



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:00 AM UTC

PDB ID : 3HQ7 / pdb_00003hq7
Title : CcpA from *G. sulfurreducens*, G94K/K97Q/R100I variant
Authors : Hoffmann, M.; Seidel, J.; Einsle, O.
Deposited on : 2009-06-05
Resolution : 2.31 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

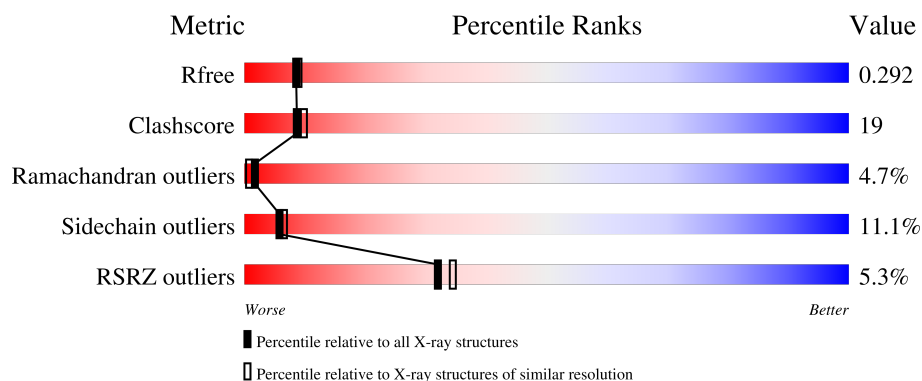
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	345	5% 43% 35% 8% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2557 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.

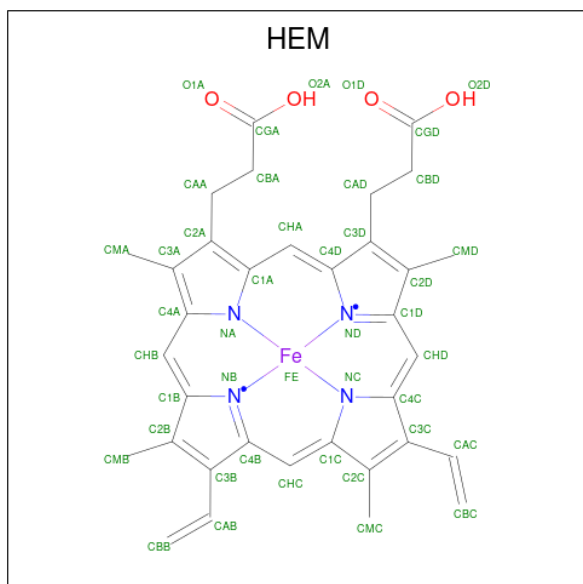
- Molecule 1 is a protein called Cytochrome c551 peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2287	1465	388	425	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	GLY	engineered mutation	UNP Q749D0
A	97	GLN	LYS	engineered mutation	UNP Q749D0
A	100	ILE	ARG	engineered mutation	UNP Q749D0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

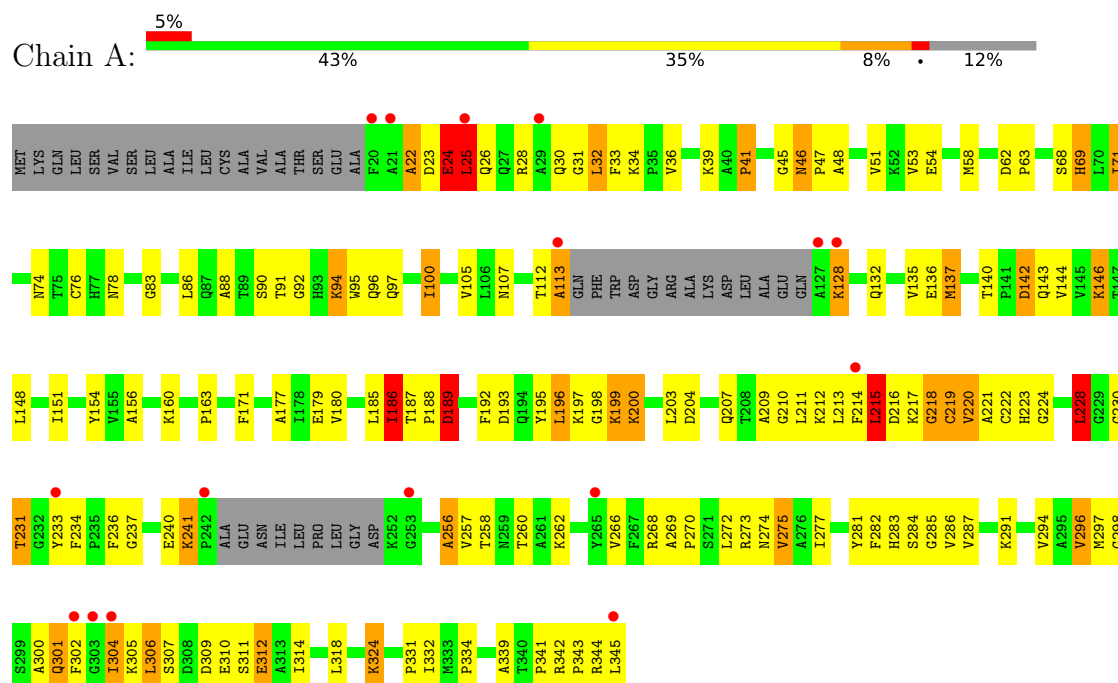
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total	O	0	0
			183	183		

