



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:51 AM UTC

PDB ID : 9G6B / pdb_00009g6b
Title : cbb3-2 NOH complex
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Deposited on : 2024-07-18
Resolution : 2.90 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

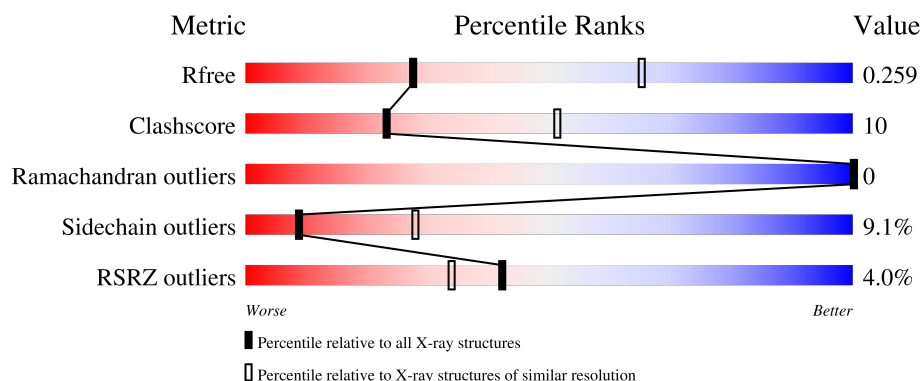
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	475	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>..</div> </div> </div>
2	B	203	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>11%</div> </div> </div>
3	C	166	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6571 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	1	0
			3717	2475	603	614	25			

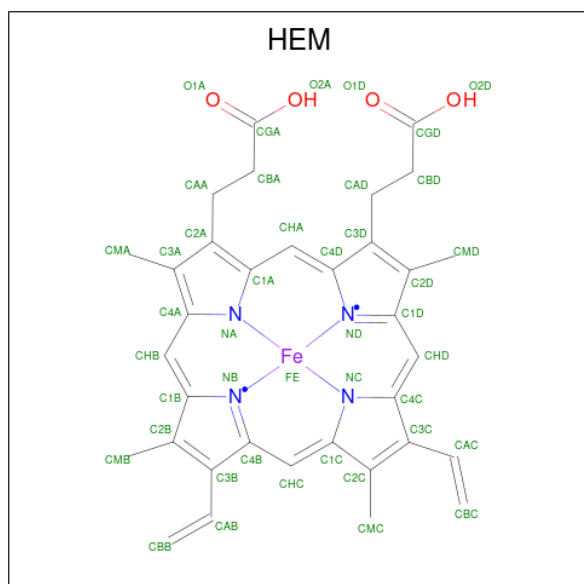
- Molecule 2 is a protein called Cbb3-type cytochrome c oxidase subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1423	896	253	265	9			

- Molecule 3 is a protein called FixH family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	S	0	0	0
			1274	802	230	240	2			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

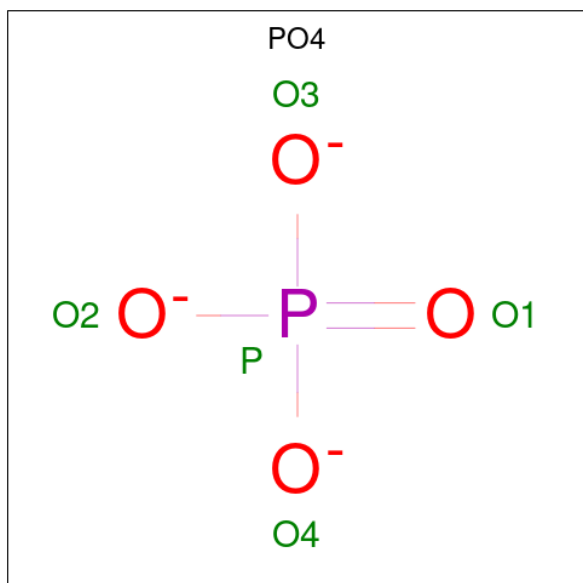
- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu		
			1	1	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca		
			2	2	0	0

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

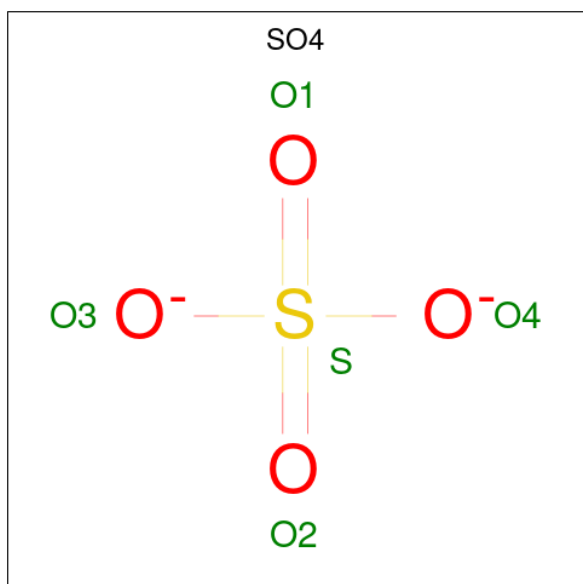


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P		
			5	4	1	0	0
7	A	1	Total	O	P		
			5	4	1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

