



Full wwPDB X-ray Structure Validation Report i

Nov 29, 2022 – 12:26 pm GMT

PDB ID : 7QZG

Title : SFX structure of dye-type peroxidase DtpB N245A variant in the ferric state

Authors : Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Shilova, A.; Axford, D.A.; Owen, R.L.; Tosha, T.; Sugimoto, H.; Owada, S.

Deposited on : 2022-01-31

Resolution : 2.10 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.31.3

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.31.3

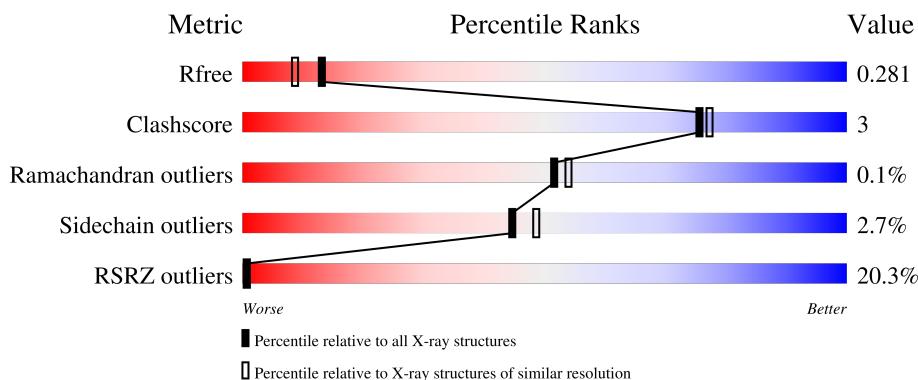
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

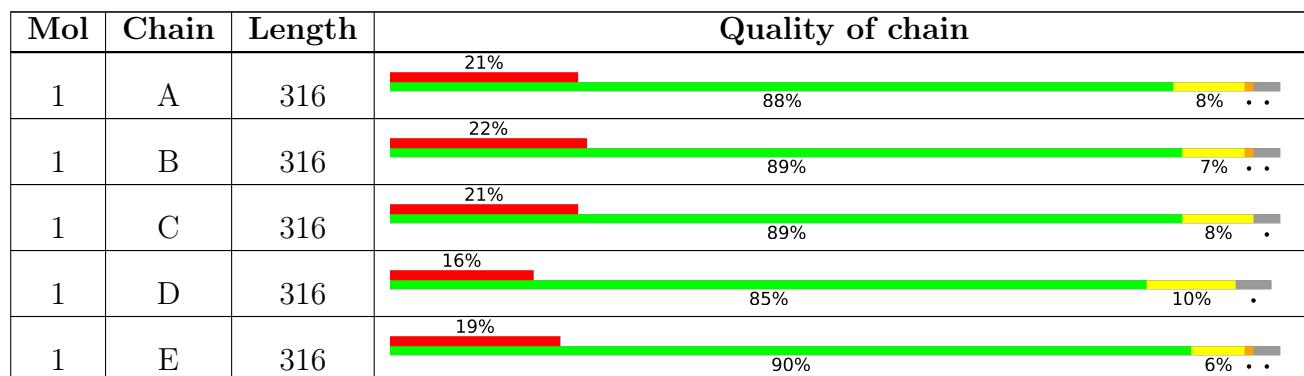
The reported resolution of this entry is 2.10 Å.

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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.



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Mol	Chain	Length	Quality of chain	
1	F	316	18%	90% 7% •

2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 15073 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.

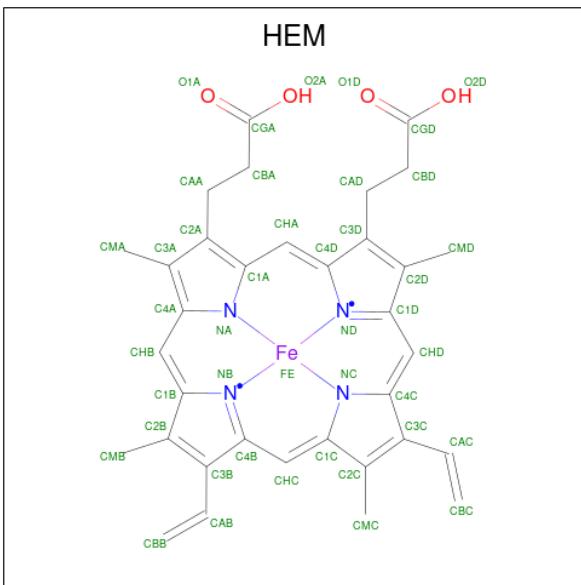
- Molecule 1 is a protein called Dyp-type peroxidase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total 2348	C 1476	N 406	O 456	S 10	0	2	0
1	B	306	Total 2326	C 1465	N 399	O 453	S 9	0	1	0
1	C	306	Total 2355	C 1481	N 407	O 458	S 9	0	4	0
1	D	304	Total 2333	C 1468	N 402	O 454	S 9	0	3	0
1	E	305	Total 2324	C 1466	N 404	O 445	S 9	0	2	0
1	F	306	Total 2334	C 1470	N 402	O 452	S 10	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
B	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
C	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
D	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
E	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
F	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total	O	0	0
			144	144		

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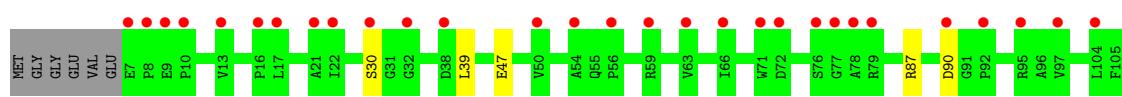
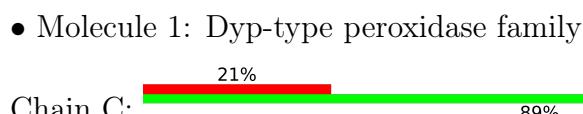
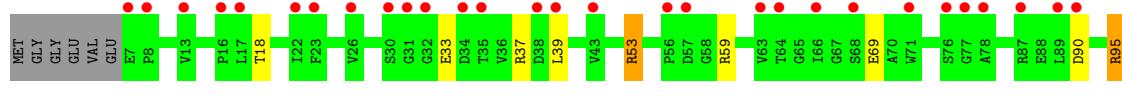
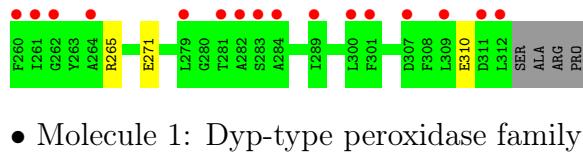
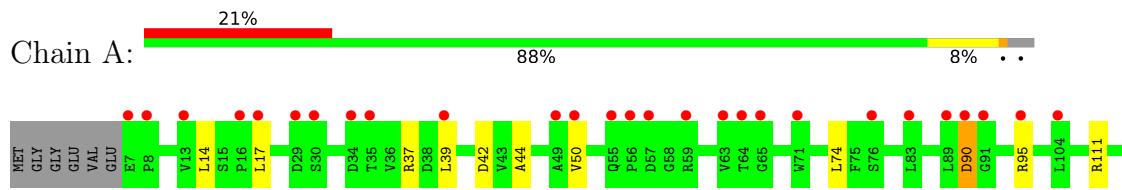
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	123	Total O 123 123	0	0
4	C	126	Total O 126 126	0	0
4	D	130	Total O 130 130	0	0
4	E	143	Total O 143 143	0	0
4	F	127	Total O 127 127	0	0

3 Residue-property plots

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.

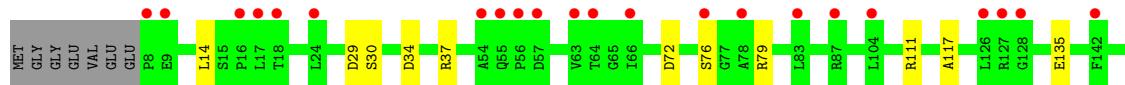
- Molecule 1: Dyp-type peroxidase family





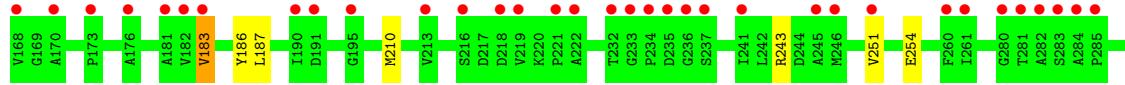
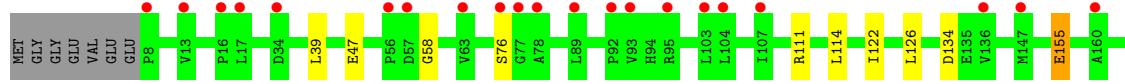
- Molecule 1: Dyp-type peroxidase family

Chain D: 16% 85% 10% •



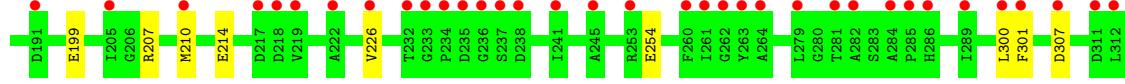
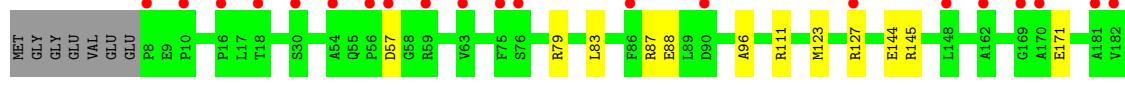
- Molecule 1: Dyp-type peroxidase family

Chain E: 19% 90% 6% •



- Molecule 1: Dyp-type peroxidase family

Chain F: 18% 90% 7% •



S313
ALA
ARG
PRO

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.95 Å 121.83 Å 199.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.10 – 2.10 32.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.10-2.10) 99.9 (32.08-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.94 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R , R_{free}	0.229 , 0.278 0.236 , 0.281	Depositor DCC
R_{free} test set	6248 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15073	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.96	3/2398 (0.1%)	1.01	2/3256 (0.1%)
1	B	0.90	3/2376 (0.1%)	0.97	3/3230 (0.1%)
1	C	0.91	2/2405 (0.1%)	1.01	3/3269 (0.1%)
1	D	0.93	3/2383 (0.1%)	0.96	4/3237 (0.1%)
1	E	0.92	3/2374 (0.1%)	1.01	2/3225 (0.1%)
1	F	0.91	3/2384 (0.1%)	0.98	2/3238 (0.1%)
All	All	0.92	17/14320 (0.1%)	0.99	16/19455 (0.1%)

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	E	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	199	GLU	CD-OE2	8.55	1.35	1.25
1	A	155	GLU	CD-OE1	-8.53	1.16	1.25
1	F	214	GLU	CD-OE1	-8.18	1.16	1.25
1	F	144	GLU	CD-OE2	-7.07	1.17	1.25
1	C	47	GLU	CD-OE1	-6.60	1.18	1.25
1	A	271	GLU	CD-OE1	-6.43	1.18	1.25
1	E	155	GLU	CD-OE1	-5.90	1.19	1.25
1	D	199	GLU	CD-OE1	5.82	1.32	1.25
1	E	47	GLU	CD-OE2	5.72	1.31	1.25
1	B	33	GLU	CD-OE2	-5.56	1.19	1.25
1	E	254	GLU	CD-OE2	5.26	1.31	1.25
1	D	135	GLU	CD-OE1	5.21	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	199	GLU	CD-OE2	5.18	1.31	1.25
1	B	240	GLU	CD-OE2	-5.17	1.20	1.25
1	A	214	GLU	CD-OE1	5.12	1.31	1.25
1	C	214	GLU	CD-OE2	-5.06	1.20	1.25
1	B	268	GLU	CD-OE1	5.02	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	243	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	145	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	E	183	VAL	CA-CB-CG1	6.49	120.64	110.90
1	C	243	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	207	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	203	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	243	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	37	ARG	CG-CD-NE	-6.00	99.20	111.80
1	F	207	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	B	53	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	243	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	243	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	189	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	307	ASP	CB-CA-C	-5.43	99.54	110.40
1	B	141	TYR	CB-CG-CD2	5.13	124.08	121.00
1	F	145	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	311	ASP	Peptide

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	2348	0	2276	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2326	0	2246	19	0
1	C	2355	0	2274	14	0
1	D	2333	0	2262	21	0
1	E	2324	0	2256	11	0
1	F	2334	0	2264	12	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	0	0
2	E	43	0	30	2	0
2	F	43	0	30	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	144	0	0	5	0
4	B	123	0	0	10	0
4	C	126	0	0	5	0
4	D	130	0	0	11	0
4	E	143	0	0	6	0
4	F	127	0	0	2	0
All	All	15073	0	13758	88	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 3.

