



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 04:07 AM EDT

PDB ID : 5E0E / pdb_00005e0e
Title : Crystal Structure of Cytochrome P450 2B37 from Desert Woodrat in complex with 4-(4-chlorophenyl)imidazole
Authors : Shah, M.B.; Halpert, J.R.; Stout, C.D.
Deposited on : 2015-09-28
Resolution : 3.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

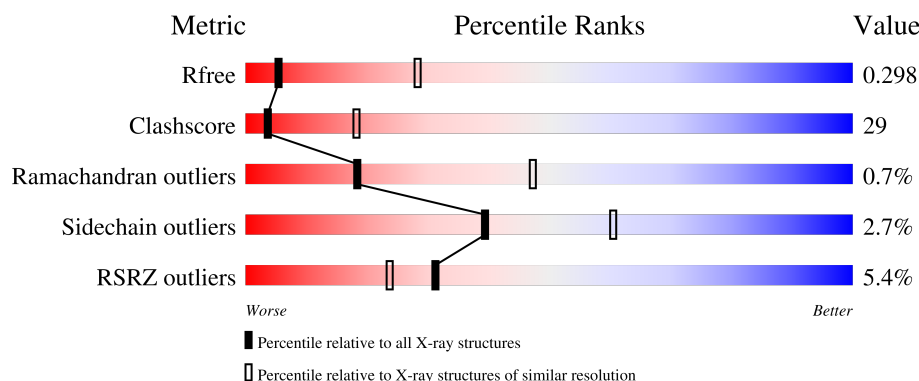
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



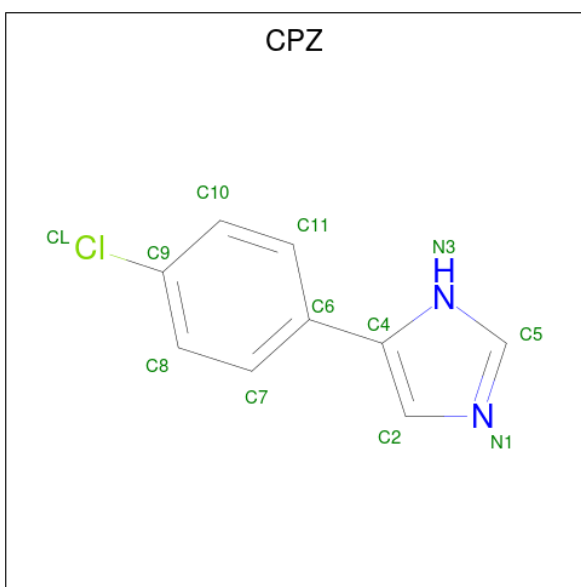
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	463	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CPZ	A	502	-	-	X	-



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N 12 9 1 2	0	0
3	A	1	Total C Cl N 12 9 1 2	0	0
3	A	1	Total C Cl N 12 9 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	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 P450 family 2 subfamily B



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	144.77 Å 144.77 Å 104.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.36 – 3.40 42.36 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.36-3.40) 97.8 (42.36-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.212 , 0.290 0.253 , 0.298	Depositor DCC
R_{free} test set	756 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	100.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3684	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CPZ

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	0.90	5/3683 (0.1%)	1.46	64/5008 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLN	C-N	8.97	1.46	1.34
1	A	456	ASN	CA-C	8.05	1.63	1.52
1	A	137	MET	CA-C	5.52	1.59	1.53
1	A	363	ILE	CA-C	-5.09	1.49	1.53
1	A	114	VAL	CA-CB	-5.00	1.47	1.54