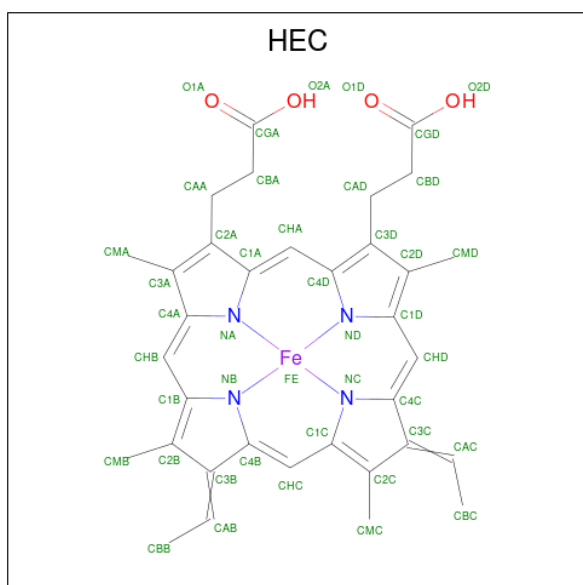
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

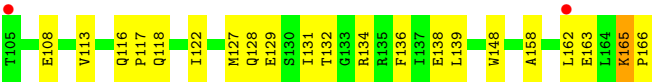
- Molecule 10 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	B	1	Total	O	0	0
			1	1		
11	C	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.00Å 84.19Å 191.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.90 48.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.37-2.90) 96.3 (48.37-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.220 , 0.259 0.221 , 0.259	Depositor DCC
R_{free} test set	1286 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6571	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: CU, HEC, HEM, SO4, CA, NA, PO4

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	0.32	0/3843	0.51	2/5247 (0.0%)
2	B	0.21	0/1458	0.43	1/1974 (0.1%)
3	C	0.20	0/1294	0.46	0/1750
All	All	0.28	0/6595	0.49	3/8971 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ASP	CB-CA-C	5.57	121.51	110.42
2	B	39	VAL	N-CA-C	-5.41	107.09	111.91
1	A	468	TYR	CB-CA-C	5.30	120.48	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3717	0	3695	95	0
2	B	1423	0	1386	34	0
3	C	1274	0	1283	25	0
4	A	86	0	60	5	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
7	A	10	0	0	0	0
8	A	1	0	0	0	0
9	A	5	0	0	0	0
10	B	43	0	30	6	0
11	A	5	0	0	0	0
11	B	1	0	0	0	0
11	C	3	0	0	0	0
All	All	6571	0	6454	134	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 10.