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 c551 peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 99.35Å 78.22Å 89.97° 89.98° 90.00°	Depositor
Resolution (Å)	70.00 – 2.31 70.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.00-2.31) 99.9 (70.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.294 0.207 , 0.292	Depositor DCC
R_{free} test set	906 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2557	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: CA, HEM

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	1.83	39/2341 (1.7%)	1.69	45/3177 (1.4%)

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	5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	LEU	CA-C	8.38	1.64	1.52
1	A	185	LEU	CA-CB	8.20	1.63	1.52
1	A	53	VAL	CA-CB	8.01	1.64	1.54
1	A	100	ILE	CA-CB	7.58	1.67	1.54
1	A	179	GLU	C-O	-7.42	1.15	1.24
1	A	273	ARG	CA-C	7.42	1.62	1.52
1	A	318	LEU	CA-C	7.23	1.62	1.52
1	A	287	VAL	CA-C	7.03	1.61	1.52
1	A	128	LYS	N-CA	6.42	1.54	1.45
1	A	275	VAL	N-CA	6.41	1.54	1.46
1	A	32	LEU	CA-C	6.33	1.63	1.52
1	A	269	ALA	CA-CB	6.10	1.62	1.53
1	A	105	VAL	CA-CB	6.08	1.61	1.54
1	A	78	ASN	C-O	-6.00	1.16	1.24
1	A	78	ASN	CA-C	-5.93	1.45	1.52
1	A	69	HIS	N-CA	5.90	1.55	1.46
1	A	163	PRO	CA-C	5.90	1.59	1.52
1	A	287	VAL	CA-CB	5.90	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	ALA	CA-CB	5.86	1.62	1.53
1	A	144	VAL	CA-CB	5.85	1.61	1.54
1	A	260	THR	CA-CB	5.82	1.62	1.53
1	A	177	ALA	N-CA	5.80	1.53	1.46
1	A	63	PRO	N-CA	5.70	1.53	1.47
1	A	294	VAL	CA-C	5.67	1.59	1.52
1	A	228	LEU	C-O	-5.67	1.16	1.24
1	A	41	PRO	N-CA	-5.61	1.40	1.47
1	A	221	ALA	CA-CB	5.45	1.60	1.53
1	A	274	ASN	CA-C	-5.36	1.44	1.52
1	A	48	ALA	CA-CB	-5.31	1.45	1.53
1	A	113	ALA	CA-C	5.28	1.64	1.52
1	A	189	ASP	CA-C	-5.26	1.46	1.53
1	A	148	LEU	CA-CB	5.24	1.61	1.53
1	A	151	ILE	CA-CB	5.18	1.60	1.54
1	A	186	ILE	N-CA	-5.14	1.40	1.46
1	A	334	PRO	CA-CB	-5.14	1.47	1.53
1	A	83	GLY	C-O	-5.08	1.17	1.24
1	A	314	ILE	C-O	-5.06	1.18	1.24
1	A	160	LYS	CA-C	5.05	1.59	1.52
1	A	281	TYR	C-O	-5.04	1.17	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	N-CA-C	-12.60	97.53	111.14
1	A	222	CYS	N-CA-C	9.90	123.09	111.71
1	A	189	ASP	N-CA-C	9.04	123.94	111.74
1	A	36	VAL	N-CA-C	-8.90	100.22	108.95
1	A	46	ASN	CA-C-N	8.67	128.71	119.78
1	A	46	ASN	C-N-CA	8.67	128.71	119.78
1	A	62	ASP	CA-C-N	-8.20	111.35	120.45
1	A	62	ASP	C-N-CA	-8.20	111.35	120.45
1	A	221	ALA	CA-C-N	7.79	131.50	120.28
1	A	221	ALA	C-N-CA	7.79	131.50	120.28
1	A	296	VAL	N-CA-C	-7.27	102.33	113.16
1	A	160	LYS	N-CA-C	7.05	118.97	111.28
1	A	256	ALA	CA-C-N	6.68	129.63	120.35
1	A	256	ALA	C-N-CA	6.68	129.63	120.35
1	A	332	ILE	CB-CA-C	6.68	120.29	112.68
1	A	331	PRO	CA-C-N	6.60	129.81	122.22
1	A	331	PRO	C-N-CA	6.60	129.81	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	VAL	N-CA-C	6.54	116.70	110.42
1	A	306	LEU	N-CA-C	6.32	119.44	108.76
1	A	112	THR	CA-C-N	6.08	132.64	121.70
1	A	112	THR	C-N-CA	6.08	132.64	121.70
1	A	86	LEU	N-CA-C	6.04	119.97	112.47
1	A	100	ILE	CB-CA-C	5.94	119.58	110.55
1	A	68	SER	N-CA-C	5.89	120.19	112.89
1	A	224	GLY	O-C-N	-5.88	118.56	123.73
1	A	332	ILE	CA-CB-CG1	-5.83	100.49	110.40
1	A	339	ALA	N-CA-C	5.81	120.10	112.89
1	A	270	PRO	N-CA-C	5.78	120.31	111.11
1	A	343	PRO	CA-C-N	-5.75	114.64	123.14
1	A	343	PRO	C-N-CA	-5.75	114.64	123.14
1	A	237	GLY	N-CA-C	5.72	120.59	110.80
1	A	342	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	74	ASN	N-CA-C	5.65	118.20	111.71
1	A	277	ILE	N-CA-C	5.60	118.38	112.83
1	A	154	TYR	N-CA-C	-5.54	104.88	111.69
1	A	105	VAL	N-CA-C	-5.47	105.64	113.07
1	A	142	ASP	N-CA-C	5.40	117.61	111.02
1	A	41	PRO	CA-C-N	5.32	128.32	120.82
1	A	41	PRO	C-N-CA	5.32	128.32	120.82
1	A	275	VAL	N-CA-C	5.32	117.69	111.05
1	A	221	ALA	O-C-N	5.29	128.10	122.38
1	A	48	ALA	N-CA-C	-5.23	101.75	110.17
1	A	83	GLY	N-CA-C	-5.15	108.17	115.43
1	A	221	ALA	N-CA-C	-5.14	100.60	110.56
1	A	71	ILE	N-CA-CB	-5.06	104.43	111.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	GLY	Peptide
1	A	230	GLY	Peptide
1	A	311	SER	Peptide
1	A	344	ARG	Peptide
1	A	45	GLY	Peptide