All (88) 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:44:ALA:N	4:A:501:HOH:O	2.06	0.88
1:C:204:VAL:HG11	4:C:625:HOH:O	1.74	0.87
1:A:140:LYS:HD3	1:A:144:GLU:OE1	1.81	0.81
1:C:210:MET:HE1	1:E:210:MET:HB2	1.63	0.80
1:A:14:LEU:HD21	1:A:166:VAL:HG21	1.66	0.76
1:B:172:ASP:OD1	4:B:501:HOH:O	2.03	0.75
1:B:116:PHE:O	1:B:120[B]:THR:HG23	1.88	0.74
1:E:114:LEU:HD23	4:E:638:HOH:O	1.86	0.74
1:B:69:GLU:OE1	4:B:502:HOH:O	2.06	0.72
2:B:401:HEM:HMB2	2:B:401:HEM:HBB2	1.70	0.71
1:A:254:GLU:OE1	4:A:502:HOH:O	2.08	0.71
1:E:134:ASP:OD2	4:E:501:HOH:O	2.08	0.70
1:D:117:ALA:HA	4:D:623:HOH:O	1.92	0.68
1:D:14:LEU:HD21	1:D:166[A]:VAL:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:SER:HB2	4:C:520:HOH:O	1.93	0.67
1:F:171:GLU:OE2	4:F:501:HOH:O	2.11	0.67
1:B:210:MET:HB2	1:F:210[A]:MET:CE	2.26	0.65
1:C:193:TRP:CZ3	4:C:625:HOH:O	2.48	0.65
1:D:29:ASP:OD1	4:D:501:HOH:O	2.14	0.65
1:D:185:LYS:NZ	4:D:505:HOH:O	2.29	0.64
1:A:42:ASP:C	4:A:501:HOH:O	2.35	0.64
1:A:209:LYS:HG2	1:A:210[B]:MET:HE2	1.80	0.64
1:A:251:VAL:O	4:A:503:HOH:O	2.15	0.63
1:D:266:THR:OG1	1:D:268:GLU:HG3	1.98	0.63
1:D:79:ARG:NH2	4:D:502:HOH:O	2.19	0.62
4:B:605:HOH:O	1:F:210[B]:MET:HE1	1.98	0.62
1:A:209:LYS:HG2	1:A:210[B]:MET:CE	2.30	0.62
2:C:401:HEM:CMC	2:C:401:HEM:HBC2	2.30	0.62
1:A:164:ARG:NH2	4:A:504:HOH:O	2.33	0.61
1:D:79:ARG:NE	4:D:502:HOH:O	2.16	0.61
1:D:147:MET:O	4:D:503:HOH:O	2.16	0.61
1:C:162:ALA:O	1:C:166[B]:VAL:HG12	2.01	0.60
1:D:251:VAL:HG12	1:F:123:MET:HG3	1.84	0.60
1:B:53:ARG:HB2	1:C:143[B]:ASP:OD1	2.02	0.59
1:D:231:VAL:HG23	1:D:239:LEU:HB2	1.85	0.59
1:C:39:LEU:HD22	1:C:126:LEU:HD11	1.85	0.59
2:E:401:HEM:HBC2	2:E:401:HEM:HMC2	1.85	0.59
1:B:90:ASP:OD1	1:B:95:ARG:HD2	2.02	0.59
1:B:18:THR:HA	4:B:514:HOH:O	2.02	0.58
1:C:210:MET:CE	1:E:210:MET:HB2	2.32	0.58
1:C:276:ARG:NH1	4:C:509:HOH:O	2.37	0.58
1:D:146:ASP:HB2	4:D:594:HOH:O	2.04	0.57
1:D:155:GLU:O	4:D:504:HOH:O	2.17	0.57
1:E:58:GLY:HA3	4:E:623:HOH:O	2.03	0.57
1:B:210:MET:HB2	1:F:210[A]:MET:HE3	1.86	0.56
1:D:239:LEU:HA	4:D:513:HOH:O	2.05	0.56
1:F:79:ARG:NH2	1:F:83:LEU:O	2.37	0.56
1:D:182:VAL:HG22	1:D:300[B]:LEU:HD23	1.87	0.56
1:F:226:VAL:HG12	4:F:538:HOH:O	2.06	0.55
1:B:211:THR:HG23	4:B:556:HOH:O	2.07	0.55
1:B:312:LEU:C	1:B:312:LEU:HD12	2.27	0.55
1:E:39:LEU:HD21	1:E:122:ILE:HG23	1.88	0.55
2:B:401:HEM:HBB2	2:B:401:HEM:CMB	2.38	0.54
1:C:250:SER:CB	4:C:520:HOH:O	2.54	0.53
1:D:72:ASP:OD2	1:D:79:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLU:OE2	4:D:504:HOH:O	2.19	0.52
1:B:213:VAL:HG12	4:B:515:HOH:O	2.09	0.52
1:B:156:ASN:O	4:B:504:HOH:O	2.18	0.50
1:A:90:ASP:OD1	1:A:95:ARG:HD2	2.11	0.50
2:C:401:HEM:HBC2	2:C:401:HEM:HMC2	1.93	0.50
1:A:37:ARG:NH1	1:A:74:LEU:O	2.43	0.50
1:C:143[B]:ASP:OD1	1:C:143[B]:ASP:O	2.30	0.50
1:D:266:THR:OG1	1:D:268:GLU:CG	2.60	0.49
1:C:166[B]:VAL:HG13	1:C:167:LEU:HG	1.94	0.49
1:C:87:ARG:NH2	1:C:271:GLU:OE1	2.45	0.49
1:A:251:VAL:CG1	1:C:123:MET:HG3	2.43	0.48
2:E:401:HEM:HBD1	4:E:519:HOH:O	2.14	0.48
1:B:213:VAL:CG1	4:B:515:HOH:O	2.60	0.47
1:D:254:GLU:OE2	1:F:127:ARG:HD2	2.15	0.47
1:B:39:LEU:HD22	1:B:126:LEU:HD11	1.96	0.46
1:B:59:ARG:NH1	4:B:514:HOH:O	2.40	0.46
1:B:120[B]:THR:HG22	1:E:251:VAL:HG12	1.98	0.45
1:B:37:ARG:O	1:B:312:LEU:HD11	2.16	0.45
1:A:50:VAL:HA	4:E:610:HOH:O	2.17	0.44
1:E:39:LEU:HD22	1:E:126:LEU:HG	1.99	0.44
1:F:88:GLU:HG3	1:F:96:ALA:O	2.18	0.44
1:A:209:LYS:CG	1:A:210[B]:MET:CE	2.96	0.44
1:B:210:MET:HB2	1:F:210[A]:MET:HE1	1.99	0.43
4:B:605:HOH:O	1:F:210[B]:MET:CE	2.63	0.43
1:E:155:GLU:O	4:E:502:HOH:O	2.21	0.42
1:A:39:LEU:HD22	1:A:39:LEU:O	2.20	0.42
1:E:187:LEU:HD12	1:E:187:LEU:N	2.35	0.41
1:F:300:LEU:HD23	1:F:301:PHE:N	2.36	0.41
1:D:162:ALA:O	1:D:166[A]:VAL:HG22	2.21	0.40
1:D:14:LEU:HD21	1:D:166[A]:VAL:CG2	2.46	0.40
1:B:213:VAL:HG21	4:D:506:HOH:O	2.21	0.40
1:E:186:TYR:C	1:E:187:LEU:HD12	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	306/316 (97%)	302 (99%)	4 (1%)	0	100	100
1	B	305/316 (96%)	297 (97%)	6 (2%)	2 (1%)	22	18
1	C	308/316 (98%)	303 (98%)	5 (2%)	0	100	100
1	D	305/316 (96%)	301 (99%)	4 (1%)	0	100	100
1	E	305/316 (96%)	300 (98%)	5 (2%)	0	100	100
1	F	306/316 (97%)	301 (98%)	5 (2%)	0	100	100
All	All	1835/1896 (97%)	1804 (98%)	29 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	GLY
1	B	235	ASP

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	246/251 (98%)	238 (97%)	8 (3%)	38	40
1	B	242/251 (96%)	238 (98%)	4 (2%)	60	67
1	C	246/251 (98%)	240 (98%)	6 (2%)	49	53
1	D	245/251 (98%)	235 (96%)	10 (4%)	30	31
1	E	240/251 (96%)	234 (98%)	6 (2%)	47	52
1	F	244/251 (97%)	238 (98%)	6 (2%)	47	52
All	All	1463/1506 (97%)	1423 (97%)	40 (3%)	44	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	90	ASP
1	A	111	ARG
1	A	237	SER
1	A	251	VAL
1	A	265[A]	ARG
1	A	265[B]	ARG
1	A	310	GLU
1	B	95	ARG
1	B	111	ARG
1	B	307	ASP
1	B	312	LEU
1	C	30	SER
1	C	90	ASP
1	C	111	ARG
1	C	217	ASP
1	C	218	ASP
1	C	307	ASP
1	D	30	SER
1	D	34	ASP
1	D	76	SER
1	D	111	ARG
1	D	216	SER
1	D	268	GLU
1	D	293	SER
1	D	307	ASP
1	D	310	GLU
1	D	311	ASP
1	E	76	SER
1	E	111	ARG
1	E	183	VAL
1	E	293	SER
1	E	307	ASP
1	E	310	GLU
1	F	57	ASP
1	F	87	ARG
1	F	111	ARG
1	F	254	GLU
1	F	307	ASP
1	F	313	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	F	401	1	41,50,50	1.73	10 (24%)	45,82,82	2.47	15 (33%)
2	HEM	C	401	1	41,50,50	2.25	16 (39%)	45,82,82	2.27	17 (37%)
2	HEM	D	401	1	41,50,50	1.70	9 (21%)	45,82,82	2.29	17 (37%)
2	HEM	E	401	1	41,50,50	1.72	10 (24%)	45,82,82	2.25	20 (44%)
2	HEM	B	401	1	41,50,50	1.78	12 (29%)	45,82,82	2.33	21 (46%)
2	HEM	A	401	1	41,50,50	1.26	6 (14%)	45,82,82	2.44	21 (46%)