All (134) 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:208:HIS:CE1	1:A:258:HIS:HE1	1.87	0.92
1:A:208:HIS:O	1:A:208:HIS:CD2	2.25	0.89
1:A:254:TRP:HB2	2:B:24:ILE:HB	1.63	0.80
1:A:208:HIS:ND1	1:A:258:HIS:HE1	1.82	0.76
1:A:254:TRP:CD2	2:B:24:ILE:HG21	2.21	0.74
1:A:208:HIS:CD2	1:A:208:HIS:C	2.68	0.72
1:A:208:HIS:CE1	1:A:258:HIS:CE1	2.75	0.68
3:C:118:GLN:HB2	3:C:122:ILE:HG13	1.76	0.68
1:A:467:GLN:HA	1:A:467:GLN:OE1	1.95	0.67
1:A:254:TRP:CB	2:B:24:ILE:HB	2.27	0.65
1:A:254:TRP:HB2	2:B:24:ILE:CB	2.27	0.65
1:A:254:TRP:CG	2:B:24:ILE:CG2	2.80	0.64
1:A:254:TRP:CD2	2:B:24:ILE:CG2	2.81	0.64
2:B:33:LEU:H	2:B:33:LEU:HD13	1.64	0.63
1:A:263:THR:HG22	2:B:72:MET:HG2	1.81	0.62
1:A:298:ALA:HB1	1:A:301:LYS:HD2	1.81	0.61
1:A:352:LEU:HB3	1:A:393:THR:HG22	1.82	0.61
1:A:387:TRP:O	1:A:391:ILE:HG12	2.01	0.61
2:B:44:GLU:OE2	3:C:64:LYS:NZ	2.33	0.61
3:C:66:ALA:HB2	3:C:148:TRP:HB2	1.83	0.60
3:C:83:LEU:HA	3:C:127:MET:H	1.66	0.60
1:A:270:GLN:HB2	1:A:331:LYS:HE3	1.84	0.60
1:A:281:LEU:HD13	1:A:326:PRO:HG2	1.86	0.58
1:A:167:ALA:O	1:A:171:VAL:HG12	2.04	0.57
2:B:149:ASP:OD1	2:B:151:LYS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:HB3	1:A:95:LEU:HB2	1.86	0.56
1:A:348:HIS:HA	1:A:351:ALA:HB3	1.86	0.56
1:A:18:PHE:CZ	1:A:100:PHE:HA	2.42	0.55
1:A:159:TYR:HB3	1:A:162:ASN:ND2	2.22	0.54
2:B:43:VAL:HG11	2:B:198:ALA:HB1	1.90	0.54
1:A:374:GLU:CD	1:A:374:GLU:H	2.16	0.54
1:A:195:ALA:HB2	2:B:96:HIS:NE2	2.23	0.54
1:A:260:LEU:HD13	1:A:265:LEU:HD11	1.90	0.54
1:A:464:LYS:HG3	1:A:470:THR:HG23	1.89	0.53
1:A:316:ALA:HB2	3:C:19:VAL:HG13	1.91	0.53
3:C:165:LYS:HG2	3:C:166:PRO:HA	1.91	0.53
1:A:465:SER:O	1:A:465:SER:OG	2.20	0.52
3:C:11:TYR:N	3:C:11:TYR:CD1	2.78	0.52
1:A:171:VAL:HG11	1:A:213:PHE:CG	2.45	0.52
1:A:347:VAL:HG22	4:A:501:HEM:C2D	2.44	0.52
1:A:77:THR:HG21	1:A:222:MET:SD	2.50	0.52
1:A:160:VAL:HG21	1:A:241:SER:HB3	1.92	0.52
1:A:302:LEU:HB3	1:A:309:ARG:HG3	1.92	0.52
1:A:377:HIS:CE1	1:A:458:ARG:HG2	2.46	0.51
1:A:159:TYR:HB3	1:A:162:ASN:HD22	1.75	0.51
1:A:195:ALA:HB2	2:B:96:HIS:CE1	2.45	0.51
1:A:254:TRP:CG	2:B:24:ILE:HG21	2.46	0.51
3:C:10:TRP:CE3	3:C:10:TRP:HA	2.46	0.51
2:B:138:PRO:HD3	10:B:301:HEC:HBC2	1.93	0.51
1:A:254:TRP:CE3	2:B:24:ILE:HG21	2.46	0.51
1:A:343:THR:O	1:A:347:VAL:HG23	2.10	0.51
4:A:502:HEM:HBB2	4:A:502:HEM:HMB2	1.93	0.50
1:A:464:LYS:CG	1:A:470:THR:HG23	2.42	0.50
2:B:124:HIS:HE1	10:B:301:HEC:C1A	2.25	0.50
3:C:100:ASN:HB2	3:C:138:GLU:HB3	1.92	0.50
1:A:253:ILE:HG23	1:A:253:ILE:O	2.12	0.50
2:B:33:LEU:H	2:B:33:LEU:CD1	2.23	0.49
1:A:208:HIS:O	1:A:208:HIS:HD2	1.88	0.49
1:A:274:MET:CG	1:A:330:ILE:HA	2.42	0.49
1:A:385:HIS:CE1	1:A:452:MET:HB2	2.47	0.49
1:A:186:SER:OG	1:A:187:LEU:N	2.44	0.49
1:A:389:ALA:O	1:A:393:THR:HG23	2.13	0.48
1:A:414:ILE:HG22	1:A:420:LEU:HD23	1.94	0.48
3:C:74:ARG:NH2	3:C:163:GLU:HB2	2.27	0.48
2:B:147:THR:HA	2:B:183:THR:HA	1.95	0.48
1:A:117:GLY:HA3	2:B:62:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:HA	4:A:501:HEM:HBB2	1.95	0.48
1:A:17:GLN:HB3	1:A:100:PHE:CE1	2.49	0.48
2:B:137:MET:HB2	10:B:301:HEC:C1D	2.44	0.48
1:A:289:ILE:O	1:A:293:MET:HG2	2.14	0.48
10:B:301:HEC:HMB3	10:B:301:HEC:HBB3	1.95	0.48
1:A:27:ILE:HD11	1:A:453:ALA:HB2	1.96	0.47
1:A:129:TRP:CG	1:A:130:PRO:HD3	2.48	0.47
2:B:33:LEU:HD22	2:B:34:PHE:CD1	2.49	0.47