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	2287	0	2298	88	0
2	A	86	0	60	9	0
3	A	1	0	0	1	0
4	A	183	0	0	14	0
All	All	2557	0	2358	89	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 19.

All (89) 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:76:CYS:SG	2:A:401:HEM:CAC	2.27	1.22
1:A:193:ASP:O	1:A:197:LYS:HG3	1.45	1.17
1:A:76:CYS:SG	2:A:401:HEM:CBC	2.50	0.99
1:A:214:PHE:O	1:A:219:CYS:HB2	1.62	0.99
1:A:146:LYS:HD3	1:A:341:PRO:HG3	1.56	0.88
1:A:216:ASP:OD1	4:A:496:HOH:O	1.92	0.87
1:A:220:VAL:HG22	1:A:220:VAL:O	1.75	0.83
1:A:285:GLY:O	4:A:470:HOH:O	1.99	0.80
1:A:113:ALA:HB1	1:A:268:ARG:HD3	1.65	0.79
1:A:302:PHE:CE1	2:A:402:HEM:HBC2	2.20	0.76
1:A:76:CYS:SG	2:A:401:HEM:C3C	2.79	0.75
1:A:54:GLU:HG3	1:A:58:MET:HE3	1.67	0.74
1:A:107:ASN:HD21	1:A:187:THR:H	1.38	0.72
1:A:233:TYR:CE2	1:A:268:ARG:HB2	2.23	0.72
1:A:192:PHE:CZ	1:A:196:LEU:HD21	2.26	0.71
1:A:22:ALA:O	1:A:24:GLU:HB3	1.91	0.70
1:A:28:ARG:NH2	4:A:496:HOH:O	1.99	0.67
1:A:113:ALA:CB	1:A:268:ARG:HD3	2.25	0.66
1:A:26:GLN:NE2	1:A:198:GLY:O	2.30	0.65
1:A:71:ILE:HD11	4:A:387:HOH:O	1.96	0.64
3:A:403:CA:CA	4:A:468:HOH:O	1.72	0.64
1:A:90:SER:HB2	2:A:401:HEM:HBC2	1.79	0.64
1:A:300:ALA:O	1:A:302:PHE:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:O	1:A:217:LYS:HG3	2.01	0.61
1:A:28:ARG:HG3	1:A:32:LEU:HD11	1.83	0.60
1:A:46:ASN:N	1:A:47:PRO:CD	2.65	0.59
1:A:220:VAL:O	1:A:220:VAL:CG2	2.49	0.59
1:A:113:ALA:CB	1:A:268:ARG:CD	2.81	0.58
1:A:22:ALA:HB1	1:A:200:LYS:HD3	1.86	0.58
1:A:256:ALA:HA	1:A:296:VAL:HG13	1.84	0.58
1:A:69:HIS:HD2	4:A:383:HOH:O	1.86	0.58
1:A:186:ILE:HG13	1:A:188:PRO:HD3	1.86	0.58
1:A:195:TYR:HA	1:A:199:LYS:O	2.05	0.56
1:A:204:ASP:OD1	1:A:204:ASP:C	2.48	0.56
1:A:28:ARG:NH1	4:A:496:HOH:O	2.39	0.56
1:A:217:LYS:O	1:A:304:ILE:HD11	2.06	0.56
1:A:132:GLN:O	1:A:136:GLU:HG3	2.07	0.55
1:A:94:LYS:HG2	1:A:137:MET:HG2	1.89	0.54
1:A:241:LYS:HB2	4:A:531:HOH:O	2.08	0.54
1:A:113:ALA:HB2	1:A:268:ARG:HD2	1.89	0.53
1:A:113:ALA:HB2	1:A:268:ARG:CD	2.39	0.53
1:A:298:GLY:HA2	1:A:304:ILE:CG2	2.39	0.53
1:A:140:THR:OG1	1:A:142:ASP:HB3	2.09	0.52
1:A:28:ARG:HG3	1:A:32:LEU:CD1	2.40	0.52
1:A:231:THR:HG22	4:A:356:HOH:O	2.10	0.51
1:A:234:PHE:HB3	1:A:236:PHE:HD1	1.76	0.50
1:A:146:LYS:HD3	1:A:341:PRO:CG	2.35	0.50
1:A:113:ALA:HA	1:A:233:TYR:OH	2.12	0.50
1:A:215:LEU:O	1:A:216:ASP:C	2.56	0.49