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	F	401	1	-	4/12/54/54	-
2	HEM	C	401	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	401	1	-	4/12/54/54	-
2	HEM	E	401	1	-	5/12/54/54	-
2	HEM	B	401	1	-	4/12/54/54	-
2	HEM	A	401	1	-	6/12/54/54	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3B-C4B	5.13	1.55	1.44
2	F	401	HEM	C1B-NB	-5.03	1.31	1.40
2	C	401	HEM	C1B-NB	-4.99	1.31	1.40
2	C	401	HEM	C4D-ND	-4.20	1.33	1.40
2	D	401	HEM	C1B-NB	-3.99	1.33	1.40
2	C	401	HEM	C3B-C2B	-3.94	1.29	1.37
2	D	401	HEM	CHB-C1B	3.87	1.44	1.35
2	B	401	HEM	C3C-C2C	-3.84	1.35	1.40
2	B	401	HEM	C4D-ND	-3.81	1.33	1.40
2	D	401	HEM	C1D-C2D	3.80	1.51	1.44
2	B	401	HEM	C1B-NB	-3.80	1.33	1.40
2	E	401	HEM	C1B-NB	-3.73	1.33	1.40
2	E	401	HEM	C4D-C3D	3.60	1.51	1.45
2	F	401	HEM	O1D-CGD	3.56	1.33	1.22
2	B	401	HEM	C3C-CAC	3.55	1.55	1.47
2	C	401	HEM	O1A-CGA	3.52	1.33	1.22
2	C	401	HEM	O1D-CGD	3.49	1.33	1.22
2	E	401	HEM	C1D-C2D	3.46	1.51	1.44
2	E	401	HEM	O1A-CGA	3.44	1.33	1.22
2	C	401	HEM	C4B-NB	-3.31	1.32	1.38
2	B	401	HEM	C1A-NA	3.25	1.42	1.36
2	C	401	HEM	CBD-CAD	3.21	1.62	1.52
2	D	401	HEM	FE-NB	3.18	2.12	1.96
2	E	401	HEM	C3D-C2D	-3.09	1.30	1.36
2	E	401	HEM	CHA-C4D	3.04	1.42	1.35
2	F	401	HEM	C1D-ND	-3.03	1.32	1.38
2	A	401	HEM	FE-NB	3.00	2.11	1.96
2	D	401	HEM	C1A-NA	2.94	1.42	1.36
2	E	401	HEM	C3B-C4B	2.90	1.50	1.44
2	A	401	HEM	C3B-C4B	2.83	1.50	1.44
2	C	401	HEM	CHB-C1B	2.70	1.41	1.35
2	B	401	HEM	CMD-C2D	2.57	1.56	1.50
2	F	401	HEM	C1A-NA	2.56	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CHB-C1B	2.54	1.41	1.35
2	C	401	HEM	CMC-C2C	2.53	1.57	1.51
2	F	401	HEM	CBD-CGD	2.53	1.56	1.50
2	E	401	HEM	CBD-CGD	2.50	1.56	1.50
2	E	401	HEM	C4A-CHB	-2.50	1.34	1.41
2	D	401	HEM	O1A-CGA	2.47	1.30	1.22
2	C	401	HEM	C1B-C2B	2.46	1.49	1.44
2	F	401	HEM	CBA-CGA	-2.43	1.44	1.50
2	F	401	HEM	CMC-C2C	-2.41	1.45	1.51
2	D	401	HEM	CMB-C2B	2.40	1.55	1.50
2	C	401	HEM	CHA-C4D	2.37	1.41	1.35
2	C	401	HEM	CMB-C2B	2.33	1.55	1.50
2	F	401	HEM	CHA-C4D	2.28	1.40	1.35
2	D	401	HEM	CHD-C1D	-2.27	1.34	1.41
2	F	401	HEM	C3C-CAC	2.24	1.52	1.47
2	D	401	HEM	CHA-C4D	2.22	1.40	1.35
2	C	401	HEM	CBD-CGD	2.20	1.55	1.50
2	C	401	HEM	C4D-C3D	2.18	1.48	1.45
2	F	401	HEM	CMD-C2D	2.17	1.55	1.50
2	C	401	HEM	CBA-CGA	2.16	1.55	1.50
2	B	401	HEM	CAA-C2A	2.10	1.55	1.52
2	A	401	HEM	O2D-CGD	-2.09	1.23	1.30
2	B	401	HEM	C1A-CHA	-2.09	1.35	1.41
2	A	401	HEM	C1B-NB	-2.08	1.36	1.40
2	A	401	HEM	CMB-C2B	2.07	1.55	1.50
2	B	401	HEM	O2D-CGD	-2.05	1.23	1.30
2	E	401	HEM	FE-NB	2.04	2.07	1.96
2	B	401	HEM	C4B-NB	-2.04	1.34	1.38
2	B	401	HEM	C4A-NA	-2.01	1.32	1.36
2	B	401	HEM	O1A-CGA	2.01	1.28	1.22

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	CHC-C4B-NB	9.06	134.27	124.43
2	B	401	HEM	CHC-C4B-NB	5.72	130.65	124.43
2	C	401	HEM	CHD-C1D-ND	5.48	130.39	124.43
2	A	401	HEM	CMB-C2B-C1B	5.34	133.18	125.04
2	A	401	HEM	CMD-C2D-C1D	5.23	133.00	125.04
2	E	401	HEM	C1B-NB-C4B	5.16	110.40	105.07
2	F	401	HEM	C2C-C3C-C4C	-5.10	103.34	106.90
2	A	401	HEM	O2A-CGA-CBA	4.97	130.00	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	C1B-NB-C4B	4.96	110.20	105.07
2	D	401	HEM	C1B-NB-C4B	4.54	109.77	105.07
2	D	401	HEM	C4A-C3A-C2A	4.54	110.15	107.00
2	A	401	HEM	O2D-CGD-CBD	4.45	128.33	114.03
2	F	401	HEM	CHB-C1B-NB	4.43	129.86	124.38
2	C	401	HEM	C4B-CHC-C1C	4.37	128.33	122.56
2	D	401	HEM	C2C-C3C-C4C	-4.29	103.90	106.90
2	F	401	HEM	CHC-C4B-C3B	-4.22	118.12	124.57
2	C	401	HEM	C4C-CHD-C1D	-4.21	117.00	122.56
2	E	401	HEM	CHB-C1B-NB	4.20	129.57	124.38
2	C	401	HEM	CHD-C1D-C2D	-4.17	118.47	124.98
2	D	401	HEM	CHD-C1D-ND	4.16	128.95	124.43
2	C	401	HEM	CAD-C3D-C4D	4.12	131.86	124.66
2	D	401	HEM	CHC-C4B-NB	4.06	128.85	124.43
2	B	401	HEM	CMC-C2C-C3C	4.04	132.24	124.68
2	D	401	HEM	CHD-C1D-C2D	-3.98	118.76	124.98
2	B	401	HEM	CHD-C1D-C2D	-3.97	118.78	124.98
2	B	401	HEM	C4C-CHD-C1D	3.96	127.79	122.56
2	C	401	HEM	CMD-C2D-C1D	3.96	131.07	125.04
2	E	401	HEM	CHD-C1D-ND	3.91	128.67	124.43
2	A	401	HEM	O2A-CGA-O1A	-3.89	113.60	123.30
2	B	401	HEM	C1B-NB-C4B	3.86	109.06	105.07
2	E	401	HEM	CHD-C1D-C2D	-3.80	119.03	124.98
2	F	401	HEM	C3B-C2B-C1B	3.80	109.31	106.49
2	F	401	HEM	C4C-CHD-C1D	3.79	127.56	122.56
2	E	401	HEM	O2D-CGD-CBD	3.77	126.15	114.03
2	D	401	HEM	CMD-C2D-C1D	3.68	130.64	125.04
2	E	401	HEM	C4C-CHD-C1D	-3.64	117.75	122.56
2	C	401	HEM	C2C-C3C-C4C	3.64	109.44	106.90
2	C	401	HEM	C4A-C3A-C2A	3.60	109.50	107.00
2	A	401	HEM	CMB-C2B-C3B	-3.43	119.90	128.30
2	A	401	HEM	O2D-CGD-O1D	-3.42	114.77	123.30
2	E	401	HEM	C4B-CHC-C1C	3.41	127.05	122.56
2	A	401	HEM	CAD-C3D-C4D	3.40	130.61	124.66
2	A	401	HEM	CAB-C3B-C2B	-3.39	117.42	128.60
2	B	401	HEM	O1A-CGA-CBA	-3.37	112.26	123.08
2	B	401	HEM	CHA-C4D-ND	3.36	128.54	124.38
2	D	401	HEM	CMB-C2B-C1B	-3.36	119.93	125.04
2	E	401	HEM	O2D-CGD-O1D	-3.35	114.96	123.30
2	B	401	HEM	C1D-C2D-C3D	-3.28	103.51	106.96
2	B	401	HEM	C4A-C3A-C2A	3.27	109.27	107.00
2	A	401	HEM	CAA-CBA-CGA	-3.22	104.74	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	C4B-C3B-C2B	-3.22	104.56	107.11
2	D	401	HEM	CHA-C4D-ND	3.20	128.34	124.38
2	E	401	HEM	CAB-C3B-C2B	-3.19	118.09	128.60
2	D	401	HEM	CHA-C4D-C3D	-3.16	119.40	125.33
2	D	401	HEM	CHB-C1B-NB	3.12	128.24	124.38
2	B	401	HEM	C2D-C1D-ND	3.12	113.61	109.88
2	A	401	HEM	CBA-CAA-C2A	3.10	117.90	112.62
2	E	401	HEM	CBA-CAA-C2A	2.96	117.67	112.62
2	B	401	HEM	CMB-C2B-C1B	2.95	129.53	125.04
2	E	401	HEM	C4B-C3B-C2B	-2.94	104.78	107.11
2	C	401	HEM	CHA-C4D-ND	2.93	128.00	124.38
2	E	401	HEM	CHA-C4D-ND	2.92	127.98	124.38
2	C	401	HEM	CAD-C3D-C2D	-2.89	122.49	127.88
2	B	401	HEM	CAA-CBA-CGA	-2.89	105.65	113.76
2	B	401	HEM	CMD-C2D-C1D	2.81	129.32	125.04
2	B	401	HEM	CHD-C1D-ND	2.81	127.48	124.43
2	C	401	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
2	C	401	HEM	C2B-C1B-NB	2.77	113.12	109.84
2	C	401	HEM	CHA-C4D-C3D	-2.74	120.18	125.33
2	B	401	HEM	O2A-CGA-CBA	2.71	122.73	114.03
2	C	401	HEM	CHC-C4B-NB	2.61	127.27	124.43
2	C	401	HEM	C3B-C2B-C1B	-2.60	104.55	106.49
2	F	401	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
2	B	401	HEM	CHC-C4B-C3B	-2.52	120.71	124.57
2	E	401	HEM	CAB-C3B-C4B	2.49	136.08	124.47
2	E	401	HEM	CHC-C4B-NB	2.49	127.13	124.43
2	A	401	HEM	CAD-C3D-C2D	-2.44	123.34	127.88
2	D	401	HEM	CBA-CAA-C2A	2.43	116.76	112.62
2	A	401	HEM	CMC-C2C-C3C	2.41	129.18	124.68
2	A	401	HEM	CAB-C3B-C4B	2.40	135.65	124.47
2	F	401	HEM	CHA-C4D-C3D	-2.39	120.85	125.33
2	E	401	HEM	CHA-C4D-C3D	-2.36	120.89	125.33
2	B	401	HEM	CBA-CAA-C2A	2.36	116.65	112.62
2	B	401	HEM	O2D-CGD-CBD	2.32	121.49	114.03
2	D	401	HEM	CMC-C2C-C3C	2.31	129.01	124.68
2	A	401	HEM	CHA-C4D-C3D	-2.31	120.99	125.33
2	A	401	HEM	CMD-C2D-C3D	-2.30	119.86	126.12
2	D	401	HEM	C1D-C2D-C3D	-2.26	104.58	106.96
2	D	401	HEM	O2A-CGA-O1A	2.26	128.93	123.30
2	D	401	HEM	C4B-C3B-C2B	-2.26	105.32	107.11
2	B	401	HEM	CMB-C2B-C3B	-2.25	122.80	128.30
2	C	401	HEM	CHB-C1B-C2B	-2.24	120.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHA-C4D-ND	2.21	127.12	124.38
2	A	401	HEM	CBD-CAD-C3D	-2.19	106.54	112.63
2	F	401	HEM	CHA-C4D-ND	2.17	127.06	124.38
2	E	401	HEM	C3C-C4C-NC	-2.15	106.89	110.94
2	F	401	HEM	CMB-C2B-C3B	-2.15	123.05	128.30
2	B	401	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
2	A	401	HEM	O1A-CGA-CBA	-2.10	116.33	123.08
2	F	401	HEM	CAD-CBD-CGD	2.10	118.12	113.60
2	A	401	HEM	C3C-C4C-NC	-2.10	106.98	110.94
2	E	401	HEM	CHB-C1B-C2B	-2.07	120.99	126.72
2	E	401	HEM	C3B-C2B-C1B	2.06	108.02	106.49
2	E	401	HEM	CBD-CAD-C3D	-2.06	106.91	112.63
2	B	401	HEM	C4B-C3B-C2B	-2.06	105.48	107.11
2	C	401	HEM	CMB-C2B-C3B	2.04	133.31	128.30
2	D	401	HEM	CMA-C3A-C2A	-2.04	121.09	124.94
2	A	401	HEM	CBB-CAB-C3B	-2.04	117.48	127.62
2	F	401	HEM	C2D-C1D-ND	2.03	112.32	109.88
2	E	401	HEM	C2D-C1D-ND	2.01	112.29	109.88
2	F	401	HEM	C4A-C3A-C2A	2.00	108.39	107.00

