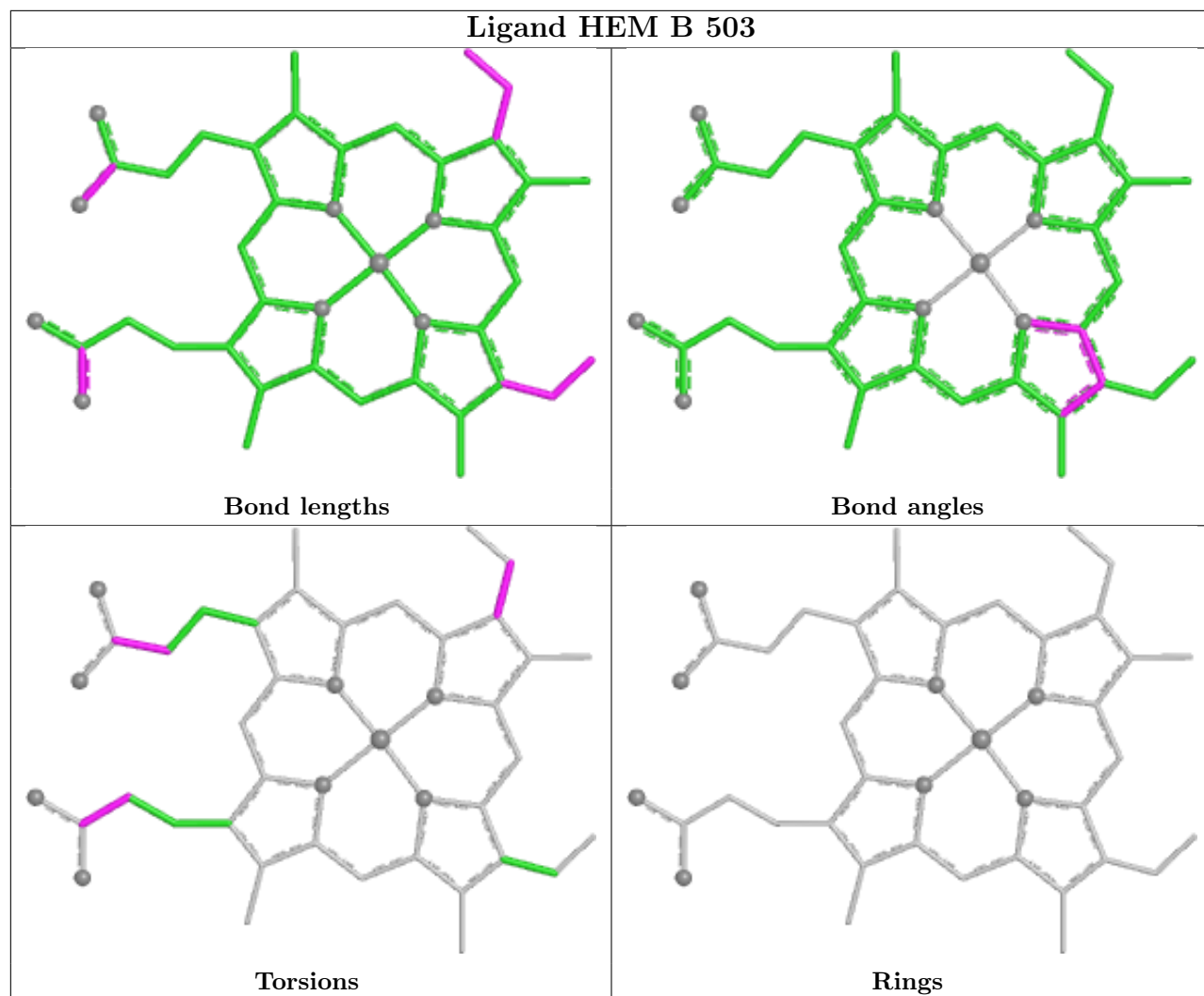
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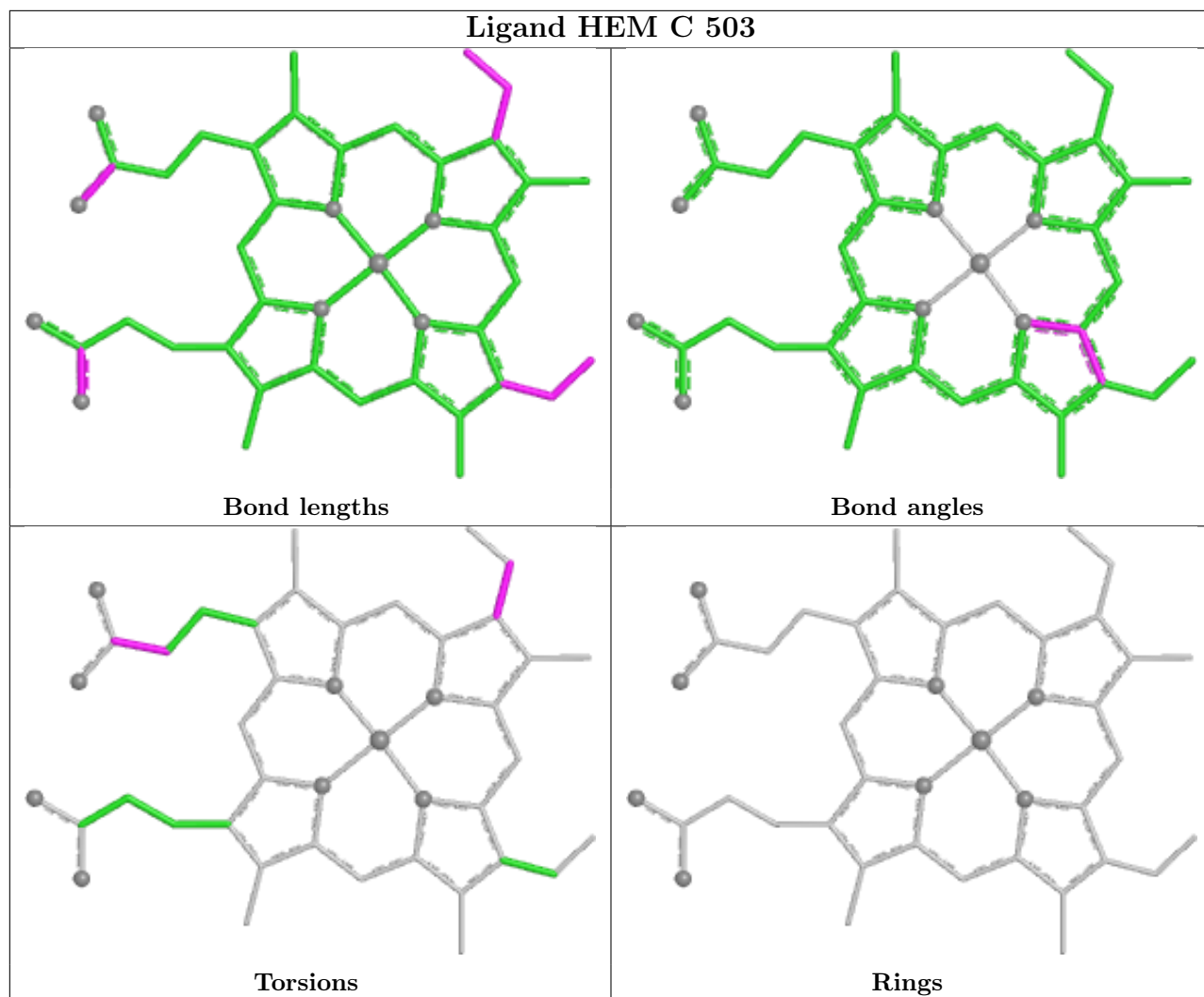