1:A:211:LEU:O	1:A:214:PHE:HB3	2.13	0.48
1:A:189:ASP:N	1:A:189:ASP:OD1	2.40	0.48
1:A:28:ARG:O	1:A:31:GLY:N	2.40	0.48
1:A:26:GLN:HG3	1:A:195:TYR:CZ	2.49	0.48
1:A:231:THR:HG21	4:A:358:HOH:O	2.13	0.48
1:A:33:PHE:CD2	1:A:228:LEU:HD22	2.49	0.47
1:A:41:PRO:O	4:A:422:HOH:O	2.20	0.47
1:A:203:LEU:HA	1:A:207:GLN:HE21	1.78	0.47
1:A:223:HIS:HE1	2:A:402:HEM:ND	2.01	0.47
1:A:272:LEU:O	1:A:275:VAL:HG12	2.14	0.47
1:A:215:LEU:O	1:A:218:GLY:N	2.28	0.47
1:A:298:GLY:HA2	1:A:304:ILE:HG22	1.95	0.47
1:A:46:ASN:N	1:A:47:PRO:HD3	2.31	0.46
1:A:217:LYS:NZ	1:A:305:LYS:O	2.37	0.46
1:A:113:ALA:HB1	1:A:268:ARG:CD	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:O	1:A:28:ARG:HB3	2.16	0.45
1:A:88:ALA:HB3	4:A:407:HOH:O	2.16	0.45
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.78	0.45
1:A:301:GLN:H	1:A:301:GLN:HG2	1.66	0.45
1:A:143:GLN:HE22	1:A:341:PRO:HB3	1.81	0.45
1:A:90:SER:HB2	2:A:401:HEM:CBC	2.46	0.44
1:A:135:VAL:HG11	1:A:171:PHE:CE1	2.52	0.44
1:A:91:THR:HA	1:A:96:GLN:HE22	1.82	0.44
1:A:95:TRP:C	1:A:95:TRP:CD1	2.95	0.44
1:A:188:PRO:O	1:A:324:LYS:HG2	2.18	0.44
1:A:195:TYR:C	1:A:197:LYS:N	2.77	0.43
1:A:71:ILE:CD1	4:A:387:HOH:O	2.63	0.43
1:A:92:GLY:HA3	2:A:401:HEM:C3C	2.53	0.43
1:A:282:PHE:O	1:A:284:SER:N	2.52	0.43
1:A:233:TYR:HB3	1:A:266:VAL:HB	2.02	0.42
1:A:188:PRO:O	1:A:324:LYS:CG	2.67	0.41
1:A:257:VAL:HG12	1:A:258:THR:N	2.35	0.41
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.38	0.41
1:A:214:PHE:CE1	1:A:219:CYS:HB3	2.56	0.41
1:A:34:LYS:HB3	1:A:34:LYS:HE2	1.82	0.41
1:A:236:PHE:CD1	2:A:402:HEM:HBC1	2.56	0.41
1:A:300:ALA:C	1:A:302:PHE:H	2.29	0.40
1:A:143:GLN:HG3	4:A:491:HOH:O	2.21	0.40
1:A:307:SER:N	1:A:310:GLU:OE1	2.36	0.40
1:A:307:SER:OG	1:A:310:GLU:HG3	2.20	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	298/345 (86%)	259 (87%)	25 (8%)	14 (5%)	2 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	CYS
1	A	301	GLN
1	A	22	ALA
1	A	23	ASP
1	A	24	GLU
1	A	30	GLN
1	A	240	GLU
1	A	283	HIS
1	A	209	ALA
1	A	210	GLY
1	A	215	LEU
1	A	312	GLU
1	A	231	THR
1	A	220	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	244/277 (88%)	217 (89%)	27 (11%)	6 6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	25	LEU
1	A	39	LYS
1	A	94	LYS
1	A	97	GLN
1	A	100	ILE
1	A	128	LYS
1	A	137	MET
1	A	146	LYS
1	A	180	VAL
1	A	186	ILE