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4B-C3B-CAB-CBB
2	E	401	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAD-CBD-CGD-O1D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A

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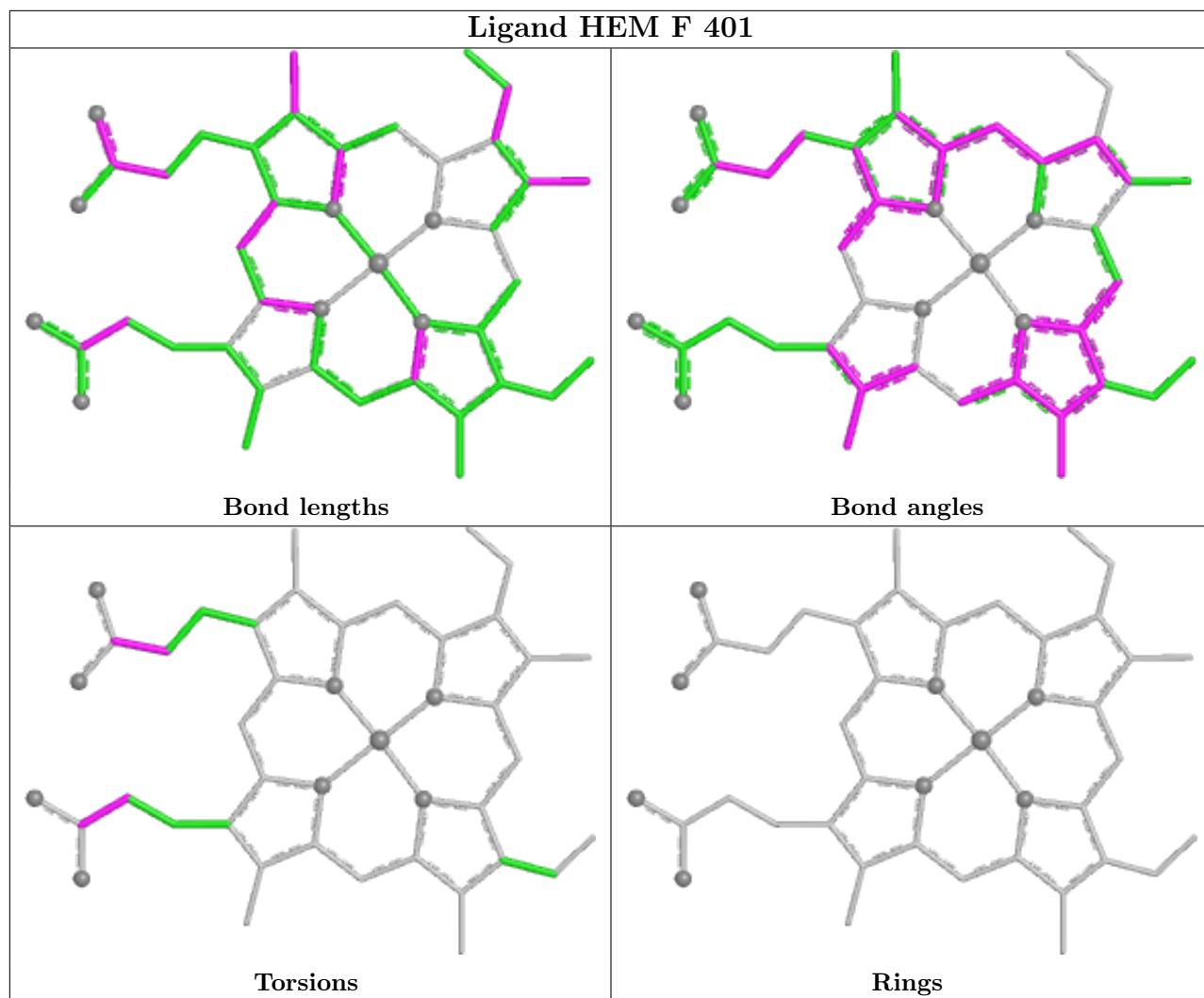
Mol	Chain	Res	Type	Atoms
2	C	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A

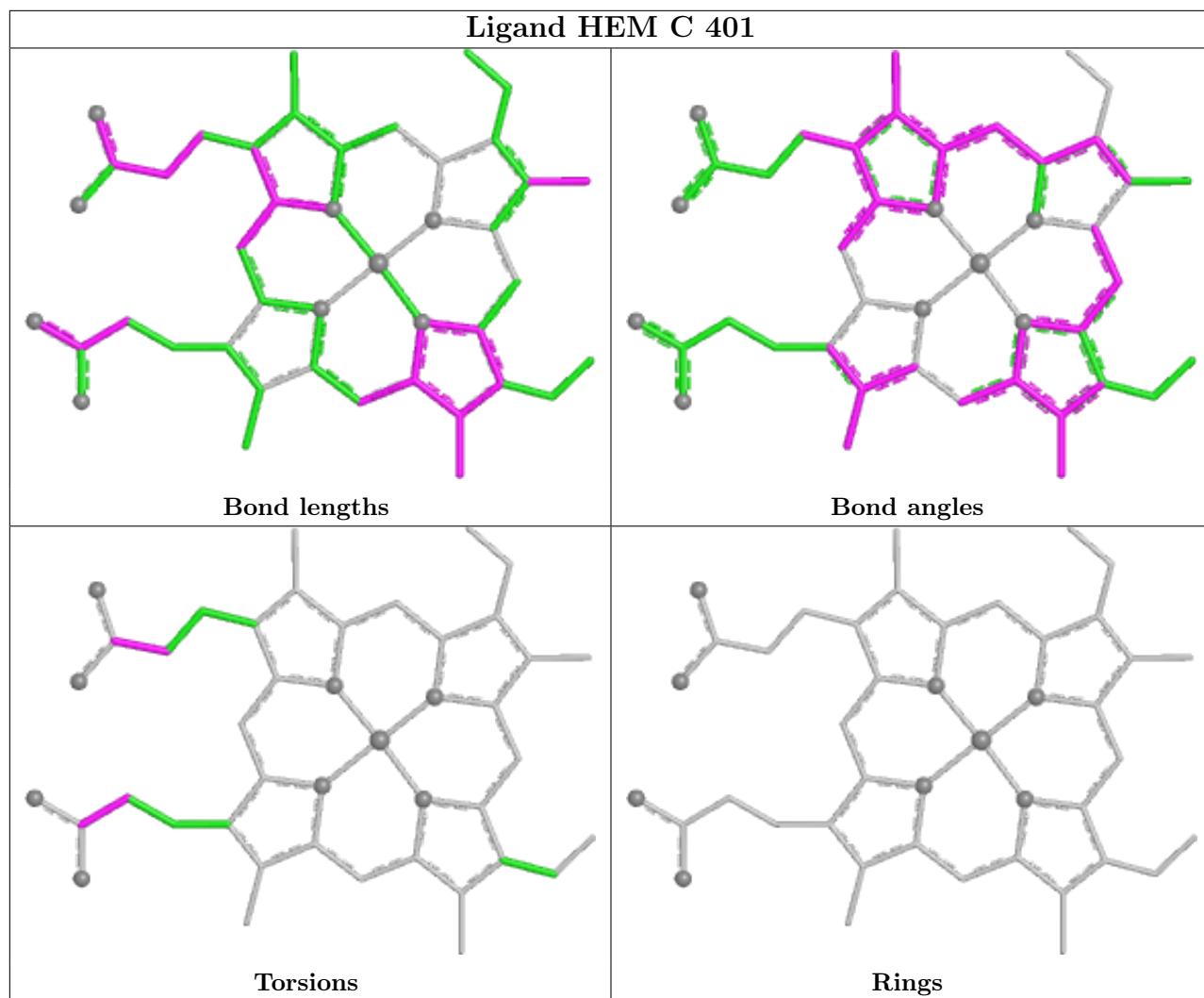
There are no ring outliers.

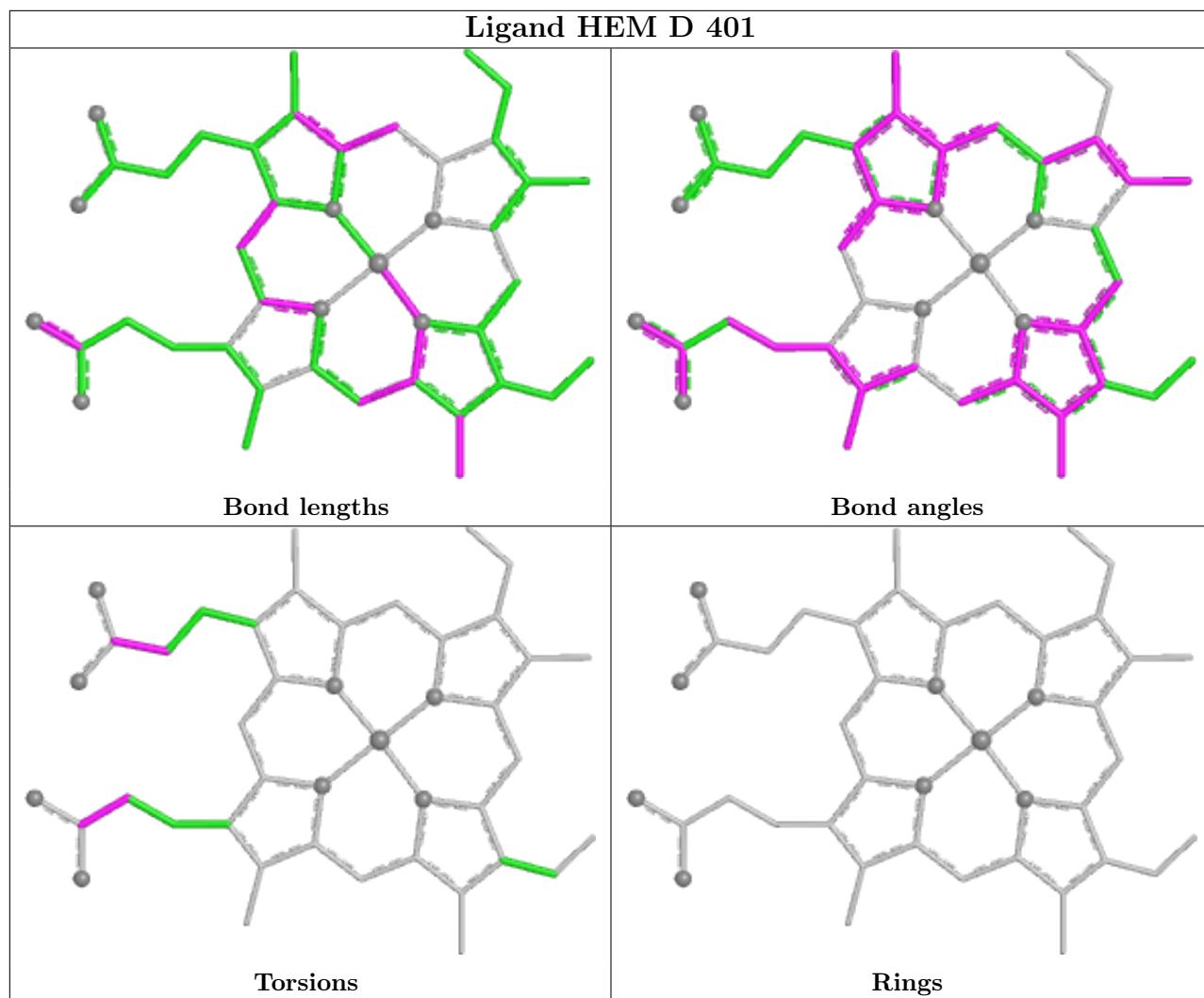
3 monomers are involved in 6 short contacts:

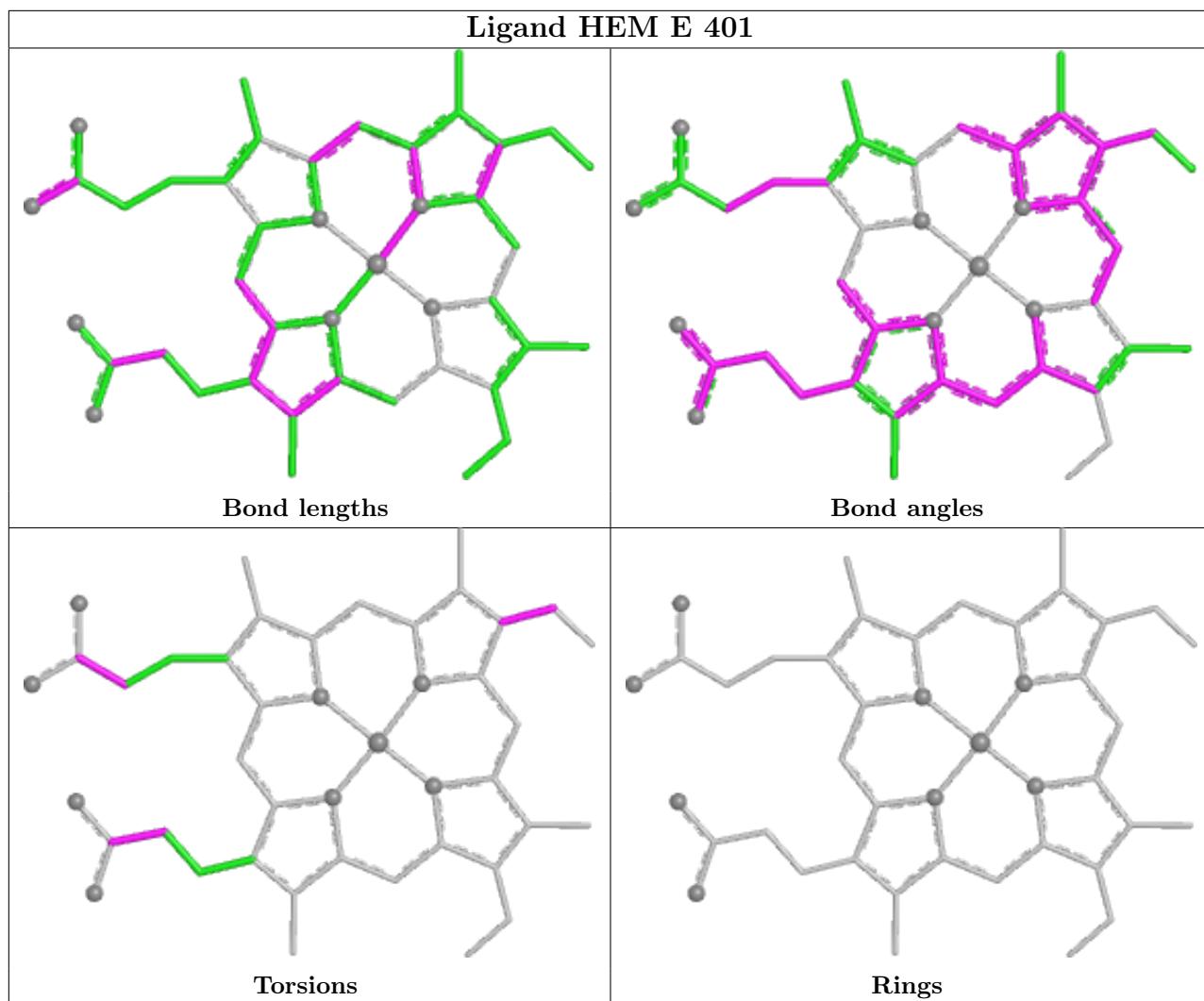
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HEM	2	0
2	E	401	HEM	2	0
2	B	401	HEM	2	0

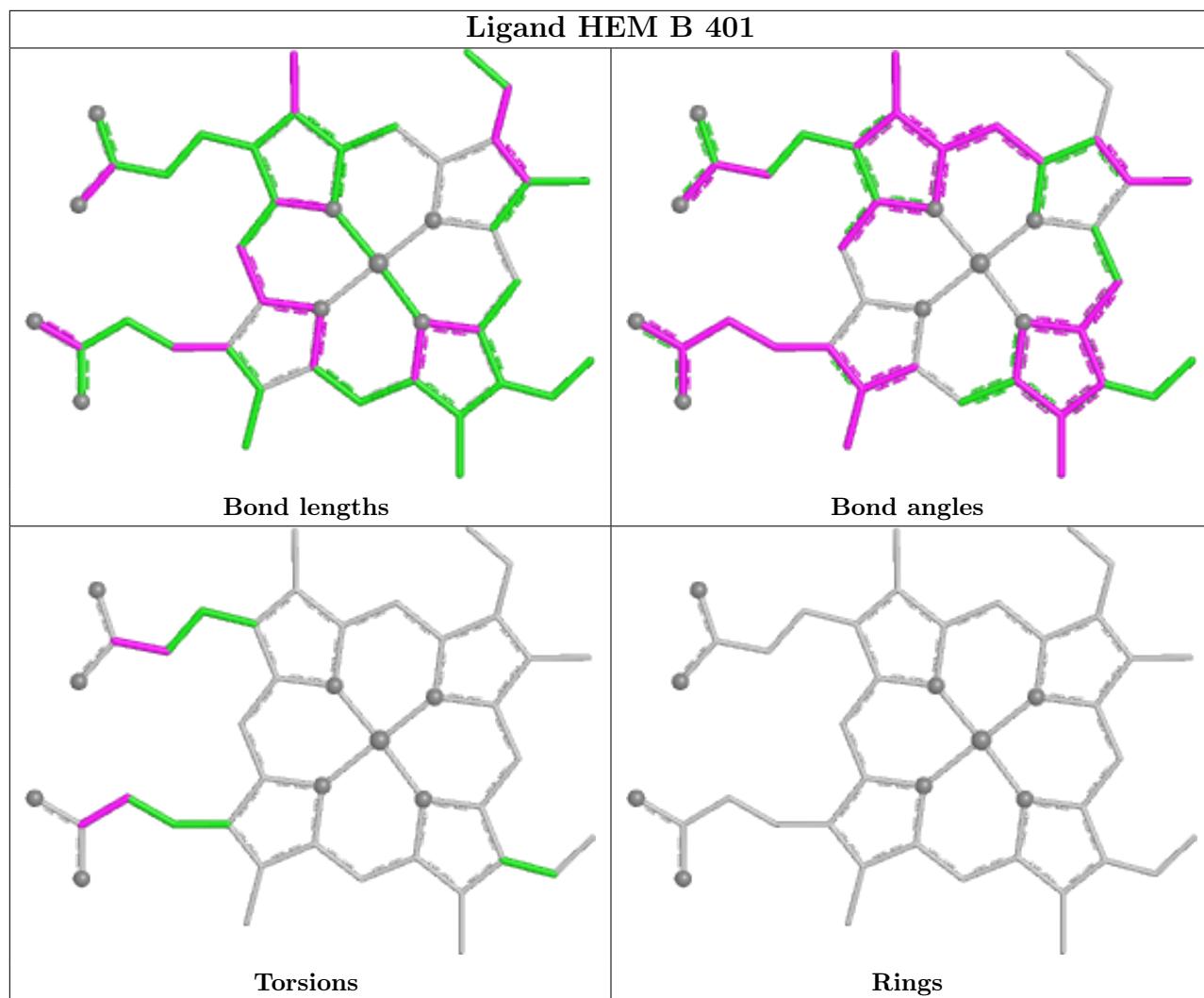
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