Mol	Chain	Res	Type	Atoms
4	C	503	HEM	C4C-C3C-CAC-CBC
4	D	503	HEM	C4C-C3C-CAC-CBC
4	D	503	HEM	CAD-CBD-CGD-O1D
4	B	503	HEM	CAA-CBA-CGA-O1A
4	D	503	HEM	CAA-CBA-CGA-O1A
4	A	503	HEM	CAA-CBA-CGA-O2A
4	A	503	HEM	C2C-C3C-CAC-CBC

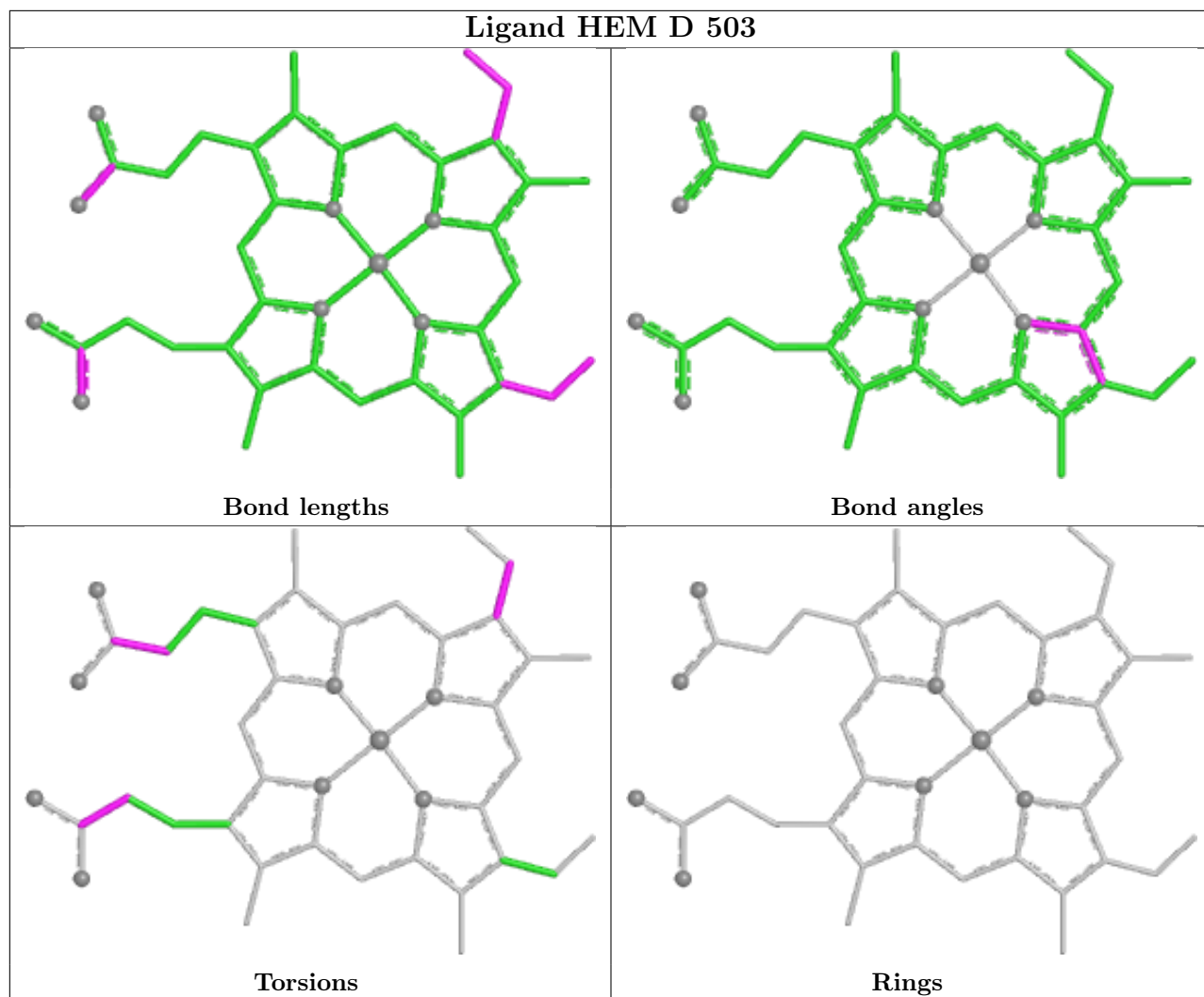
There are no ring outliers.