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Mol	Chain	Res	Type
1	A	189	ASP
1	A	196	LEU
1	A	199	LYS
1	A	200	LYS
1	A	212	LYS
1	A	228	LEU
1	A	241	LYS
1	A	262	LYS
1	A	286	VAL
1	A	291	LYS
1	A	297	MET
1	A	304	ILE
1	A	309	ASP
1	A	312	GLU
1	A	324	LYS
1	A	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	107	ASN
1	A	138	ASN
1	A	143	GLN
1	A	194	GLN
1	A	207	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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	HEM	A	401	1	50,50,50	2.18	13 (26%)	67,82,82	2.25	21 (31%)
2	HEM	A	402	1	50,50,50	2.96	13 (26%)	67,82,82	2.44	26 (38%)

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	HEM	A	401	1	-	5/14/54/54	-
2	HEM	A	402	1	-	6/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	HEM	FE-ND	10.94	2.28	1.94
2	A	402	HEM	FE-NA	8.48	2.23	1.95
2	A	402	HEM	C3D-C2D	8.47	1.55	1.36
2	A	402	HEM	FE-NC	7.58	2.20	1.95
2	A	401	HEM	C3D-C2D	6.77	1.51	1.36
2	A	401	HEM	FE-ND	5.81	2.12	1.94
2	A	401	HEM	FE-NB	5.57	2.12	1.94
2	A	402	HEM	CAC-C3C	4.08	1.58	1.47
2	A	402	HEM	CAB-C3B	3.90	1.57	1.47
2	A	401	HEM	CAB-C3B	3.81	1.57	1.47
2	A	401	HEM	CMA-C3A	3.64	1.58	1.50
2	A	401	HEM	CMC-C2C	3.50	1.57	1.50
2	A	402	HEM	FE-NB	3.41	2.05	1.94
2	A	401	HEM	CAC-C3C	3.06	1.55	1.47
2	A	402	HEM	CMD-C2D	2.90	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	HEM	CMC-C2C	2.78	1.56	1.50
2	A	401	HEM	CAA-C2A	2.69	1.58	1.51
2	A	401	HEM	C4C-NC	2.66	1.44	1.39
2	A	401	HEM	FE-NC	2.52	2.03	1.95
2	A	402	HEM	CMA-C3A	2.51	1.55	1.50
2	A	401	HEM	O1D-CGD	2.32	1.29	1.22
2	A	402	HEM	C1D-ND	2.15	1.43	1.38
2	A	401	HEM	O1A-CGA	2.13	1.29	1.22
2	A	401	HEM	CMB-C2B	2.07	1.55	1.50
2	A	402	HEM	CMB-C2B	2.07	1.55	1.50
2	A	402	HEM	CHD-C4C	2.03	1.42	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	HEM	C4D-ND-C1D	8.71	115.52	105.21
2	A	402	HEM	C2A-C1A-NA	-7.07	102.31	110.15
2	A	401	HEM	CHC-C1C-NC	6.17	131.17	124.45
2	A	401	HEM	C3C-C2C-C1C	5.07	111.84	107.05
2	A	401	HEM	C4D-ND-C1D	4.90	111.00	105.21
2	A	402	HEM	C3D-C4D-ND	-4.80	104.91	110.17
2	A	401	HEM	CAC-C3C-C4C	4.65	135.91	124.82
2	A	401	HEM	C4C-CHD-C1D	-4.62	116.20	126.02
2	A	401	HEM	CHA-C4D-ND	4.59	130.05	124.37
2	A	401	HEM	C3B-C4B-NB	-4.55	106.20	109.47
2	A	402	HEM	C4A-NA-C1A	4.32	112.86	105.82
2	A	402	HEM	O1A-CGA-CBA	-3.89	110.74	123.09
2	A	401	HEM	CAA-CBA-CGA	3.80	123.75	113.67
2	A	401	HEM	CAC-C3C-C2C	-3.67	116.49	128.43
2	A	402	HEM	C3B-C4B-NB	-3.58	106.90	109.47
2	A	401	HEM	C1B-NB-C4B	3.56	109.42	105.21
2	A	402	HEM	C1B-NB-C4B	3.55	109.42	105.21
2	A	402	HEM	C3B-C2B-C1B	3.55	109.07	106.41
2	A	402	HEM	C2D-C1D-ND	-3.53	105.82	109.90
2	A	402	HEM	CHB-C1B-NB	3.23	128.36	124.37
2	A	402	HEM	CHD-C4C-C3C	2.97	130.22	125.21
2	A	402	HEM	CMA-C3A-C2A	2.97	131.93	125.62
2	A	402	HEM	CHA-C1A-C2A	2.95	131.75	125.30
2	A	401	HEM	O2A-CGA-CBA	2.94	123.28	114.00
2	A	401	HEM	C4A-CHB-C1B	-2.82	119.60	126.25
2	A	401	HEM	O1A-CGA-CBA	-2.76	114.34	123.09
2	A	402	HEM	CMA-C3A-C4A	-2.74	121.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	HEM	CMB-C2B-C1B	-2.73	120.77	125.03
2	A	402	HEM	CHC-C1C-NC	2.64	127.33	124.45
2	A	402	HEM	C4C-NC-C1C	2.55	109.97	105.82
2	A	402	HEM	O2A-CGA-CBA	2.51	121.94	114.00
2	A	401	HEM	CHA-C4D-C3D	-2.42	120.77	125.23
2	A	402	HEM	C2B-C1B-NB	-2.35	107.14	109.84
2	A	401	HEM	CMA-C3A-C4A	-2.33	121.87	125.42
2	A	402	HEM	C1A-C2A-C3A	2.27	110.38	106.87
2	A	401	HEM	CHD-C1D-C2D	2.26	128.60	125.03
2	A	402	HEM	CAC-C3C-C4C	2.22	130.12	124.82
2	A	402	HEM	CHD-C1D-C2D	2.21	128.52	125.03
2	A	402	HEM	CHA-C4D-C3D	2.21	129.29	125.23
2	A	401	HEM	CMC-C2C-C3C	-2.17	123.18	128.43
2	A	401	HEM	CMB-C2B-C1B	-2.14	121.69	125.03
2	A	401	HEM	CBA-CAA-C2A	-2.07	106.82	112.53
2	A	401	HEM	CHC-C4B-C3B	2.06	129.19	125.07
2	A	402	HEM	C3C-C2C-C1C	2.06	109.00	107.05
2	A	401	HEM	C2B-C1B-NB	-2.03	107.50	109.84
2	A	402	HEM	CAC-C3C-C2C	-2.02	121.86	128.43
2	A	402	HEM	CBC-CAC-C3C	-2.01	117.50	127.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