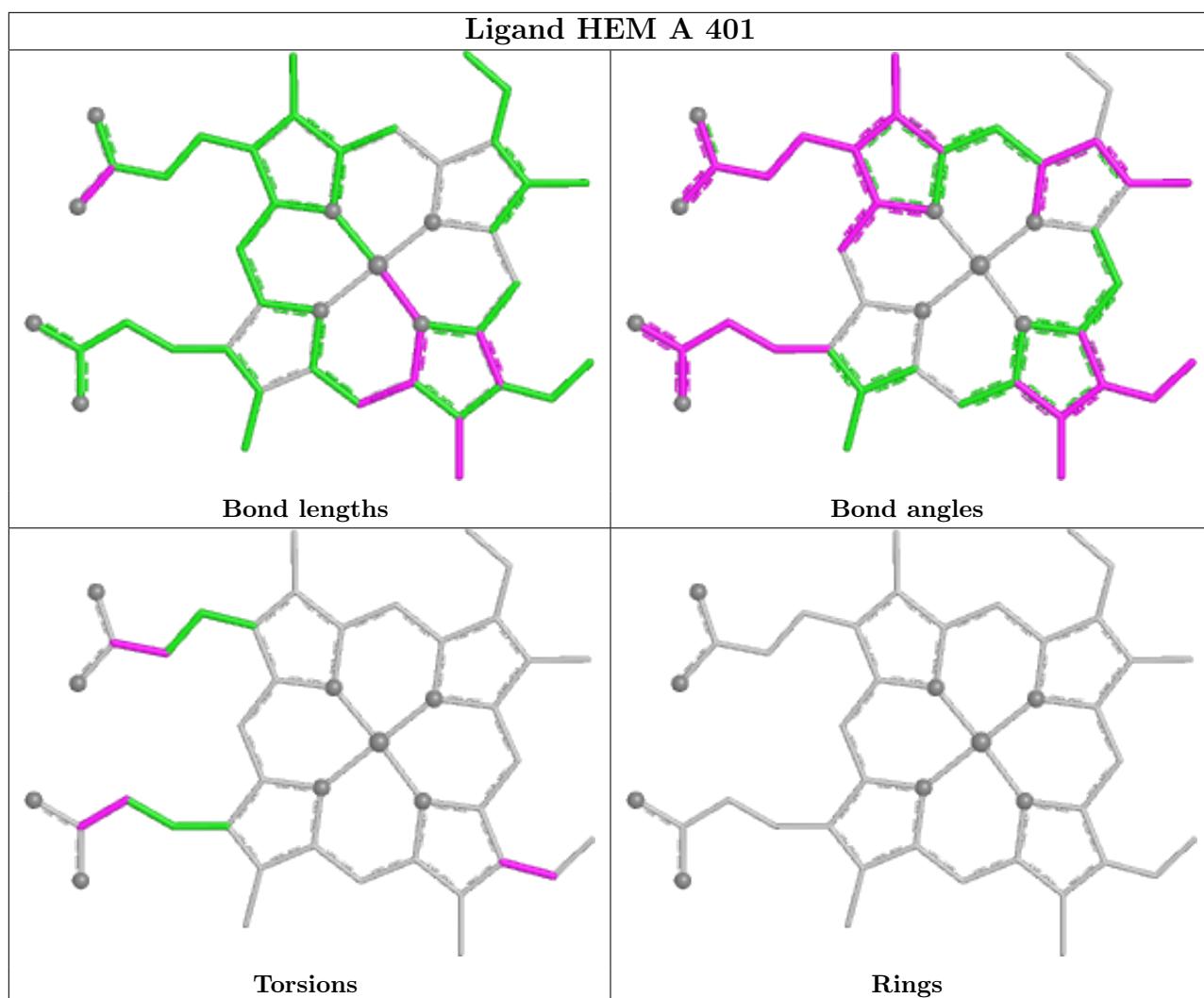












5.7 Other polymers [\(i\)](#)

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	306/316 (96%)	1.30	65 (21%) 0 0	19, 28, 49, 68	0
1	B	306/316 (96%)	1.43	70 (22%) 0 0	19, 31, 54, 74	0
1	C	306/316 (96%)	1.42	67 (21%) 0 0	20, 30, 54, 74	0
1	D	304/316 (96%)	1.29	52 (17%) 1 1	18, 29, 52, 74	0
1	E	305/316 (96%)	1.32	61 (20%) 1 1	18, 29, 49, 94	0
1	F	306/316 (96%)	1.32	57 (18%) 1 1	18, 29, 51, 88	0
All	All	1833/1896 (96%)	1.35	372 (20%) 1 1	18, 29, 52, 94	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	234	PRO	8.6
1	C	312	LEU	8.3
1	B	312	LEU	6.7
1	F	234	PRO	6.7
1	F	236	GLY	6.5
1	D	234	PRO	6.4
1	E	235	ASP	6.1
1	A	17	LEU	6.0
1	F	313	SER	6.0
1	C	233	GLY	6.0
1	C	235	ASP	6.0
1	D	76	SER	5.7
1	A	7	GLU	5.7
1	E	76	SER	5.7
1	D	8	PRO	5.7
1	B	234	PRO	5.6
1	F	237	SER	5.6
1	F	235	ASP	5.5
1	B	236	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	219	VAL	5.5
1	C	311	ASP	5.4
1	E	236	GLY	5.4
1	E	232	THR	5.4
1	C	261	ILE	5.4
1	E	312	LEU	5.4
1	B	76	SER	5.3
1	A	282	ALA	5.2
1	B	170	ALA	5.2
1	B	8	PRO	5.2
1	C	237	SER	5.2
1	A	30	SER	5.1
1	E	311	ASP	5.1
1	C	218	ASP	5.0
1	D	217	ASP	4.8
1	E	233	GLY	4.8
1	C	8	PRO	4.8
1	C	234	PRO	4.8
1	C	219	VAL	4.8
1	E	261	ILE	4.8
1	F	90	ASP	4.7
1	E	183	VAL	4.7
1	B	16	PRO	4.7
1	B	217	ASP	4.6
1	E	77	GLY	4.6
1	D	232	THR	4.5
1	B	233	GLY	4.5
1	C	76	SER	4.5
1	D	235	ASP	4.5
1	D	218	ASP	4.4
1	C	17	LEU	4.4
1	B	104	LEU	4.4
1	C	90	ASP	4.3
1	B	56	PRO	4.3
1	D	56	PRO	4.3
1	E	92	PRO	4.3
1	B	261	ILE	4.3
1	F	210[A]	MET	4.2
1	D	16	PRO	4.2
1	F	8	PRO	4.2
1	C	238	ASP	4.2
1	C	169	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	182	VAL	4.0
1	F	232	THR	4.0
1	B	31	GLY	4.0
1	B	216	SER	4.0
1	A	312	LEU	3.9
1	D	170	ALA	3.9
1	A	16	PRO	3.9
1	B	7	GLU	3.9
1	C	142	PHE	3.9
1	C	260	PHE	3.9
1	B	238	ASP	3.9
1	D	261	ILE	3.9
1	F	219	VAL	3.8
1	E	8	PRO	3.8
1	C	30	SER	3.8
1	F	76	SER	3.8
1	A	56	PRO	3.7
1	F	281	THR	3.7
1	B	173	PRO	3.7
1	A	261	ILE	3.7
1	D	236	GLY	3.7
1	B	279	LEU	3.7
1	B	282	ALA	3.7
1	D	17	LEU	3.7
1	F	282	ALA	3.7
1	B	182	VAL	3.7
1	B	30	SER	3.7
1	B	66	ILE	3.7
1	E	104	LEU	3.6
1	A	57	ASP	3.6
1	D	233	GLY	3.6
1	F	260	PHE	3.6
1	A	218	ASP	3.6
1	E	56	PRO	3.6
1	F	312	LEU	3.5
1	F	261	ILE	3.5
1	A	279	LEU	3.5
1	B	181	ALA	3.5
1	A	234	PRO	3.5
1	A	89	LEU	3.4
1	A	34	ASP	3.4
1	B	218	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	181	ALA	3.4
1	E	170	ALA	3.4
1	D	237	SER	3.3
1	D	289	ILE	3.3
1	B	232	THR	3.3
1	B	183	VAL	3.3
1	C	182	VAL	3.3
1	D	168	VAL	3.3
1	B	68	SER	3.3
1	C	263	TYR	3.3
1	E	285	PRO	3.3
1	A	160	ALA	3.3
1	C	170	ALA	3.3
1	E	181	ALA	3.3
1	B	13	VAL	3.3
1	C	104	LEU	3.2
1	F	54	ALA	3.2
1	C	59	ARG	3.2
1	C	97	VAL	3.2
1	C	183	VAL	3.2
1	A	221	PRO	3.1
1	E	16	PRO	3.1
1	D	260	PHE	3.1
1	C	92	PRO	3.1
1	C	95	ARG	3.1
1	A	151	VAL	3.1
1	C	7	GLU	3.1
1	D	128	GLY	3.1
1	A	281	THR	3.1
1	F	205	ILE	3.1
1	E	182	VAL	3.1
1	E	218	ASP	3.1
1	E	237	SER	3.1
1	D	311	ASP	3.1
1	C	16	PRO	3.0
1	B	63	VAL	3.0
1	D	231	VAL	3.0
1	E	260	PHE	3.0
1	B	283	SER	3.0
1	D	307	ASP	3.0
1	A	210[A]	MET	3.0
1	B	281	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	ASP	3.0
1	C	54	ALA	2.9
1	C	236	GLY	2.9
1	F	289	ILE	2.9
1	B	89	LEU	2.9
1	B	237	SER	2.9
1	B	300	LEU	2.9
1	B	97	VAL	2.9
1	D	142	PHE	2.9
1	C	78	ALA	2.9
1	D	54	ALA	2.9
1	E	282	ALA	2.9
1	A	190	ILE	2.9
1	E	160	ALA	2.9
1	E	281	THR	2.9
1	D	104	LEU	2.9
1	F	285	PRO	2.9
1	B	301	PHE	2.8
1	F	59	ARG	2.8
1	E	78	ALA	2.8
1	E	95	ARG	2.8
1	B	38	ASP	2.8
1	A	226	VAL	2.8
1	C	38	ASP	2.8
1	C	251	VAL	2.8
1	F	217	ASP	2.8
1	F	56	PRO	2.8
1	A	90	ASP	2.8
1	A	183	VAL	2.8
1	C	9	GLU	2.8
1	F	169	GLY	2.8
1	A	127	ARG	2.8
1	B	148	LEU	2.8
1	F	300	LEU	2.8
1	A	8	PRO	2.7
1	D	9	GLU	2.7
1	A	217	ASP	2.7
1	E	307	ASP	2.7
1	E	216	SER	2.7
1	F	162	ALA	2.7
1	C	253	ARG	2.7
1	B	260	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	71	TRP	2.7
1	D	245	ALA	2.7
1	F	170	ALA	2.7
1	A	182	VAL	2.6
1	C	77	GLY	2.6
1	C	10	PRO	2.6
1	B	78	ALA	2.6
1	F	86	PHE	2.6
1	A	283	SER	2.6
1	D	182	VAL	2.6
1	D	262	GLY	2.6
1	D	306	ALA	2.6
1	A	311	ASP	2.6
1	B	168	VAL	2.6
1	B	160	ALA	2.6
1	D	87	ARG	2.6
1	E	283	SER	2.6
1	B	280	GLY	2.6
1	A	141	TYR	2.6
1	F	218	ASP	2.5
1	D	183	VAL	2.5
1	F	241	ILE	2.5
1	F	10	PRO	2.5
1	D	148	LEU	2.5
1	A	284	ALA	2.5
1	C	50	VAL	2.5
1	F	301	PHE	2.5
1	F	148	LEU	2.5
1	D	78	ALA	2.5
1	C	63	VAL	2.5
1	B	90	ASP	2.5
1	C	141	TYR	2.5
1	B	262	GLY	2.5
1	D	181	ALA	2.5
1	E	93	VAL	2.5
1	A	142	PHE	2.5
1	A	301	PHE	2.5
1	A	39	LEU	2.5
1	E	284	ALA	2.5
1	D	83	LEU	2.4
1	D	161	ALA	2.4
1	F	181	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	75	PHE	2.4
1	B	235	ASP	2.4
1	C	136	VAL	2.4
1	E	251	VAL	2.4
1	A	205	ILE	2.4
1	D	55	GLN	2.4
1	E	190	ILE	2.4
1	B	64	THR	2.4
1	E	57	ASP	2.4
1	A	76	SER	2.4
1	D	126	LEU	2.4
1	B	87	ARG	2.4
1	C	310	GLU	2.4
1	B	57	ASP	2.4
1	C	232	THR	2.4
1	C	266	THR	2.4
1	A	104	LEU	2.4
1	C	262	GLY	2.4
1	E	195	GLY	2.4
1	A	168	VAL	2.4
1	B	26	VAL	2.4
1	D	57	ASP	2.4
1	A	49	ALA	2.4
1	B	176	ALA	2.4
1	B	245	ALA	2.4
1	C	304	PRO	2.4
1	D	274	LEU	2.4
1	F	311	ASP	2.4
1	B	253	ARG	2.4
1	F	262	GLY	2.4
1	F	238	ASP	2.4
1	B	43	VAL	2.3
1	A	95	ARG	2.3
1	E	107	ILE	2.3
1	A	83	LEU	2.3
1	E	300	LEU	2.3
1	E	221	PRO	2.3
1	F	16	PRO	2.3
1	F	286	HIS	2.3
1	A	235	ASP	2.3
1	B	77	GLY	2.3
1	D	160	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	22	ILE	2.3
1	E	289	ILE	2.3
1	A	29	ASP	2.3
1	B	32	GLY	2.3
1	E	63	VAL	2.3
1	E	245	ALA	2.3
1	E	241	ILE	2.3
1	B	17	LEU	2.3
1	A	13	VAL	2.3
1	C	13	VAL	2.3
1	C	181	ALA	2.3
1	D	310	GLU	2.3
1	F	57	ASP	2.3
1	A	241	ILE	2.3
1	B	304	PRO	2.3
1	E	173	PRO	2.3
1	F	233	GLY	2.3
1	E	219	VAL	2.3
1	B	204	VAL	2.2
1	A	289	ILE	2.2
1	C	106	HIS	2.2
1	B	219	VAL	2.2
1	F	127	ARG	2.2
1	A	91	GLY	2.2
1	A	307	ASP	2.2
1	C	190	ILE	2.2
1	C	245	ALA	2.2
1	E	246	MET	2.2
1	F	284	ALA	2.2
1	A	309	LEU	2.2
1	A	63	VAL	2.2
1	A	65	GLY	2.2
1	B	23	PHE	2.2
1	F	30	SER	2.2
1	B	190	ILE	2.2
1	F	222	ALA	2.2
1	F	245	ALA	2.2
1	D	64	THR	2.2
1	F	279	LEU	2.2
1	B	247	PRO	2.2
1	E	168	VAL	2.2
1	A	35	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	18	THR	2.2
1	C	66	ILE	2.2
1	C	71	TRP	2.2
1	C	241	ILE	2.2
1	C	217	ASP	2.2
1	A	148	LEU	2.2
1	C	79	ARG	2.2
1	A	264	ALA	2.2
1	C	56	PRO	2.2
1	C	164	ARG	2.2
1	E	89	LEU	2.1
1	E	13[A]	VAL	2.1
1	E	136	VAL	2.1
1	C	72	ASP	2.1
1	F	307	ASP	2.1
1	C	107	ILE	2.1
1	D	24	LEU	2.1
1	E	103	LEU	2.1
1	E	309	LEU	2.1
1	F	63	VAL	2.1
1	A	170	ALA	2.1
1	C	22	ILE	2.1
1	F	191	ASP	2.1
1	A	50	VAL	2.1
1	A	232	THR	2.1
1	E	222	ALA	2.1
1	E	213	VAL	2.1
1	A	260	PHE	2.1
1	F	263	TYR	2.1
1	F	253	ARG	2.1
1	A	262	GLY	2.1
1	C	32	GLY	2.1
1	B	39	LEU	2.1
1	C	300[A]	LEU	2.1
1	E	176	ALA	2.1
1	C	127	ARG	2.0
1	D	66	ILE	2.0
1	A	55	GLN	2.0
1	D	63	VAL	2.0
1	F	226	VAL	2.0
1	A	71	TRP	2.0
1	D	127	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	34	ASP	2.0
1	D	246	MET	2.0
1	E	147	MET	2.0
1	E	17	LEU	2.0
1	B	35	THR	2.0
1	C	21	ALA	2.0
1	F	264	ALA	2.0
1	A	59	ARG	2.0
1	E	280	GLY	2.0
1	B	172	ASP	2.0
1	E	191	ASP	2.0
1	A	64	THR	2.0
1	A	300	LEU	2.0
1	D	18	THR	2.0
1	D	165	ALA	2.0
1	B	307	ASP	2.0
1	C	226	VAL	2.0