2:B:75:PRO:HG3	3:C:49:TYR:CD2	2.49	0.47
2:B:113:GLY:HA2	2:B:193:GLN:HA	1.96	0.47
1:A:302:LEU:HD12	3:C:15:TRP:HB3	1.95	0.47
2:B:30:ILE:HD12	2:B:30:ILE:HA	1.69	0.47
1:A:54:PHE:CZ	1:A:58:ARG:HG3	2.50	0.47
1:A:253:ILE:HG22	2:B:24:ILE:HG13	1.97	0.47
1:A:295:LEU:HD21	1:A:308:LEU:HD21	1.96	0.47
1:A:254:TRP:CD1	1:A:254:TRP:O	2.68	0.47
1:A:306:PRO:HB2	1:A:382:ILE:HG22	1.96	0.46
1:A:5:ILE:HG12	1:A:91:PHE:O	2.15	0.46
1:A:373:ARG:HG3	1:A:463:ALA:HB2	1.96	0.46
3:C:97:LEU:HD13	3:C:139:LEU:HD11	1.97	0.46
2:B:177:ASP:OD1	2:B:177:ASP:N	2.43	0.46
1:A:46:ASN:CG	2:B:138:PRO:HB3	2.41	0.46
1:A:103:TRP:O	1:A:107:ILE:HG12	2.16	0.46
1:A:139:TRP:HD1	1:A:173:ALA:HB2	1.81	0.46
1:A:239:ARG:H	1:A:239:ARG:HE	1.63	0.46
1:A:342:TRP:HE1	1:A:401:TRP:CD1	2.33	0.46
1:A:400:MET:HE3	1:A:438:ARG:HB2	1.97	0.46
3:C:132:THR:HG21	3:C:158:ALA:HB2	1.97	0.45
1:A:323:PHE:CE1	3:C:27:VAL:HA	2.52	0.45
1:A:64:ALA:O	1:A:68:ALA:HB3	2.17	0.45
3:C:78:ASN:ND2	3:C:85:GLU:OE2	2.48	0.45
2:B:140:TYR:CE1	10:B:301:HEC:HBB2	2.53	0.44
1:A:129:TRP:CD1	1:A:130:PRO:HD3	2.52	0.44
1:A:288:MET:HE2	1:A:288:MET:HB3	1.94	0.44
1:A:220:LEU:HD13	1:A:244:HIS:CE1	2.52	0.44
3:C:104:PRO:HB3	3:C:136:PHE:CZ	2.52	0.44
3:C:128:GLN:OE1	3:C:128:GLN:N	2.45	0.44
2:B:138:PRO:HD3	10:B:301:HEC:CBC	2.48	0.43
1:A:171:VAL:HG11	1:A:213:PHE:CD1	2.53	0.43
1:A:248:LEU:O	1:A:252:TYR:HB2	2.18	0.43
1:A:278:ILE:O	1:A:281:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:LEU:HD12	3:C:131:ILE:HD13	2.00	0.43
3:C:116:GLN:NE2	3:C:117:PRO:HD2	2.33	0.43
1:A:65:VAL:HG21	4:A:502:HEM:C4C	2.54	0.43
1:A:51:TRP:CD1	1:A:51:TRP:H	2.35	0.43
1:A:127:LEU:HD13	1:A:131:ILE:HG21	2.00	0.43
1:A:153:ARG:HE	1:A:156:LYS:HA	1.83	0.43
3:C:11:TYR:N	3:C:11:TYR:HD1	2.16	0.43
3:C:104:PRO:HG3	3:C:134:ARG:HG2	2.01	0.43
1:A:295:LEU:HD13	1:A:299:TRP:HA	2.01	0.42
1:A:314:SER:HB3	1:A:357:MET:HB2	2.02	0.42
1:A:12:TYR:O	1:A:16:ARG:HG2	2.19	0.42
1:A:328:MET:HE1	1:A:346:HIS:CG	2.55	0.42
1:A:347:VAL:HG22	4:A:501:HEM:C3D	2.55	0.42
1:A:175:LEU:HD22	1:A:206:TYR:HA	2.02	0.41
1:A:215:LEU:HD22	1:A:355:VAL:HG21	2.01	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.86	0.41
2:B:80:THR:HG21	3:C:45:VAL:HG21	2.02	0.41
3:C:12:THR:HG23	3:C:13:GLN:HE21	1.84	0.41
1:A:328:MET:HE3	1:A:328:MET:HB2	1.81	0.41
1:A:212:GLY:HA2	1:A:252:TYR:CE2	2.55	0.41
1:A:254:TRP:CG	2:B:24:ILE:HB	2.55	0.41
1:A:274:MET:HB3	1:A:274:MET:HE3	1.73	0.41
2:B:176:ARG:HH21	2:B:180:ARG:CZ	2.34	0.41
1:A:11:ASN:N	1:A:89:ARG:HD2	2.36	0.41
2:B:30:ILE:HG22	2:B:31:VAL:HG23	2.03	0.41
1:A:309:ARG:HD3	3:C:15:TRP:CZ2	2.57	0.40
1:A:208:HIS:C	1:A:208:HIS:HD2	2.27	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	466/475 (98%)	459 (98%)	7 (2%)	0	100	100
2	B	178/203 (88%)	174 (98%)	4 (2%)	0	100	100
3	C	157/166 (95%)	152 (97%)	5 (3%)	0	100	100
All	All	801/844 (95%)	785 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	379/383 (99%)	349 (92%)	30 (8%)	11	34
2	B	149/170 (88%)	137 (92%)	12 (8%)	11	33
3	C	134/141 (95%)	116 (87%)	18 (13%)	4	12
All	All	662/694 (95%)	602 (91%)	60 (9%)	9	28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	32	LEU
1	A	44	SER
1	A	51	TRP
1	A	58	ARG
1	A	119	THR
1	A	123	GLU
1	A	160	VAL
1	A	168	PHE
1	A	177	ILE
1	A	186	SER
1	A	229	LYS
1	A	235	VAL
1	A	239	ARG
1	A	242	ILE