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLN	N-CA-C	18.54	136.82	111.24
1	A	141	SER	CA-CB-OG	17.35	145.79	111.10
1	A	31	PRO	CB-CA-C	-16.39	95.99	111.39
1	A	141	SER	N-CA-CB	14.32	134.70	110.49
1	A	457	PHE	N-CA-CB	13.90	133.99	110.49
1	A	456	ASN	CA-CB-CG	-12.19	100.41	112.60
1	A	456	ASN	CA-C-O	-11.66	106.56	119.97
1	A	114	VAL	N-CA-C	-11.48	85.45	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	MET	O-C-N	11.18	136.83	122.19
1	A	141	SER	N-CA-C	-10.98	87.42	110.80
1	A	456	ASN	N-CA-C	10.68	124.21	111.82
1	A	137	MET	N-CA-C	10.50	124.15	111.02
1	A	240	GLU	O-C-N	10.46	132.97	122.09
1	A	240	GLU	CA-C-O	-10.18	110.00	120.90
1	A	114	VAL	CB-CA-C	9.83	127.42	111.29
1	A	403	GLU	N-CA-C	9.49	125.70	112.04
1	A	161	GLN	CB-CA-C	-9.45	97.54	112.09
1	A	439	GLU	N-CA-C	-9.36	98.76	111.96
1	A	59	ARG	N-CA-C	-8.98	99.36	110.41
1	A	374	ASP	N-CA-C	-8.83	98.77	110.24
1	A	457	PHE	CB-CA-C	-8.52	93.46	110.42
1	A	404	GLN	N-CA-C	-8.38	91.28	109.81
1	A	336	ARG	N-CA-C	8.23	120.95	110.33
1	A	456	ASN	CA-C-N	7.62	136.09	121.54
1	A	456	ASN	C-N-CA	7.62	136.09	121.54
1	A	236	ARG	O-C-N	-7.13	114.56	122.12
1	A	61	LYS	CB-CA-C	-7.01	96.77	110.10
1	A	113	VAL	N-CA-C	6.99	123.89	109.34
1	A	58	ILE	CB-CA-C	-6.95	99.90	111.29
1	A	61	LYS	N-CA-C	6.70	129.75	111.00
1	A	130	VAL	N-CA-C	-6.67	103.82	110.62
1	A	455	GLN	CA-C-N	6.64	130.41	120.31
1	A	455	GLN	C-N-CA	6.64	130.41	120.31
1	A	114	VAL	CA-C-N	6.39	133.08	122.54
1	A	114	VAL	C-N-CA	6.39	133.08	122.54
1	A	121	TRP	N-CA-C	6.31	117.82	111.07
1	A	170	LEU	N-CA-C	-6.30	104.30	112.23
1	A	365	ILE	N-CA-C	-6.20	106.95	112.90
1	A	366	GLY	CA-C-N	-6.17	117.36	123.04
1	A	366	GLY	C-N-CA	-6.17	117.36	123.04
1	A	135	PHE	N-CA-C	-6.17	105.88	113.41
1	A	104	VAL	N-CA-C	-6.07	106.83	112.83
1	A	317	TYR	CA-C-N	5.97	126.08	119.87
1	A	317	TYR	C-N-CA	5.97	126.08	119.87
1	A	52	LEU	N-CA-C	-5.94	107.85	114.62
1	A	281	THR	N-CA-C	5.82	117.84	110.33
1	A	320	VAL	N-CA-C	-5.64	104.87	110.62
1	A	199	LEU	N-CA-C	-5.59	106.30	113.01
1	A	62	TYR	N-CA-C	5.47	120.83	113.72
1	A	205	SER	N-CA-C	-5.46	104.36	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	LEU	N-CA-C	5.45	117.26	108.32
1	A	205	SER	N-CA-CB	5.42	118.06	109.82
1	A	367	VAL	CA-C-N	5.41	126.61	119.84
1	A	367	VAL	C-N-CA	5.41	126.61	119.84
1	A	121	TRP	CB-CA-C	-5.38	102.43	110.88
1	A	141	SER	CA-C-N	5.36	127.80	120.46
1	A	141	SER	C-N-CA	5.36	127.80	120.46
1	A	447	PHE	N-CA-C	5.35	120.14	111.37
1	A	456	ASN	N-CA-CB	5.32	118.53	110.28
1	A	37	LEU	CA-C-N	-5.12	114.51	120.04
1	A	37	LEU	C-N-CA	-5.12	114.51	120.04
1	A	456	ASN	CB-CA-C	-5.12	100.85	110.67
1	A	102	ALA	N-CA-C	5.07	118.96	112.87
1	A	403	GLU	CB-CA-C	-5.06	101.30	110.56

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	VAL	Peptide
1	A	125	ARG	Sidechain
1	A	139	LYS	Peptide
1	A	187	ARG	Sidechain
1	A	456	ASN	Peptide
1	A	46	MET	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	3589	0	3394	202	0
2	A	43	0	30	9	0
3	A	36	0	21	8	0
4	A	16	0	0	1	0
All	All	3684	0	3445	207	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 29.