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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

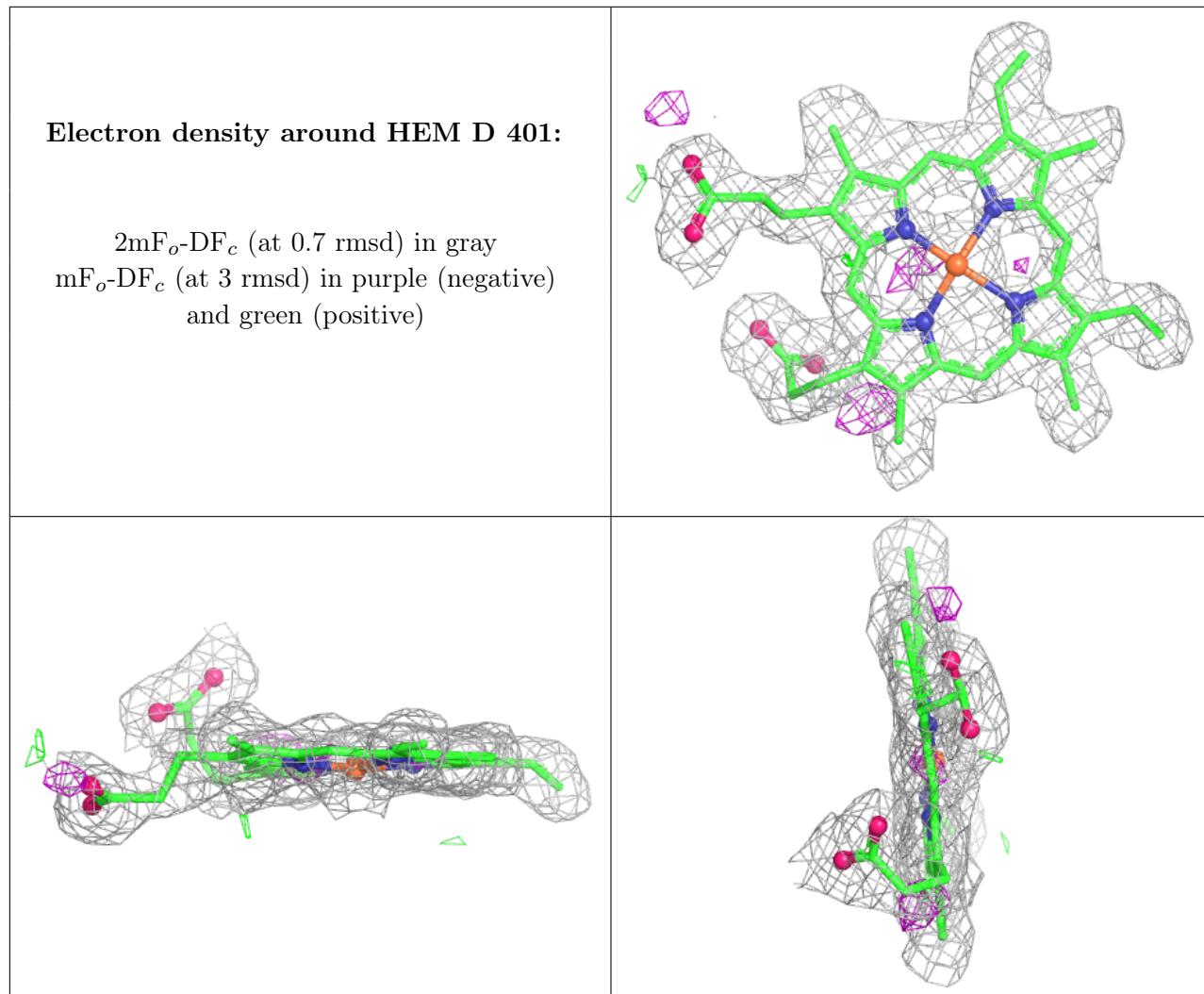
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	402	1/1	0.82	0.14	42,42,42,42	0
2	HEM	D	401	43/43	0.86	0.23	16,23,27,31	0
2	HEM	A	401	43/43	0.87	0.20	18,21,26,29	0
2	HEM	B	401	43/43	0.87	0.20	17,23,29,36	0
2	HEM	F	401	43/43	0.88	0.21	18,21,27,32	0
2	HEM	C	401	43/43	0.89	0.20	17,21,28,29	0

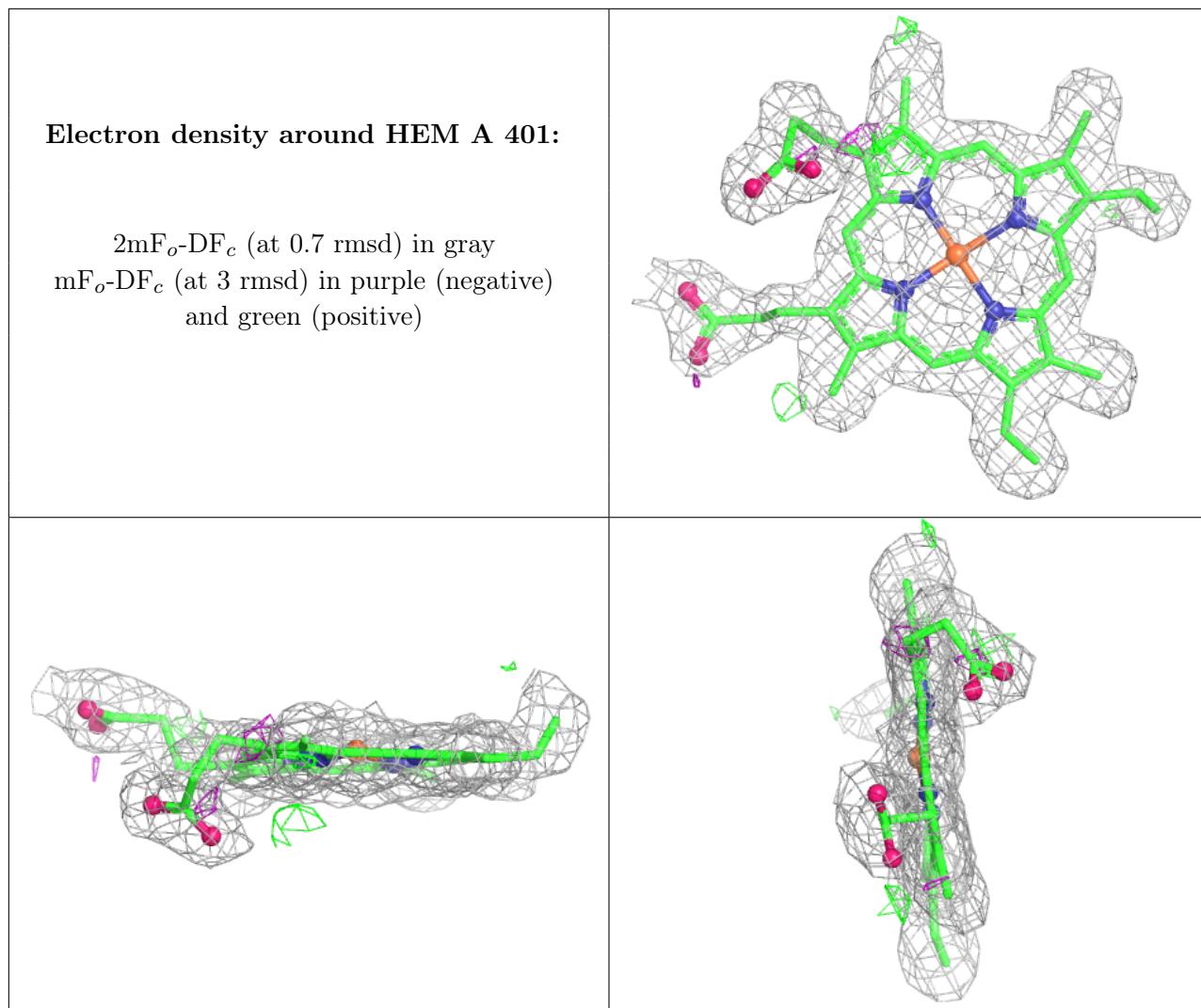
Continued on next page...

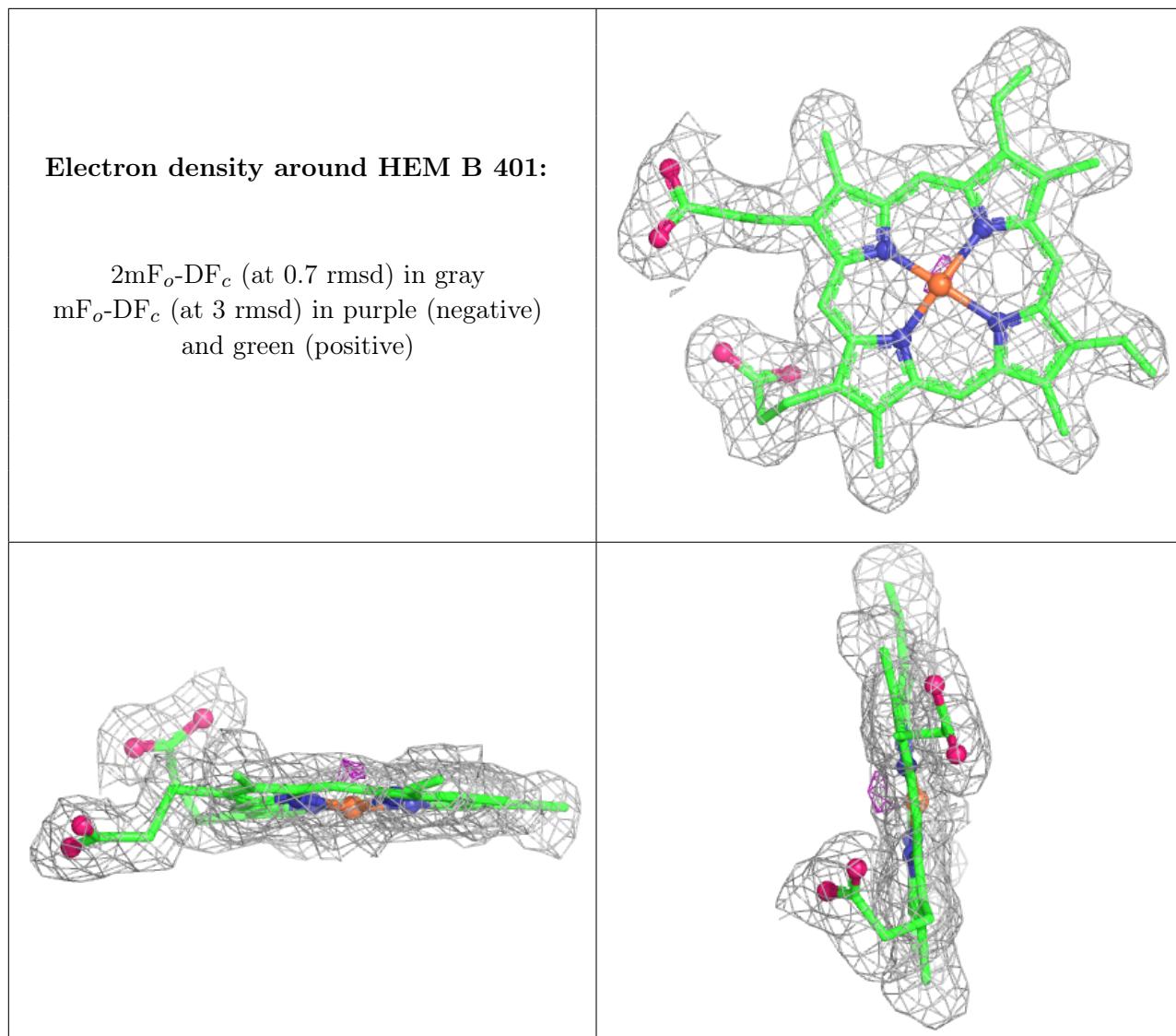
Continued from previous page...