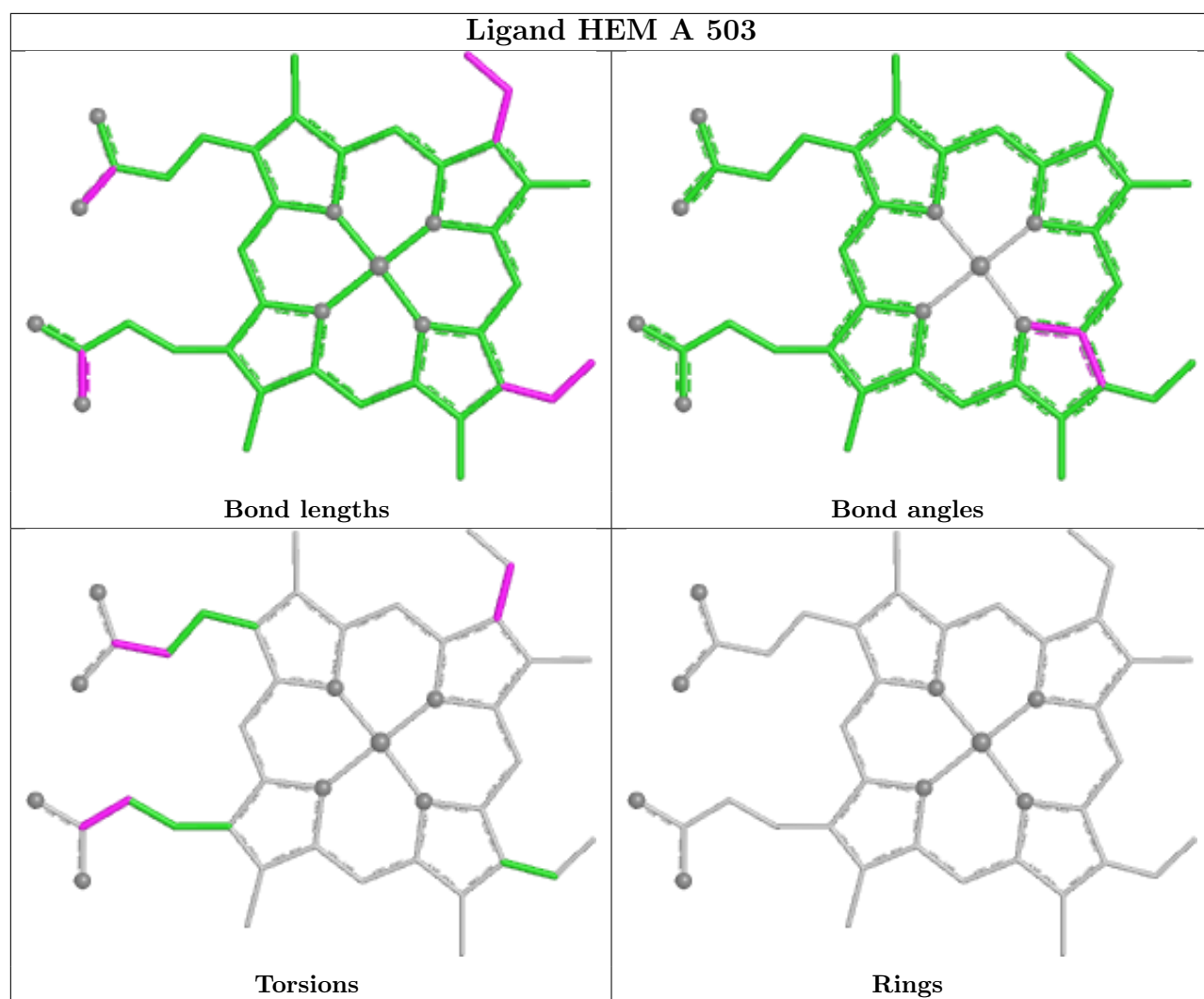
No monomer is involved in short contacts.

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	484/488 (99%)	0.13	10 (2%) 63 59	19, 29, 53, 85	0
1	B	488/488 (100%)	0.14	12 (2%) 58 54	19, 29, 51, 81	3 (0%)
1	C	488/488 (100%)	-0.21	11 (2%) 61 57	18, 31, 50, 90	3 (0%)
1	D	488/488 (100%)	0.34	17 (3%) 47 43	21, 35, 55, 81	3 (0%)
All	All	1948/1952 (99%)	0.10	50 (2%) 57 53	18, 31, 53, 90	9 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	GLN	10.4
1	C	457	PRO	10.0
1	D	457	PRO	9.9
1	B	457	PRO	9.3
1	B	456	GLN	8.7
1	C	455	LYS	8.0
1	D	455	LYS	7.9