All (207) 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:391:ILE:O	1:A:394:SER:OG	1.67	1.09
1:A:165:LEU:O	1:A:167:PRO:HD3	1.63	0.98
1:A:105:GLU:OE2	1:A:106:PRO:N	2.00	0.93
1:A:278:ASN:HB2	1:A:281:THR:HG23	1.48	0.93
1:A:60:GLU:HA	1:A:61:LYS:C	1.91	0.92
1:A:392:LEU:O	1:A:395:ALA:N	2.03	0.91
1:A:268:TYR:CE2	1:A:288:LEU:HB2	2.07	0.88
1:A:143:GLU:HG3	1:A:340:LEU:HD23	1.58	0.86
1:A:168:THR:O	1:A:172:GLN:HG3	1.75	0.85
1:A:367:VAL:CG1	2:A:501:HEM:HAA1	2.08	0.84
1:A:58:ILE:HG22	1:A:58:ILE:O	1.78	0.83
1:A:160:SER:C	1:A:161:GLN:HG3	2.04	0.82
1:A:37:LEU:HD21	1:A:44:LEU:HD12	1.61	0.80
1:A:59:ARG:O	1:A:60:GLU:C	2.23	0.80
1:A:81:THR:HG21	1:A:401:TYR:CE2	2.17	0.79
1:A:121:TRP:CE3	1:A:122:LYS:HG3	2.16	0.79
1:A:278:ASN:CB	1:A:281:THR:HG23	2.16	0.76
1:A:105:GLU:OE2	1:A:105:GLU:C	2.29	0.75
1:A:60:GLU:N	1:A:63:GLY:H	1.85	0.74
1:A:371:VAL:HG11	1:A:375:THR:HG21	1.69	0.74
1:A:461:SER:CB	1:A:486:ILE:HG22	2.18	0.73
1:A:346:MET:HE2	1:A:349:THR:OG1	1.88	0.73
1:A:169:PHE:HA	1:A:172:GLN:OE1	1.89	0.72
1:A:311:PHE:O	1:A:315:LEU:HD23	1.90	0.72
1:A:403:GLU:O	1:A:405:PRO:HD3	1.90	0.71
1:A:60:GLU:HA	1:A:62:TYR:N	2.05	0.70
1:A:113:VAL:HG13	1:A:124:LEU:HB2	1.72	0.70
1:A:44:LEU:O	1:A:47:ASP:OD2	2.09	0.69
1:A:81:THR:HG23	1:A:82:GLU:H	1.56	0.69
1:A:96:SER:O	1:A:434:ARG:NE	2.24	0.69
1:A:160:SER:O	1:A:161:GLN:HG3	1.92	0.69
1:A:256:LEU:HD11	1:A:270:LEU:HD21	1.73	0.68
1:A:462:PRO:HD2	1:A:485:GLN:O	1.93	0.68
1:A:59:ARG:O	1:A:61:LYS:N	2.26	0.68
1:A:200:TYR:O	1:A:201:LEU:HD23	1.94	0.68
1:A:139:LYS:CB	1:A:140:ARG:HA	2.22	0.68
1:A:81:THR:HG23	1:A:82:GLU:N	2.10	0.67
1:A:324:VAL:O	1:A:328:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:146:ILE:HG13	1.95	0.67
1:A:350:GLU:HB3	1:A:420:LEU:HD21	1.77	0.67
1:A:473:LYS:O	1:A:474:GLU:HG3	1.95	0.66
1:A:288:LEU:O	1:A:292:VAL:HG23	1.96	0.65
1:A:133:ARG:NH1	4:A:601:HOH:O	2.29	0.65
1:A:340:LEU:HD22	1:A:448:LEU:HD21	1.79	0.65
1:A:268:TYR:CG	1:A:288:LEU:HD23	2.33	0.64
1:A:105:GLU:N	1:A:106:PRO:HD2	2.13	0.64
1:A:47:ASP:HA	3:A:504:CPZ:H10	1.80	0.63
1:A:286:GLN:HA	1:A:289:VAL:HG12	1.78	0.63
1:A:54:SER:O	1:A:58:ILE:HG13	1.99	0.63
1:A:367:VAL:HG23	1:A:368:PRO:HD2	1.82	0.62
1:A:475:SER:O	1:A:478:GLY:N	2.32	0.62
1:A:98:ARG:HH12	1:A:367:VAL:HG13	1.65	0.62
1:A:349:THR:O	1:A:353:ILE:HG13	1.99	0.62
1:A:360:SER:CB	1:A:362:LEU:HD11	2.30	0.61
1:A:37:LEU:HD13	1:A:41:GLY:O	1.99	0.61
1:A:373:LYS:C	1:A:374:ASP:O	2.39	0.61
1:A:105:GLU:OE2	1:A:106:PRO:CA	2.48	0.61
1:A:132:MET:HA	1:A:135:PHE:HB2	1.83	0.61
1:A:367:VAL:HG12	2:A:501:HEM:HAA1	1.83	0.61
1:A:59:ARG:HG3	1:A:63:GLY:O	2.01	0.60
1:A:179:ILE:O	1:A:183:VAL:HG22	2.02	0.60
1:A:105:GLU:O	1:A:107:ILE:N	2.34	0.60
1:A:327:GLU:OE2	1:A:348:TYR:HB3	2.02	0.59
1:A:278:ASN:HB2	1:A:281:THR:CG2	2.28	0.59
1:A:121:TRP:CZ3	1:A:122:LYS:HG3	2.38	0.59
2:A:501:HEM:C4B	3:A:502:CPZ:H5	2.37	0.59
1:A:85:ARG:NH1	1:A:424:GLU:HB3	2.17	0.59
1:A:73:ARG:HD3	1:A:387:GLU:CD	2.27	0.59
1:A:243:ASP:O	1:A:247:GLN:HB2	2.03	0.59
1:A:478:GLY:O	1:A:479:LYS:C	2.45	0.58
1:A:153:LEU:HD21	1:A:157:PHE:HE2	1.66	0.58
1:A:361:ASP:OD1	1:A:393:SER:HA	2.04	0.58
1:A:305:THR:HA	1:A:308:ARG:HD3	1.84	0.58
1:A:315:LEU:HG	1:A:486:ILE:HG21	1.84	0.58
1:A:113:VAL:CG1	1:A:124:LEU:HB2	2.34	0.58