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Mol	Chain	Res	Type
1	A	253	ILE
1	A	274	MET
1	A	280	LEU
1	A	281	LEU
1	A	295	LEU
1	A	304	THR
1	A	342	TRP
1	A	357	MET
1	A	379	VAL
1	A	383	ASN
1	A	412	ARG
1	A	426	GLU
1	A	429	GLU
1	A	464	LYS
1	A	467	GLN
2	B	24	ILE
2	B	30	ILE
2	B	33	LEU
2	B	39	VAL
2	B	40	ASN
2	B	43	VAL
2	B	46	MET
2	B	79	GLU
2	B	131	VAL
2	B	161	ARG
2	B	177	ASP
2	B	203	ARG
3	C	10	TRP
3	C	11	TYR
3	C	24	LEU
3	C	31	VAL
3	C	43	THR
3	C	47	ASP
3	C	54	LYS
3	C	70	GLU
3	C	72	GLN
3	C	75	ILE
3	C	85	GLU
3	C	89	SER
3	C	102	LEU
3	C	108	GLU
3	C	113	VAL

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Mol	Chain	Res	Type
3	C	129	GLU
3	C	162	LEU
3	C	165	LYS

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

Mol	Chain	Res	Type
2	B	29	GLN
3	C	13	GLN
3	C	58	GLN
3	C	96	GLN
3	C	106	GLN
3	C	116	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 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
4	HEM	A	501	6,1	50,50,50	1.62	7 (14%)	67,82,82	1.28	8 (11%)
7	PO4	A	505	-	4,4,4	0.95	0	6,6,6	0.38	0
7	PO4	A	509	-	4,4,4	0.99	0	6,6,6	0.47	0
4	HEM	A	502	6,1	50,50,50	1.44	9 (18%)	67,82,82	1.22	7 (10%)
10	HEC	B	301	2	46,50,50	1.85	5 (10%)	58,82,82	1.73	4 (6%)
9	SO4	A	508	6	4,4,4	0.26	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	501	6,1	-	6/14/54/54	-
10	HEC	B	301	2	-	8/14/54/54	-
4	HEM	A	502	6,1	-	0/14/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	HEC	CAC-C3C	6.39	1.55	1.35
10	B	301	HEC	CAB-C3B	6.19	1.55	1.35
10	B	301	HEC	C3D-C2D	5.60	1.53	1.38
4	A	501	HEM	FE-NB	5.53	2.11	1.94
4	A	501	HEM	FE-NC	5.03	2.11	1.95
4	A	502	HEM	FE-NA	4.05	2.08	1.95
4	A	501	HEM	FE-ND	3.61	2.06	1.94
4	A	502	HEM	FE-NB	3.55	2.05	1.94
4	A	502	HEM	CAB-C3B	3.00	1.55	1.47
4	A	502	HEM	CAC-C3C	2.91	1.55	1.47
4	A	501	HEM	CAC-C3C	2.90	1.55	1.47
4	A	502	HEM	FE-NC	2.77	2.04	1.95
4	A	501	HEM	CAB-C3B	2.73	1.54	1.47
4	A	502	HEM	FE-ND	2.29	2.02	1.94
10	B	301	HEC	CMB-C2B	2.25	1.55	1.50
4	A	501	HEM	CMC-C2C	2.25	1.55	1.50
4	A	501	HEM	FE-NA	2.17	2.02	1.95
4	A	502	HEM	CMB-C2B	2.15	1.55	1.50
4	A	502	HEM	CMA-C3A	2.11	1.55	1.50
4	A	502	HEM	CMC-C2C	2.10	1.55	1.50
10	B	301	HEC	CMC-C2C	2.06	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	301	HEC	CBB-CAB-C3B	-7.84	111.77	127.43
10	B	301	HEC	CBC-CAC-C3C	-6.38	114.68	127.43
10	B	301	HEC	C4D-ND-C1D	3.38	111.33	105.82
4	A	501	HEM	C2A-C1A-NA	-2.63	107.23	110.15
4	A	501	HEM	C4D-ND-C1D	2.55	108.22	105.21
4	A	502	HEM	C4D-ND-C1D	2.54	108.22	105.21
4	A	501	HEM	CAD-CBD-CGD	-2.50	107.03	113.67
4	A	502	HEM	C2A-C1A-NA	-2.49	107.39	110.15
4	A	501	HEM	C3B-C4B-NB	-2.49	107.68	109.47
4	A	502	HEM	C3D-C4D-ND	-2.48	107.45	110.17
4	A	502	HEM	CHD-C1D-ND	2.41	127.02	124.42
4	A	501	HEM	C3D-C4D-ND	-2.40	107.54	110.17
4	A	502	HEM	O1A-CGA-CBA	-2.37	115.59	123.09
10	B	301	HEC	C2A-C1A-NA	-2.36	108.04	110.32
4	A	502	HEM	C1B-NB-C4B	2.35	107.98	105.21
4	A	501	HEM	C3B-C2B-C1B	2.17	108.04	106.41
4	A	501	HEM	C1B-NB-C4B	2.17	107.78	105.21
4	A	502	HEM	O2A-CGA-CBA	2.11	120.66	114.00
4	A	501	HEM	CAA-CBA-CGA	-2.03	108.29	113.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