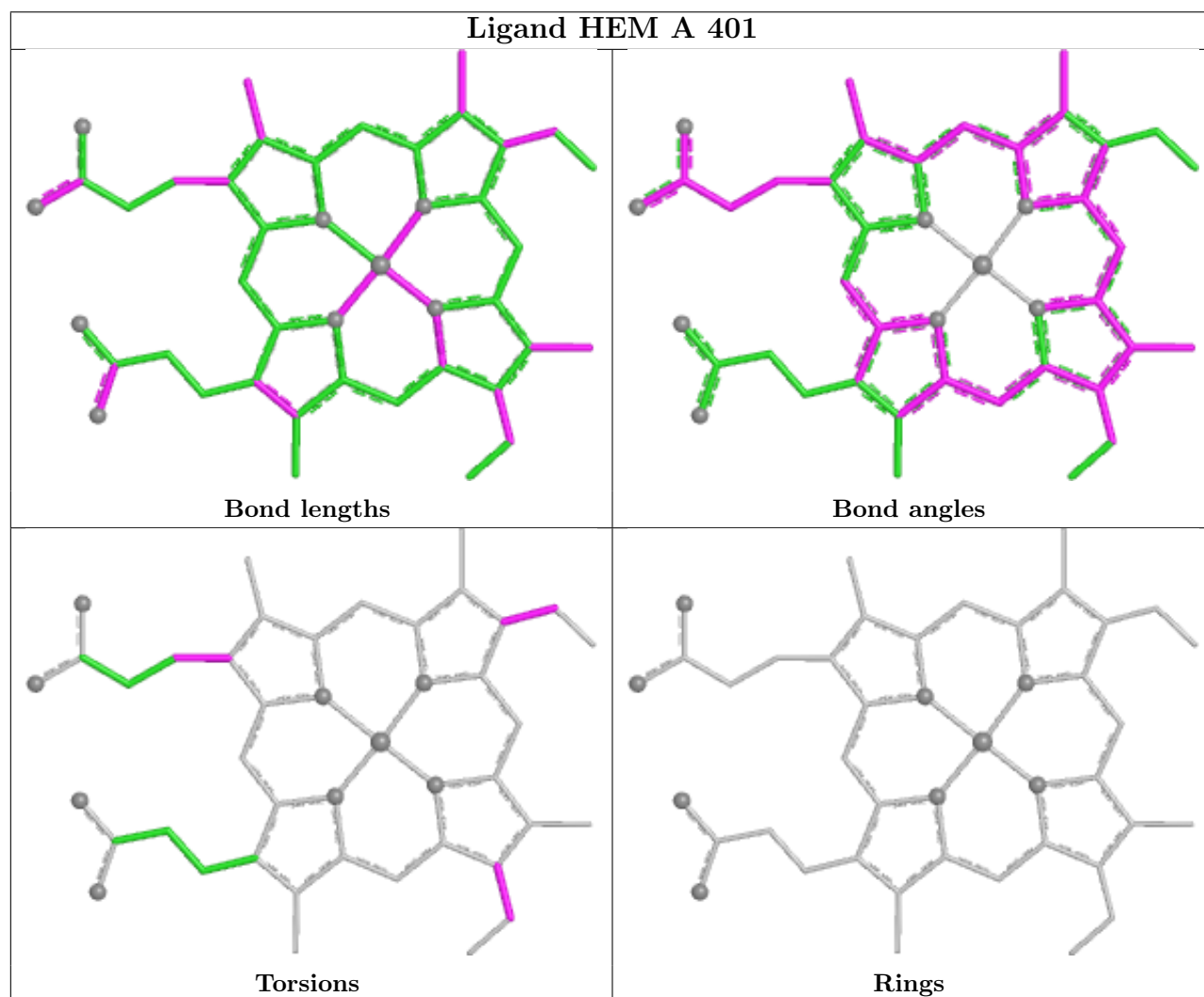
Mol	Chain	Res	Type	Atoms
2	A	402	HEM	C2C-C3C-CAC-CBC
2	A	402	HEM	C4C-C3C-CAC-CBC
2	A	401	HEM	C2B-C3B-CAB-CBB
2	A	402	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4C-C3C-CAC-CBC
2	A	401	HEM	C4B-C3B-CAB-CBB
2	A	401	HEM	C3A-C2A-CAA-CBA
2	A	401	HEM	C1A-C2A-CAA-CBA
2	A	402	HEM	CAA-CBA-CGA-O2A
2	A	402	HEM	C4B-C3B-CAB-CBB
2	A	402	HEM	CAA-CBA-CGA-O1A