1:A:143:GLU:HG3	1:A:340:LEU:CD2	2.32	0.57
1:A:429:PHE:O	1:A:430:SER:HB3	2.03	0.57
1:A:141:SER:O	1:A:145:ARG:HD2	2.04	0.57
1:A:37:LEU:HD21	1:A:44:LEU:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HB2	1:A:67:THR:HG23	1.86	0.56
1:A:202:PHE:CZ	1:A:241:ILE:HD13	2.41	0.56
1:A:360:SER:C	1:A:362:LEU:HD12	2.31	0.56
1:A:373:LYS:HG3	1:A:374:ASP:O	2.05	0.56
1:A:275:GLU:HB3	1:A:281:THR:HG21	1.87	0.55
1:A:101:ILE:HD11	3:A:502:CPZ:CL	2.43	0.55
1:A:60:GLU:H	1:A:63:GLY:H	1.54	0.55
1:A:105:GLU:O	1:A:106:PRO:C	2.48	0.55
1:A:355:GLU:HG3	1:A:410:PRO:HA	1.89	0.55
1:A:491:ARG:O	1:A:491:ARG:HG3	2.07	0.54
1:A:168:THR:O	1:A:172:GLN:CG	2.52	0.54
1:A:196:LEU:C	1:A:198:LEU:H	2.15	0.54
1:A:392:LEU:O	1:A:393:SER:C	2.49	0.54
1:A:121:TRP:HE3	1:A:122:LYS:HG3	1.69	0.54
1:A:268:TYR:CZ	1:A:288:LEU:HB2	2.43	0.53
1:A:278:ASN:HD22	1:A:281:THR:CG2	2.21	0.53
1:A:342:ASP:O	1:A:345:LYS:N	2.38	0.53
1:A:259:SER:O	1:A:261:PRO:HD3	2.08	0.53
1:A:347:PRO:HA	1:A:420:LEU:HD11	1.90	0.53
2:A:501:HEM:C4D	3:A:502:CPZ:H2	2.43	0.53
1:A:170:LEU:O	1:A:174:ILE:HG12	2.08	0.53
1:A:101:ILE:HG22	1:A:368:PRO:HG2	1.91	0.53
1:A:410:PRO:C	1:A:412:HIS:H	2.15	0.53
1:A:457:PHE:CD1	1:A:488:PHE:HB3	2.44	0.52
1:A:173:CYS:O	1:A:177:ASN:HB2	2.09	0.52
1:A:132:MET:O	1:A:133:ARG:HB2	2.10	0.52
1:A:286:GLN:HA	1:A:289:VAL:CG1	2.39	0.52
1:A:376:LEU:C	1:A:376:LEU:HD13	2.35	0.52
1:A:128:SER:O	1:A:131:THR:HG22	2.10	0.52
1:A:430:SER:HB2	2:A:501:HEM:HMA2	1.91	0.52
1:A:267:THR:O	1:A:268:TYR:C	2.52	0.51
1:A:165:LEU:O	1:A:167:PRO:CD	2.47	0.51
1:A:152:CYS:SG	1:A:187:ARG:CZ	2.98	0.51
2:A:501:HEM:CHA	3:A:502:CPZ:H2	2.40	0.51
1:A:373:LYS:O	1:A:374:ASP:C	2.53	0.51
2:A:501:HEM:C1A	3:A:502:CPZ:H2	2.46	0.51
1:A:339:THR:O	1:A:342:ASP:HB2	2.10	0.51
1:A:172:GLN:HB3	1:A:203:TYR:CZ	2.45	0.51
1:A:310:GLY:O	1:A:314:MET:HG2	2.11	0.51
1:A:434:ARG:O	1:A:435:ILE:C	2.54	0.50
1:A:465:PRO:O	1:A:466:LYS:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:CA	1:A:62:TYR:N	2.74	0.50
1:A:453:ILE:HG23	1:A:488:PHE:HE2	1.76	0.50
1:A:169:PHE:CZ	1:A:173:CYS:SG	3.04	0.50
1:A:410:PRO:C	1:A:412:HIS:N	2.69	0.50
1:A:475:SER:O	1:A:476:GLY:C	2.54	0.50
1:A:457:PHE:HA	1:A:490:ALA:HA	1.93	0.50
1:A:303:SER:HA	1:A:306:THR:HG22	1.94	0.50
1:A:392:LEU:HD12	1:A:392:LEU:H	1.76	0.50
1:A:113:VAL:HG13	1:A:124:LEU:CB	2.41	0.49
1:A:206:PHE:HE1	1:A:297:PHE:CE1	2.31	0.49
1:A:47:ASP:O	1:A:49:GLY:O	2.31	0.49
1:A:150:ALA:O	1:A:151:ARG:C	2.55	0.49
1:A:264:PHE:HA	1:A:267:THR:HG22	1.94	0.49
1:A:256:LEU:C	1:A:256:LEU:HD13	2.38	0.49
1:A:456:ASN:HB2	1:A:457:PHE:CE2	2.48	0.49
1:A:348:TYR:O	1:A:349:THR:C	2.55	0.49
1:A:101:ILE:CD1	3:A:502:CPZ:CL	2.98	0.48
1:A:29:HIS:O	1:A:380:TYR:HB3	2.13	0.48
1:A:108:PHE:O	1:A:109:ARG:C	2.56	0.48
1:A:149:GLU:OE2	1:A:187:ARG:HD2	2.13	0.47
1:A:414:LEU:HD12	1:A:418:GLY:C	2.39	0.47
1:A:105:GLU:OE2	1:A:106:PRO:HA	2.14	0.47
1:A:232:ARG:HB3	1:A:236:ARG:HH21	1.80	0.47
1:A:473:LYS:C	1:A:474:GLU:HG3	2.40	0.47
1:A:60:GLU:CA	1:A:61:LYS:C	2.74	0.47
1:A:429:PHE:O	1:A:430:SER:CB	2.62	0.47
1:A:85:ARG:HA	1:A:89:VAL:HG23	1.97	0.46
1:A:392:LEU:HD21	1:A:430:SER:HA	1.97	0.46
1:A:105:GLU:C	1:A:107:ILE:N	2.73	0.46
1:A:269:LEU:HA	1:A:272:MET:HE2	1.98	0.46