1	C	456	GLN	7.2
1	B	455	LYS	6.7
1	D	15	ASP	5.9
1	A	15	ASP	4.6
1	C	15	ASP	4.4
1	B	448	ASN	4.4
1	A	448	ASN	4.2
1	C	448	ASN	4.2
1	D	448	ASN	3.9
1	D	451	ARG	3.8
1	B	477	GLN	3.6
1	A	223	ASN	3.6
1	D	500	VAL	3.2
1	B	97	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASN	3.0
1	D	223	ASN	3.0
1	A	480	GLN	2.9
1	D	496	ALA	2.9
1	D	501	ALA	2.9
1	B	15	ASP	2.9
1	B	284	ARG	2.8
1	B	408	SER	2.7
1	C	287	LYS	2.6
1	A	187	GLN	2.6
1	D	497	ILE	2.5
1	D	31	ASN	2.5
1	D	379	LYS	2.5
1	D	477	GLN	2.4
1	A	16	VAL	2.4
1	C	18	GLU	2.4
1	A	477	GLN	2.3
1	B	187	GLN	2.3
1	D	443	PHE	2.3
1	B	461	LYS	2.3
1	C	458	GLY	2.3
1	D	498	LYS	2.2
1	B	414	GLN	2.2
1	C	187	GLN	2.2
1	D	18	GLU	2.2
1	C	406	ASP	2.1
1	A	453	LEU	2.1
1	A	97	LYS	2.1
1	A	458	GLY	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

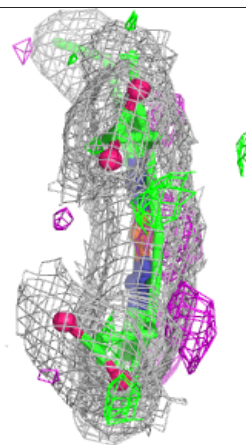
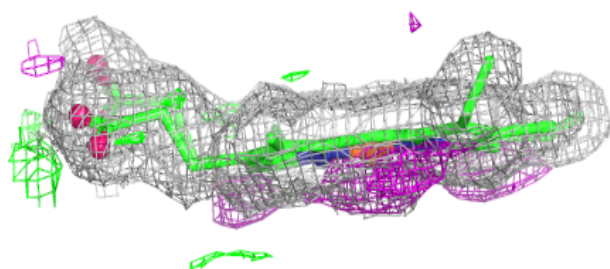
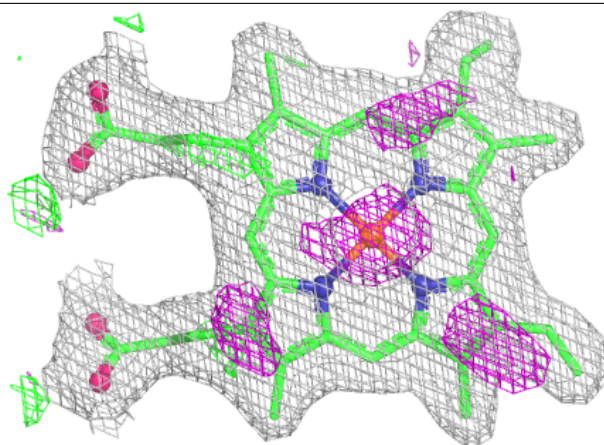
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1	5/5	0.87	0.39	79,82,85,87	0
2	AZI	B	504	3/3	0.90	0.11	25,25,27,27	0
3	SO4	D	2	5/5	0.90	0.44	70,77,79,80	0
2	AZI	D	504	3/3	0.93	0.10	27,27,28,32	0
2	AZI	A	504	3/3	0.95	0.10	25,25,28,28	0
4	HEM	B	503	43/43	0.95	0.10	18,22,25,28	0