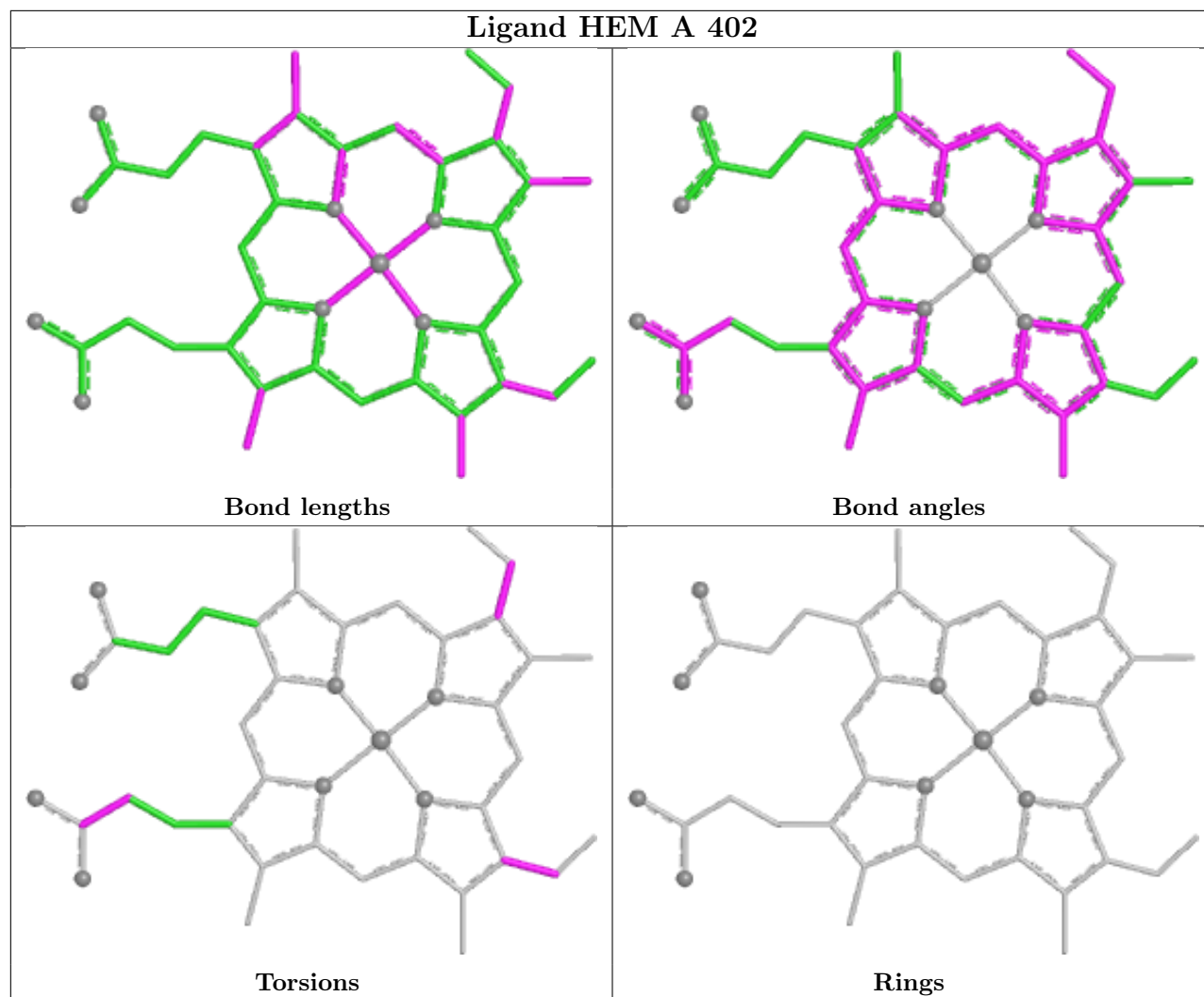
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	6	0
2	A	402	HEM	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/345 (88%)	0.35	16 (5%) 32 34	18, 37, 66, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	5.1
1	A	113	ALA	5.1
1	A	345	LEU	5.1
1	A	127	ALA	4.5
1	A	302	PHE	4.5
1	A	242	PRO	4.2
1	A	265	TYR	3.8
1	A	303	GLY	3.6
1	A	25	LEU	3.2
1	A	128	LYS	2.8
1	A	21	ALA	2.8
1	A	253	GLY	2.8
1	A	29	ALA	2.5
1	A	304	ILE	2.4
1	A	214	PHE	2.3
1	A	233	TYR	2.2

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](#)

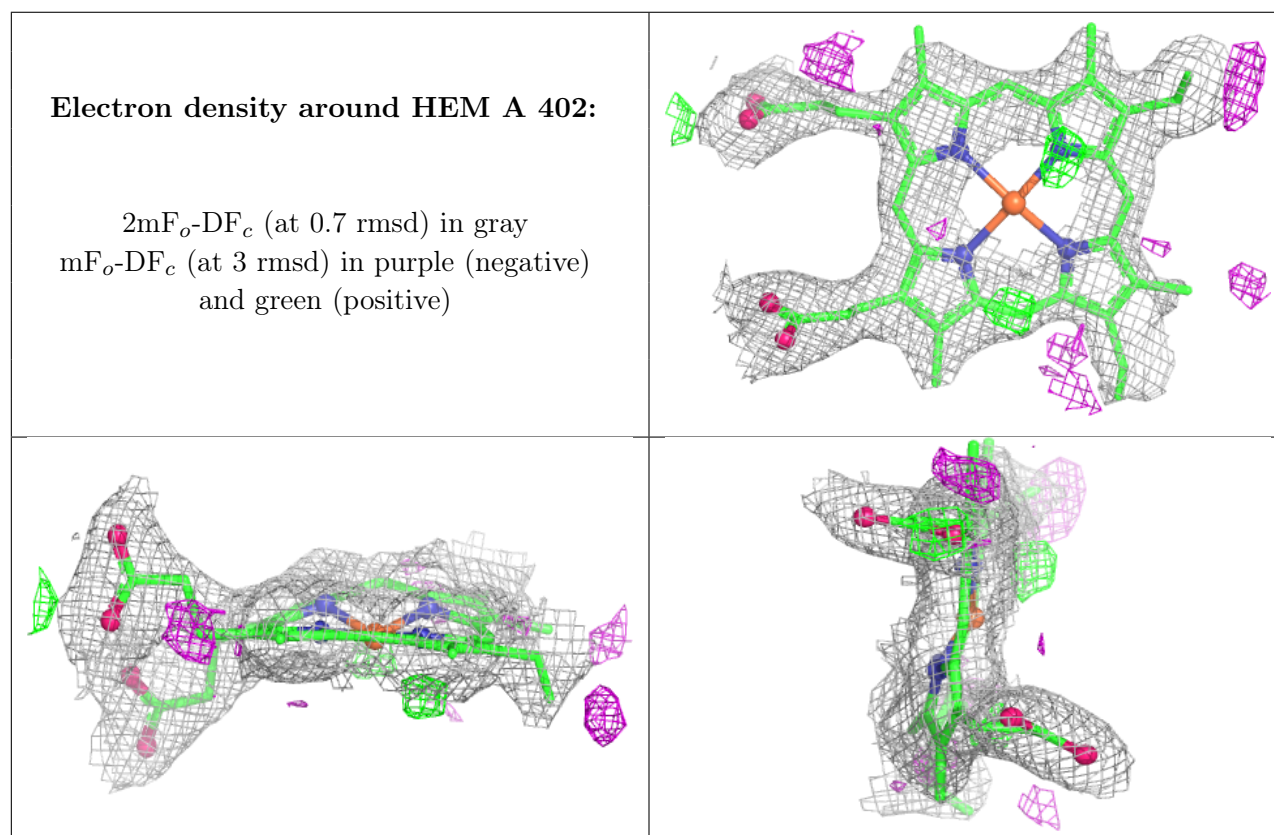
There are no oligosaccharides in this entry.