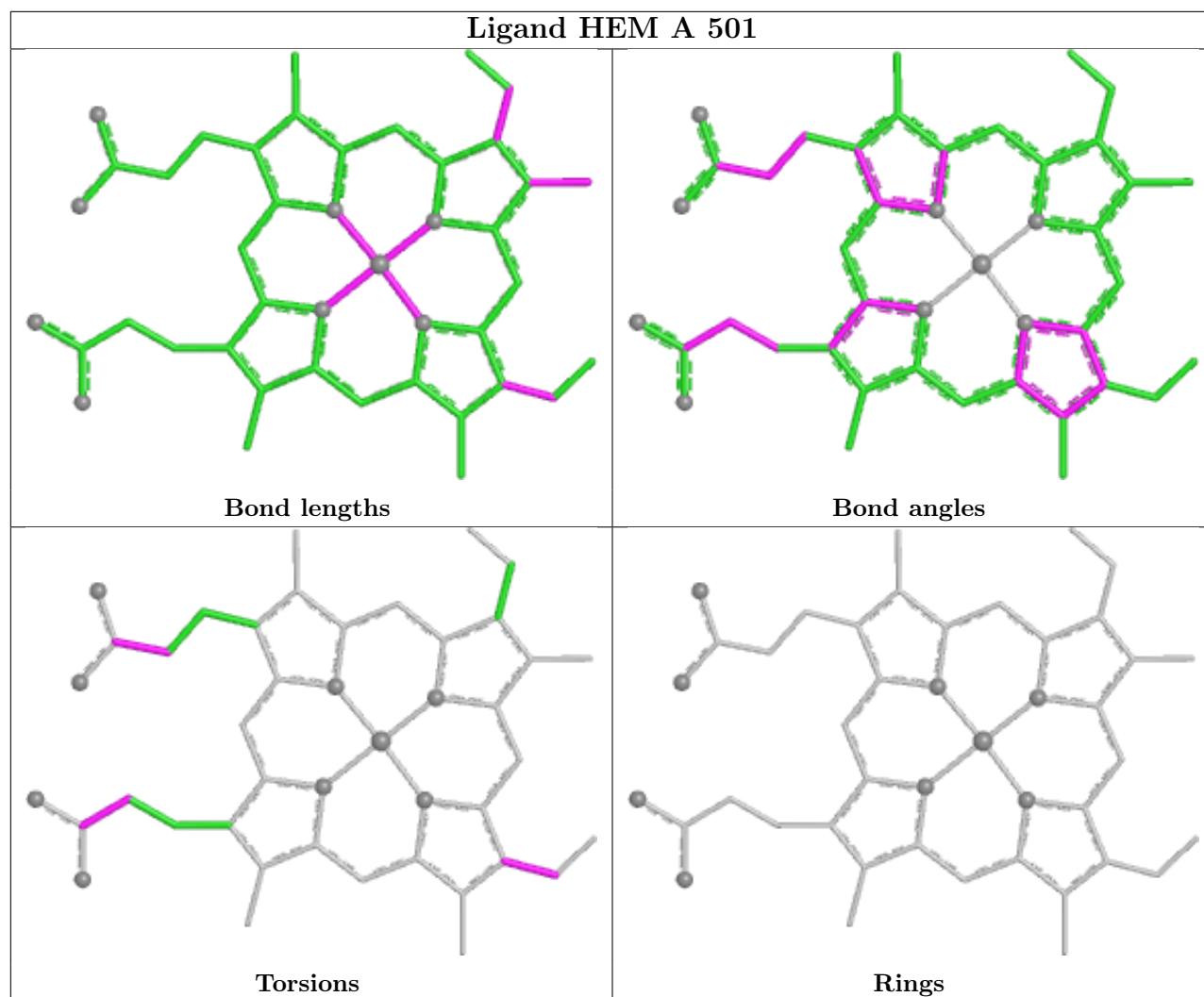
Mol	Chain	Res	Type	Atoms
4	A	501	HEM	C2B-C3B-CAB-CBB
4	A	501	HEM	C4B-C3B-CAB-CBB
10	B	301	HEC	C2B-C3B-CAB-CBB
10	B	301	HEC	C4B-C3B-CAB-CBB
10	B	301	HEC	C2C-C3C-CAC-CBC
10	B	301	HEC	C4C-C3C-CAC-CBC
4	A	501	HEM	CAA-CBA-CGA-O1A
10	B	301	HEC	CAD-CBD-CGD-O1D
4	A	501	HEM	CAA-CBA-CGA-O2A
10	B	301	HEC	CAD-CBD-CGD-O2D
4	A	501	HEM	CAD-CBD-CGD-O2D
4	A	501	HEM	CAD-CBD-CGD-O1D
10	B	301	HEC	CAA-CBA-CGA-O1A
10	B	301	HEC	CAA-CBA-CGA-O2A