1:A:87:ALA:HB2	1:A:377:PHE:CZ	2.51	0.46
1:A:153:LEU:HD21	1:A:157:PHE:CE2	2.51	0.45
1:A:256:LEU:HD11	1:A:270:LEU:CD2	2.41	0.45
1:A:255:THR:HB	1:A:262:ARG:NH2	2.32	0.45
1:A:396:LEU:HD12	1:A:396:LEU:N	2.32	0.45
1:A:200:TYR:C	1:A:201:LEU:HD23	2.41	0.45
2:A:501:HEM:NB	3:A:502:CPZ:H5	2.30	0.45
1:A:132:MET:O	1:A:134:ASP:N	2.44	0.45
1:A:113:VAL:C	1:A:114:VAL:HG23	2.42	0.44
1:A:278:ASN:O	1:A:280:HIS:N	2.50	0.44
1:A:77:MET:HB3	1:A:391:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:O	1:A:343:ARG:C	2.60	0.44
1:A:59:ARG:HG2	1:A:60:GLU:N	2.33	0.44
1:A:73:ARG:HA	1:A:74:PRO:HD2	1.81	0.44
1:A:273:GLU:O	1:A:276:LYS:HB2	2.18	0.44
1:A:392:LEU:C	1:A:394:SER:N	2.76	0.44
1:A:37:LEU:N	1:A:37:LEU:HD12	2.32	0.43
1:A:362:LEU:HD12	1:A:362:LEU:N	2.33	0.43
1:A:367:VAL:HG12	2:A:501:HEM:CAA	2.46	0.43
1:A:367:VAL:CG2	1:A:368:PRO:HD2	2.47	0.43
1:A:98:ARG:HB2	1:A:434:ARG:NH1	2.34	0.43
1:A:105:GLU:N	1:A:106:PRO:CD	2.81	0.43
1:A:381:LEU:C	1:A:381:LEU:HD13	2.44	0.43
1:A:194:GLN:O	1:A:198:LEU:HB2	2.18	0.43
1:A:262:ARG:HG3	1:A:266:ASP:OD1	2.19	0.43
1:A:342:ASP:O	1:A:344:THR:N	2.51	0.42
1:A:108:PHE:O	1:A:110:GLY:N	2.52	0.42
1:A:256:LEU:HD13	1:A:257:ASP:N	2.34	0.42
1:A:52:LEU:O	1:A:55:PHE:HB2	2.20	0.42
1:A:81:THR:CG2	1:A:82:GLU:H	2.29	0.42
1:A:132:MET:C	1:A:134:ASP:N	2.78	0.42
1:A:447:PHE:HD2	1:A:448:LEU:HD23	1.84	0.42
1:A:358:ARG:HA	1:A:396:LEU:HD23	2.01	0.42
1:A:367:VAL:HA	1:A:368:PRO:HD3	1.98	0.41
1:A:462:PRO:HG2	1:A:463:VAL:H	1.85	0.41
1:A:232:ARG:CB	1:A:236:ARG:HH21	2.34	0.41
1:A:278:ASN:HD22	1:A:281:THR:HG21	1.86	0.41
1:A:305:THR:HG22	1:A:362:LEU:HD21	2.02	0.41
1:A:361:ASP:OD1	1:A:396:LEU:HD22	2.20	0.41
1:A:371:VAL:CG1	1:A:375:THR:HG21	2.44	0.41
1:A:318:PRO:HD2	1:A:319:HIS:CE1	2.55	0.41
1:A:383:PRO:O	1:A:384:LYS:C	2.63	0.41
1:A:202:PHE:CE2	1:A:241:ILE:HD13	2.56	0.41
1:A:361:ASP:OD1	1:A:396:LEU:HB2	2.20	0.41
1:A:456:ASN:O	1:A:491:ARG:N	2.45	0.41
1:A:143:GLU:CG	1:A:340:LEU:HD23	2.39	0.41
1:A:206:PHE:HE1	1:A:297:PHE:CD1	2.39	0.41
1:A:278:ASN:C	1:A:280:HIS:H	2.29	0.41
1:A:137:MET:HA	1:A:138:GLY:HA3	1.87	0.40
1:A:205:SER:O	1:A:206:PHE:C	2.64	0.40
1:A:107:ILE:H	1:A:107:ILE:HG13	1.54	0.40
1:A:67:THR:HG22	1:A:76:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:O	1:A:86:GLU:C	2.64	0.40
1:A:268:TYR:O	1:A:269:LEU:C	2.64	0.40
1:A:291:SER:O	1:A:292:VAL:C	2.65	0.40
1:A:372:THR:H	1:A:372:THR:HG23	1.56	0.40
1:A:92:ALA:HB1	1:A:433:LYS:HG2	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	459/463 (99%)	362 (79%)	94 (20%)	3 (1%)	18 47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	343	ARG
1	A	430	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	368/412 (89%)	358 (97%)	10 (3%)	39 60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	A	60	GLU
1	A	101	ILE
1	A	107	ILE
1	A	113	VAL
1	A	161	GLN
1	A	165	LEU
1	A	309	TYR
1	A	392	LEU
1	A	457	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	278	ASN
1	A	286	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	CPZ	A	503	-	12,13,13	1.02	1 (8%)	16,17,17	1.02	1 (6%)
3	CPZ	A	502	2	12,13,13	1.01	1 (8%)	16,17,17	1.01	1 (6%)
3	CPZ	A	504	-	12,13,13	1.01	2 (16%)	16,17,17	1.01	1 (6%)
2	HEM	A	501	1,3	50,50,50	1.79	7 (14%)	67,82,82	1.60	10 (14%)