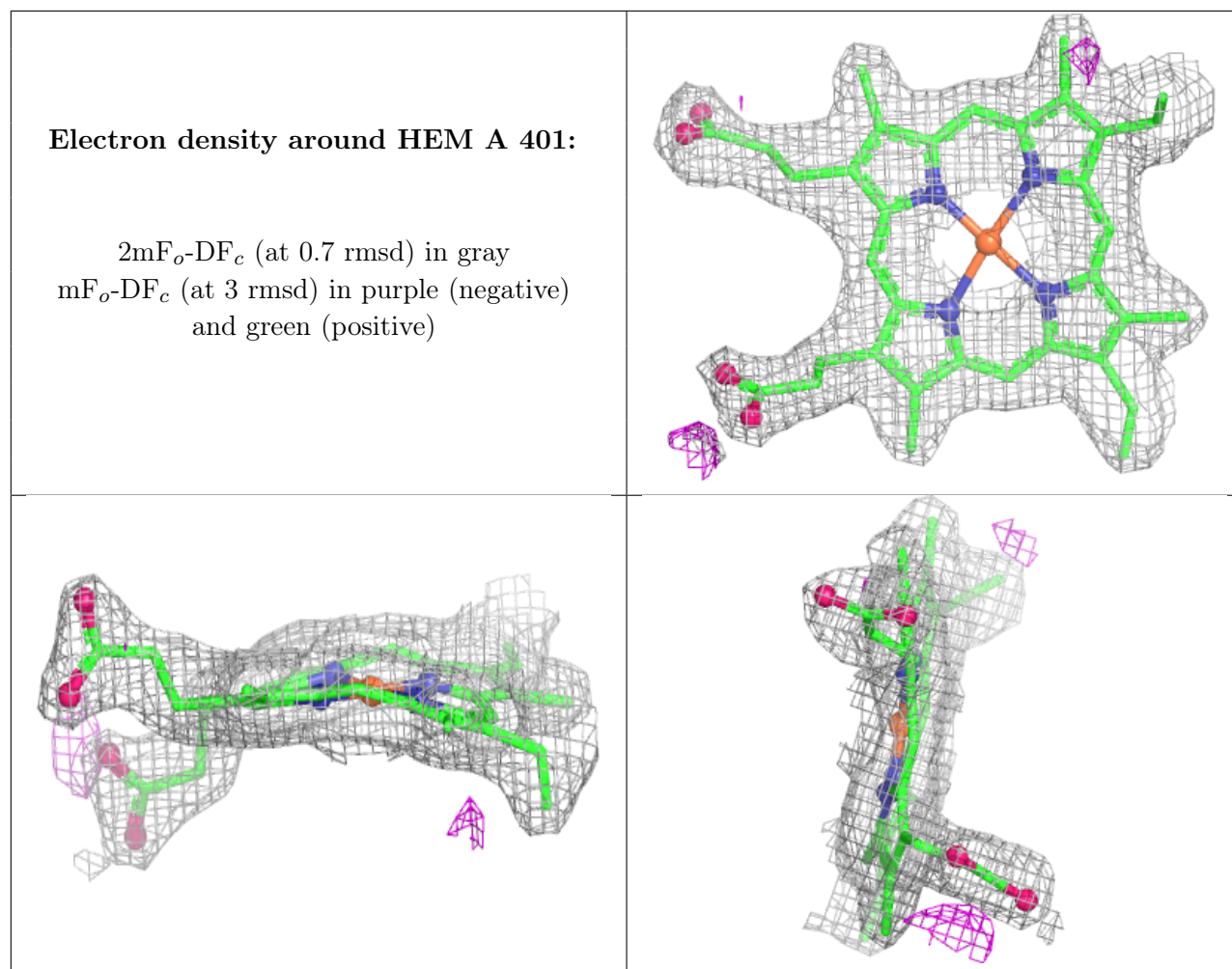
6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	402	43/43	0.95	0.10	24,48,53,55	0
2	HEM	A	401	43/43	0.98	0.08	21,27,49,53	0
3	CA	A	403	1/1	0.99	0.04	19,19,19,19	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.