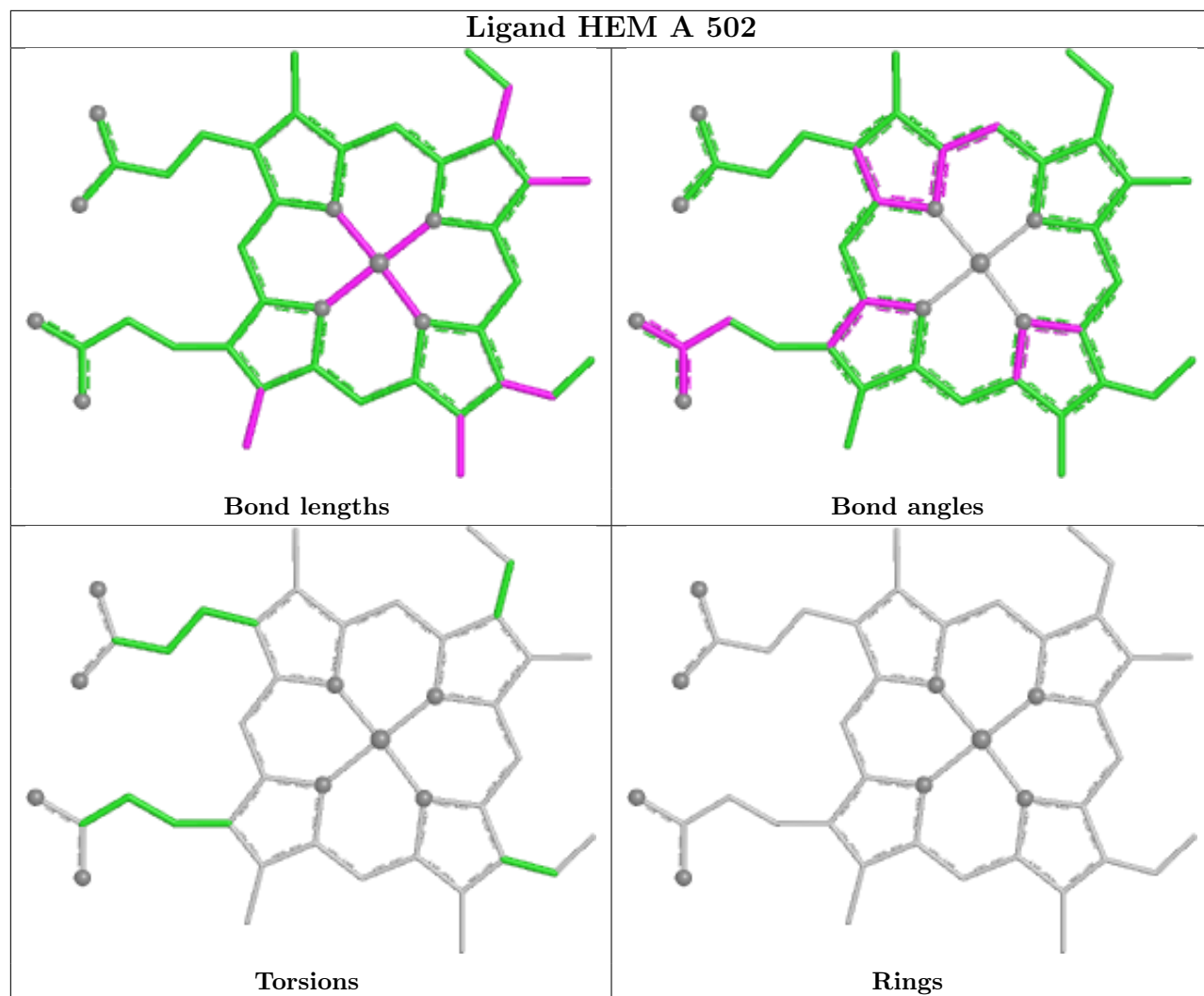
There are no ring outliers.