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
3	CPZ	A	503	-	-	0/4/4/4	0/2/2/2
3	CPZ	A	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	A	504	-	-	4/4/4/4	0/2/2/2
2	HEM	A	501	1,3	-	6/14/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	6.82	1.51	1.36
2	A	501	HEM	FE-ND	6.14	2.13	1.94
2	A	501	HEM	C3B-C2B	-3.10	1.30	1.37
2	A	501	HEM	CAC-C3C	2.87	1.55	1.47
2	A	501	HEM	FE-NA	2.51	2.03	1.95
2	A	501	HEM	CAB-C3B	2.42	1.53	1.47
3	A	503	CPZ	C4-N3	-2.31	1.35	1.38
3	A	504	CPZ	C4-N3	-2.26	1.35	1.38
3	A	502	CPZ	C4-N3	-2.24	1.35	1.38
2	A	501	HEM	CMA-C3A	2.17	1.55	1.50
3	A	504	CPZ	C2-N1	-2.00	1.34	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	4.99	111.11	105.21
2	A	501	HEM	CAA-CBA-CGA	-4.78	100.97	113.67
2	A	501	HEM	CAD-C3D-C4D	3.26	130.37	124.70
2	A	501	HEM	CMA-C3A-C2A	3.06	132.12	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CPZ	C6-C4-N3	3.01	127.22	123.72
3	A	503	CPZ	C6-C4-N3	2.99	127.19	123.72
3	A	504	CPZ	C6-C4-N3	2.98	127.17	123.72
2	A	501	HEM	CMA-C3A-C4A	-2.81	121.14	125.42
2	A	501	HEM	CHB-C4A-NA	2.76	128.86	123.86
2	A	501	HEM	C2A-C1A-NA	-2.31	107.59	110.15
2	A	501	HEM	CHB-C4A-C3A	-2.27	120.84	127.43
2	A	501	HEM	CHD-C1D-ND	2.21	126.80	124.42
2	A	501	HEM	CAB-C3B-C2B	-2.06	121.74	128.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	CPZ	C2-C4-C6-C11
3	A	504	CPZ	C2-C4-C6-C7
3	A	504	CPZ	N3-C4-C6-C7
3	A	504	CPZ	N3-C4-C6-C11
2	A	501	HEM	C2B-C3B-CAB-CBB
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	C4B-C3B-CAB-CBB