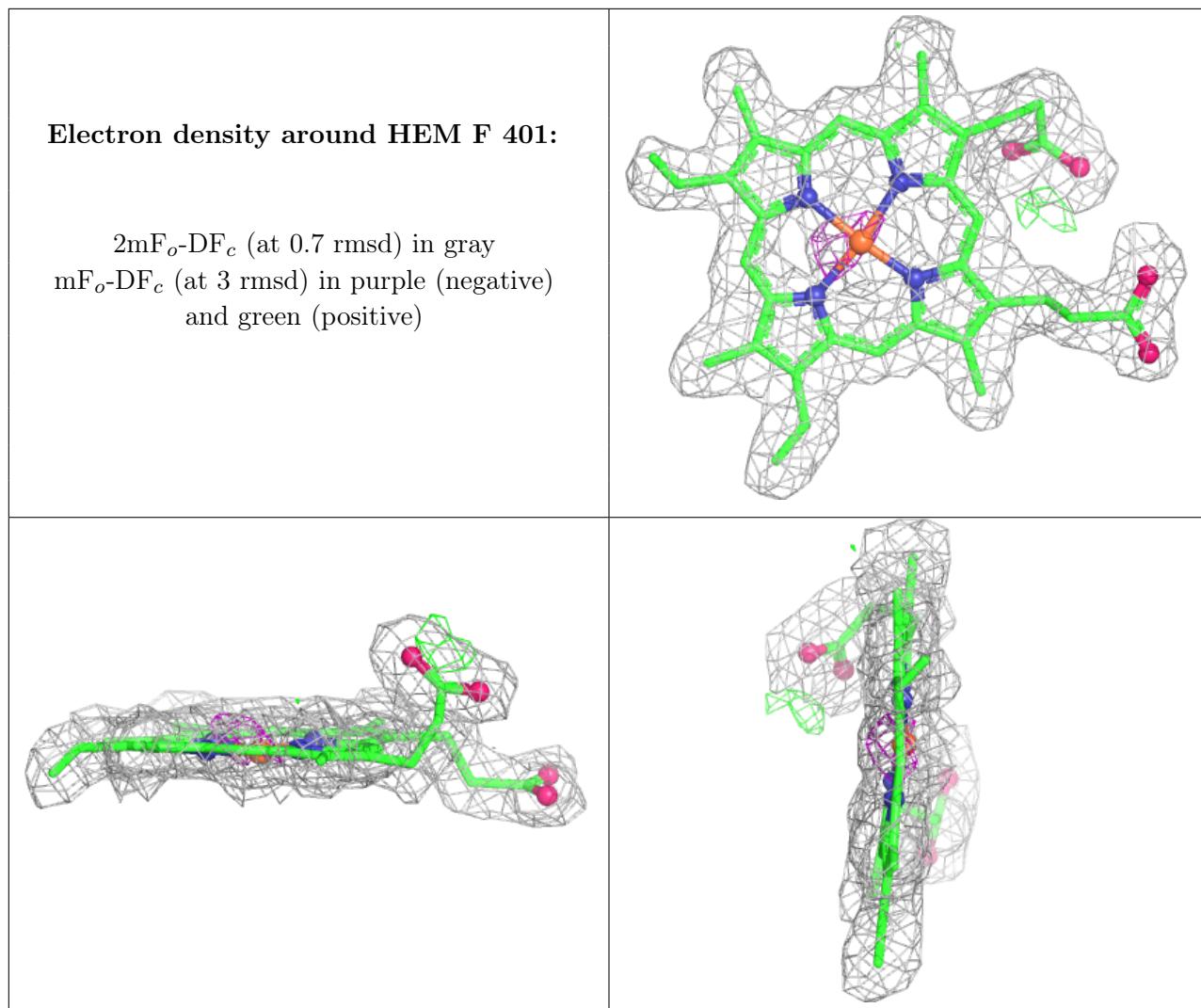
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	E	401	43/43	0.89	0.21	18,23,29,37	0
3	MG	A	402	1/1	0.96	0.16	25,25,25,25	0

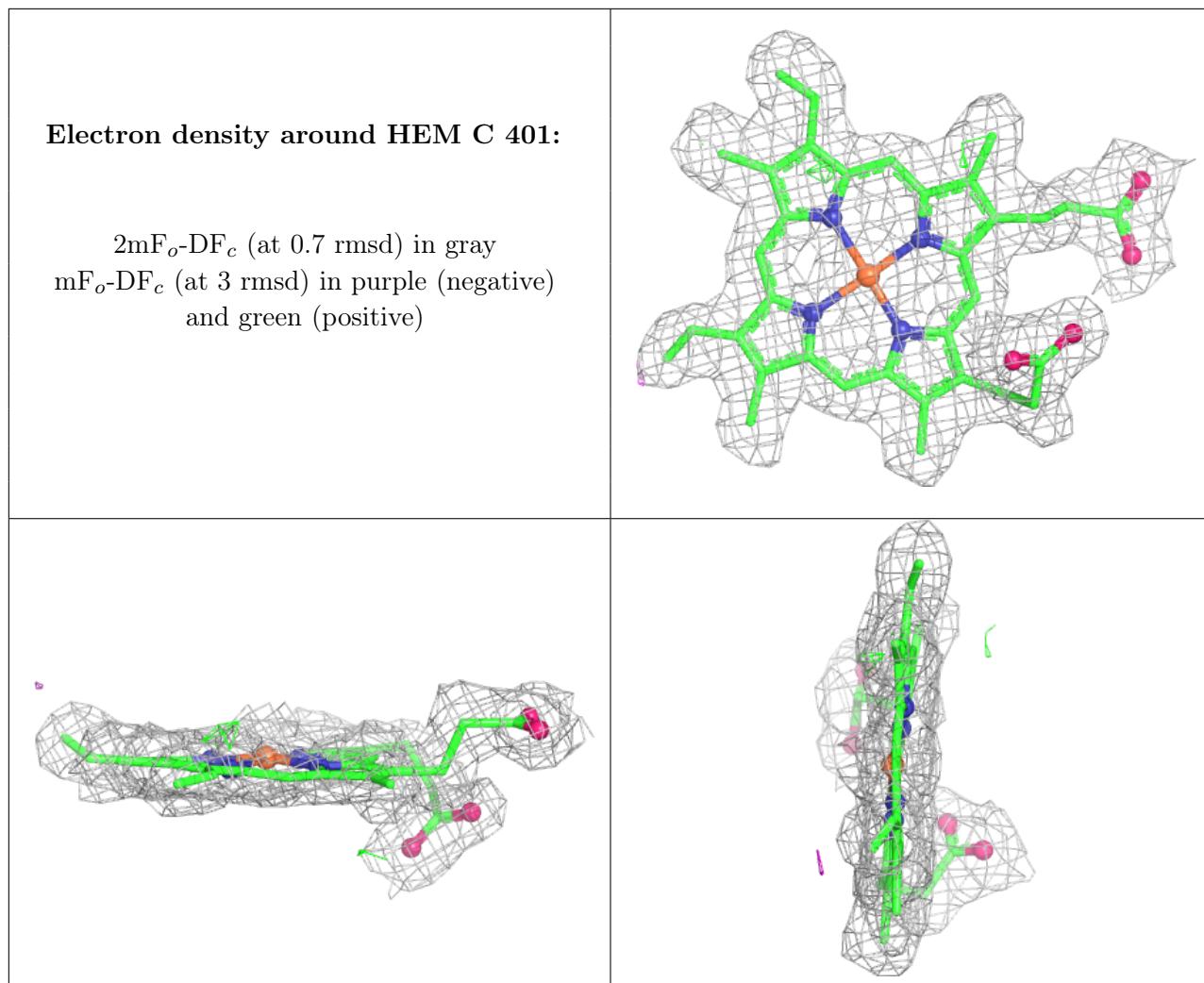
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

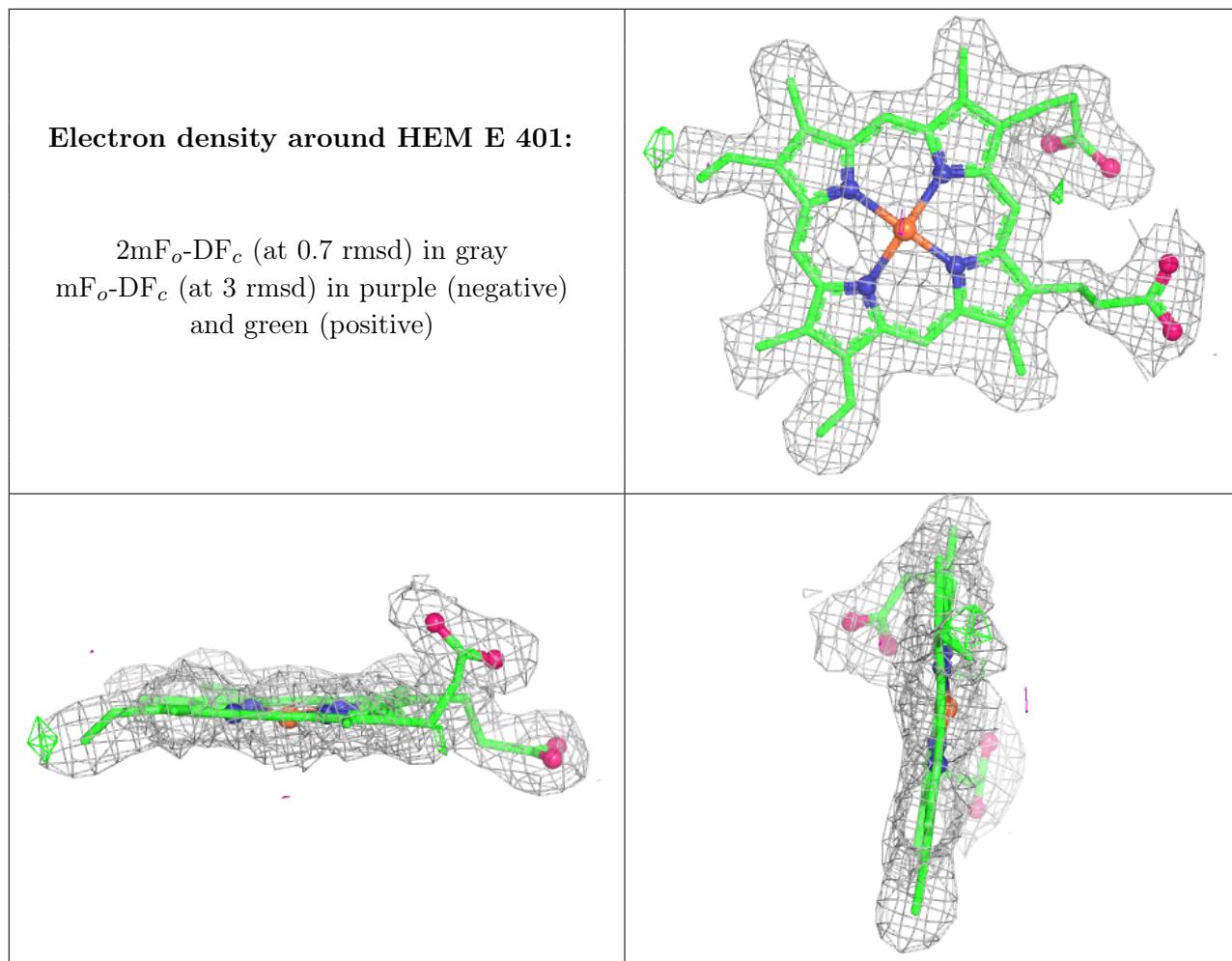












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.