4	HEM	D	503	43/43	0.95	0.10	21,26,28,30	0
4	HEM	A	503	43/43	0.97	0.07	18,23,25,27	0
4	HEM	C	503	43/43	0.98	0.06	12,22,25,29	0
2	AZI	C	504	3/3	0.99	0.05	20,20,21,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

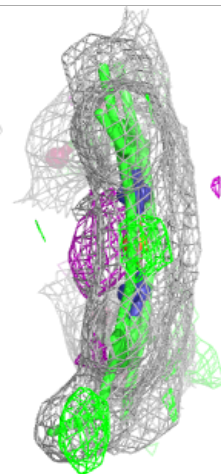
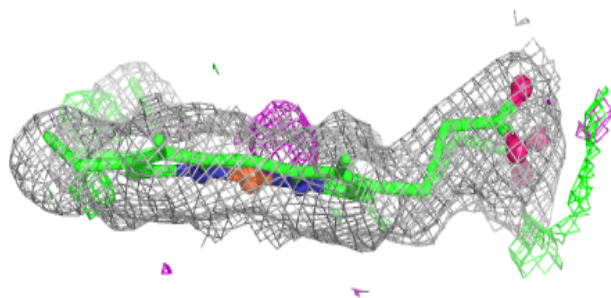
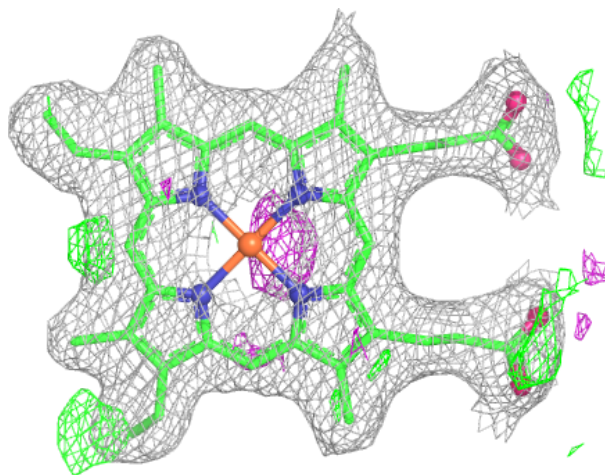
**Electron density around HEM B 503:**

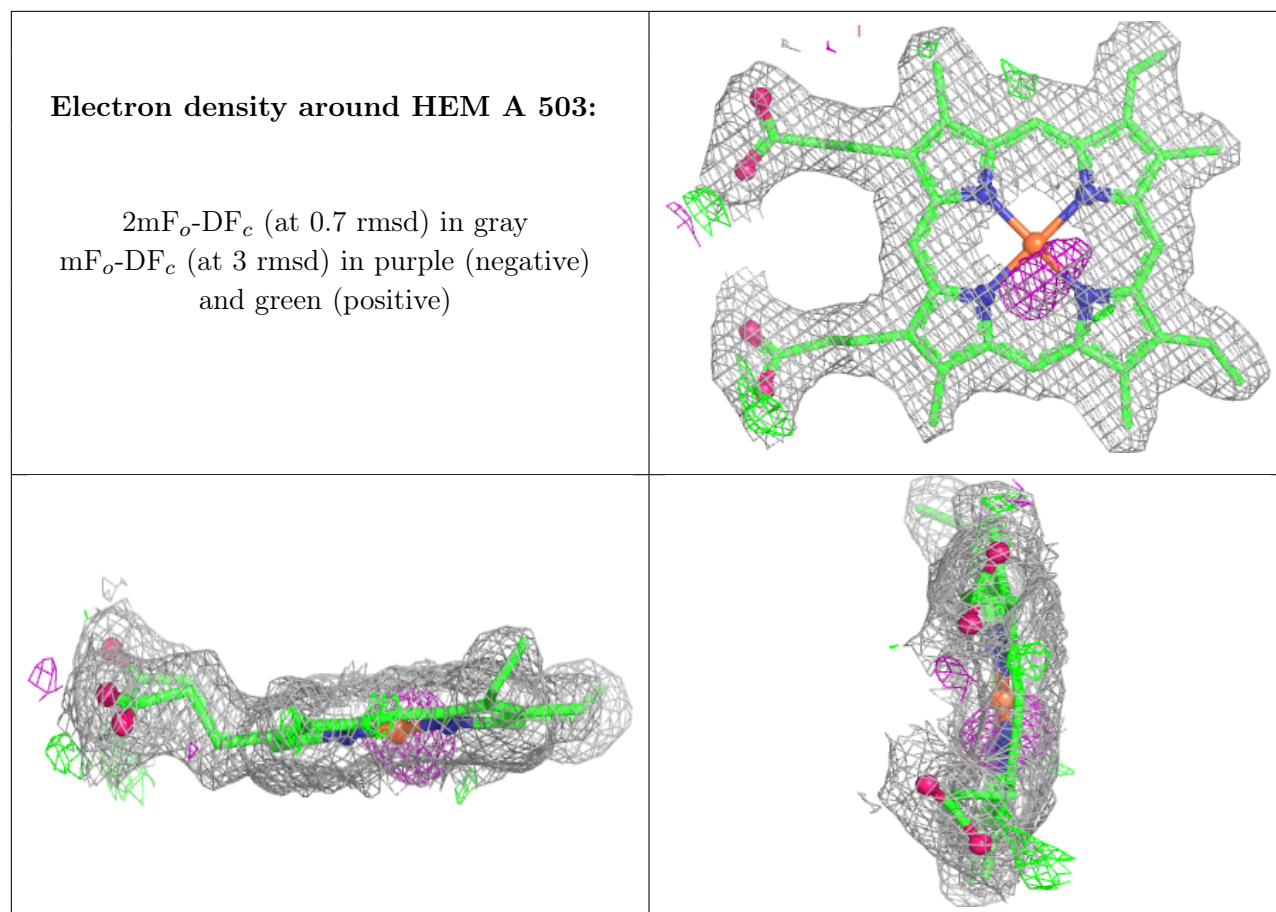
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

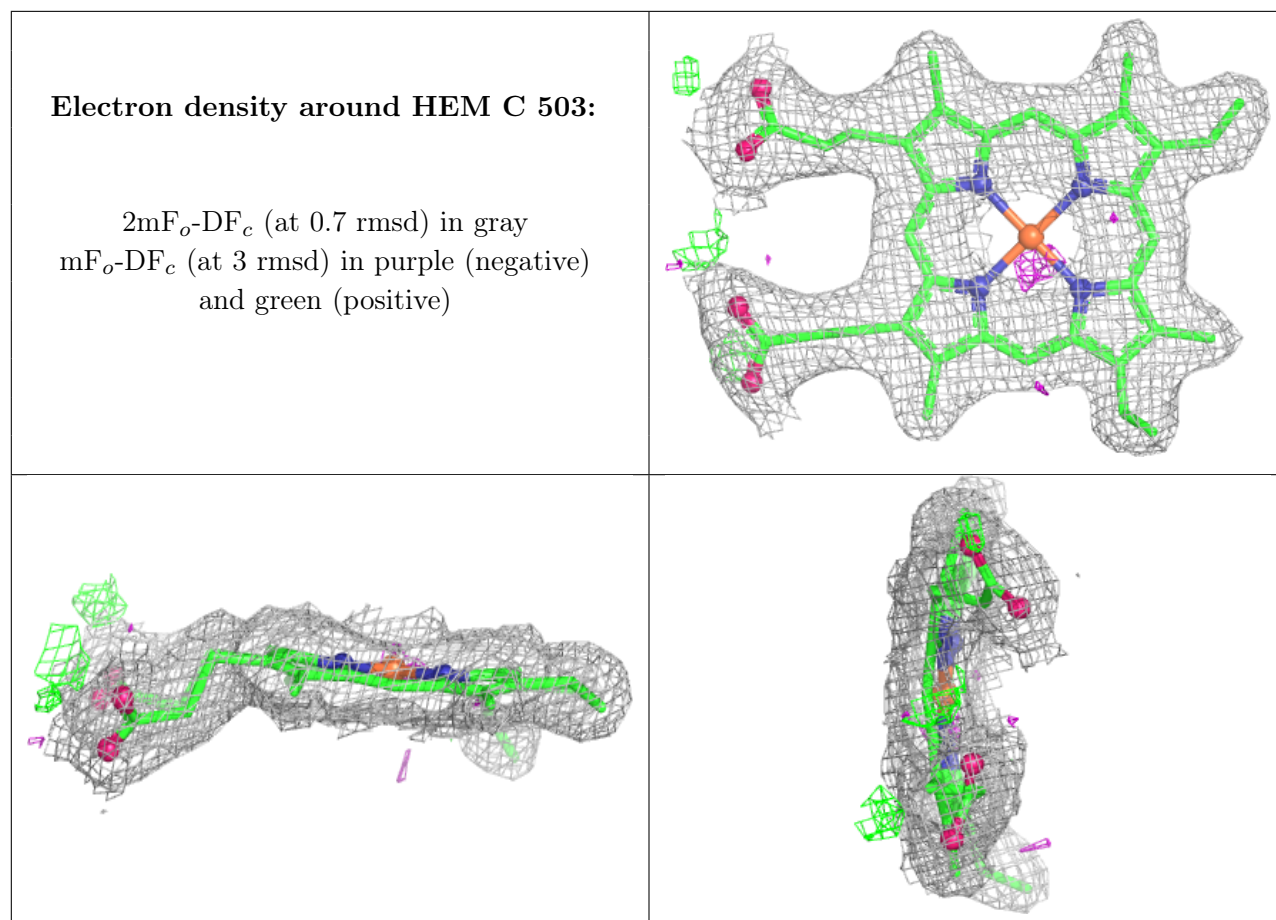


**Electron density around HEM D 503:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.