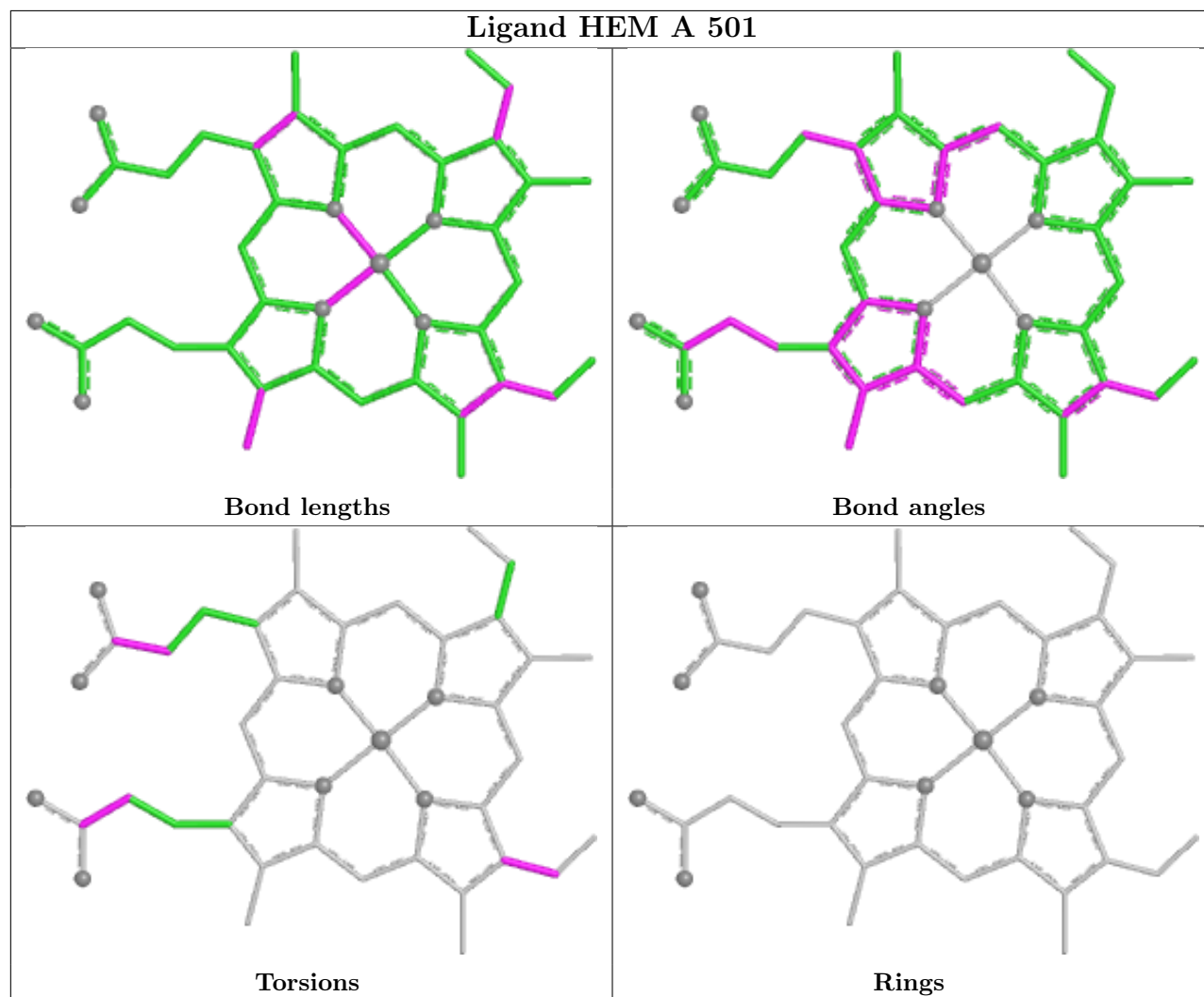
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CPZ	7	0
3	A	504	CPZ	1	0
2	A	501	HEM	9	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

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, 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	463/463 (100%)	0.49	25 (5%)	31 24	56, 87, 128, 138	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	PHE	4.3
1	A	113	VAL	3.9
1	A	139	LYS	3.5
1	A	476	GLY	3.4
1	A	482	GLN	3.2
1	A	479	LYS	3.1
1	A	286	GLN	3.0
1	A	281	THR	3.0
1	A	473	LYS	3.0
1	A	416	ALA	2.9
1	A	201	LEU	2.9
1	A	137	MET	2.7
1	A	47	ASP	2.7
1	A	411	ASP	2.6
1	A	387	GLU	2.5
1	A	361	ASP	2.4
1	A	338	PRO	2.4
1	A	142	VAL	2.4
1	A	133	ARG	2.4
1	A	200	TYR	2.4
1	A	420	LEU	2.3
1	A	438	GLY	2.2
1	A	161	GLN	2.1
1	A	475	SER	2.1
1	A	167	PRO	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](#)

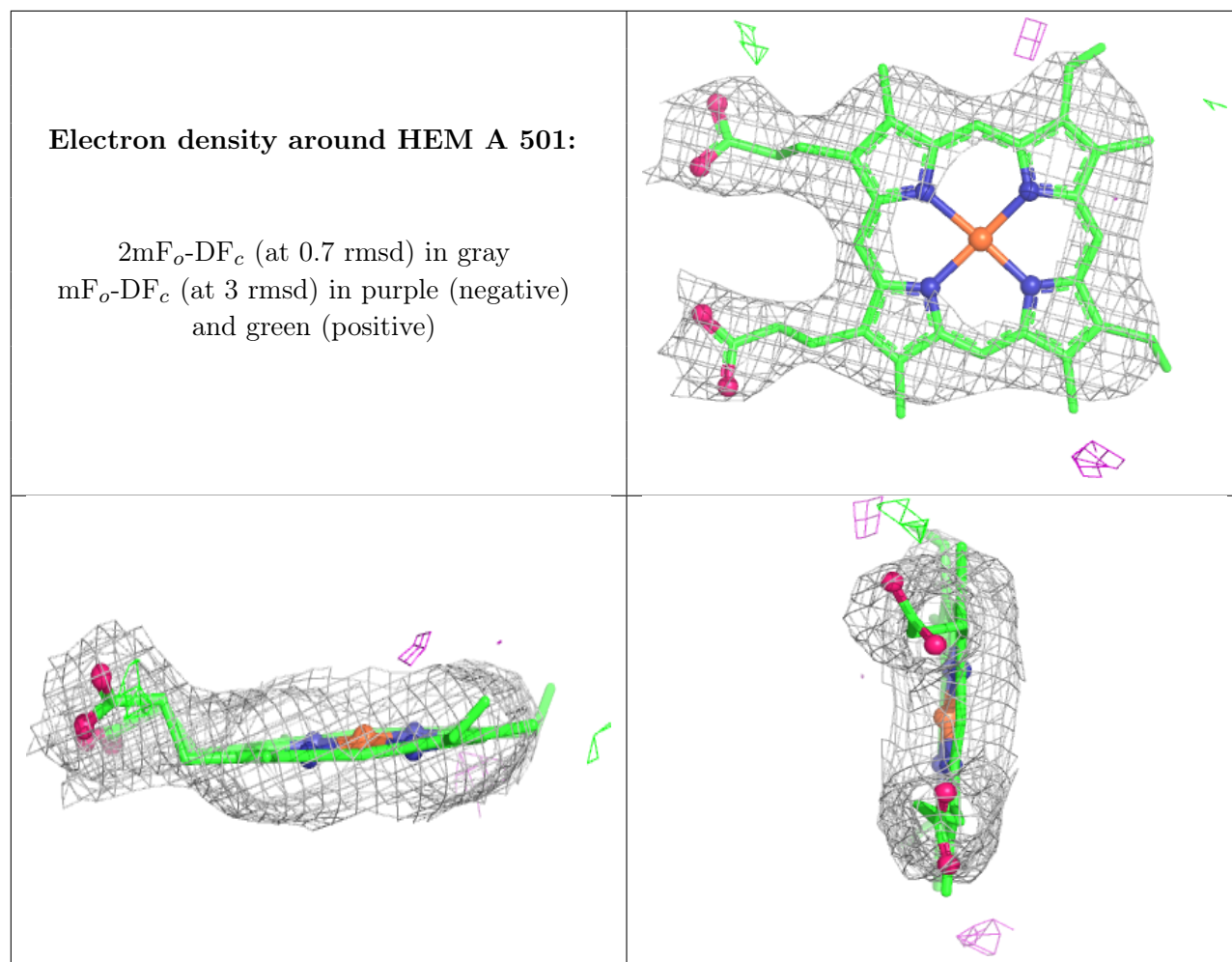
There are no oligosaccharides in this entry.

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
3	CPZ	A	503	12/12	0.92	0.20	95,106,113,113	0
3	CPZ	A	502	12/12	0.93	0.18	85,88,92,100	0
3	CPZ	A	504	12/12	0.94	0.17	105,108,113,113	0
2	HEM	A	501	43/43	0.98	0.08	56,59,64,66	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.