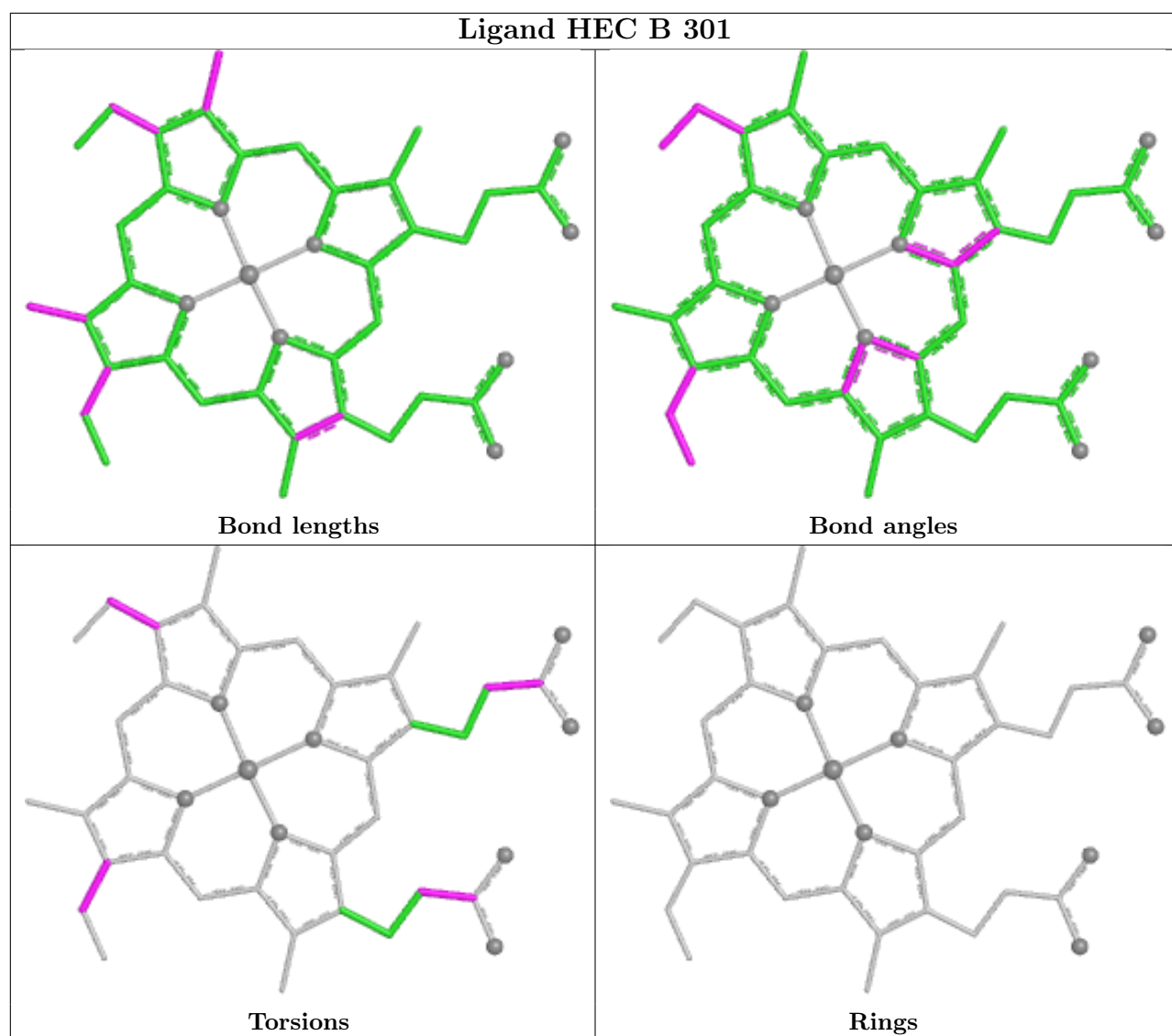
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HEM	3	0
4	A	502	HEM	2	0
10	B	301	HEC	6	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	467/475 (98%)	0.12	16 (3%)	48 39	52, 73, 108, 177	1 (0%)
2	B	180/203 (88%)	0.06	12 (6%)	24 19	54, 71, 171, 186	0
3	C	159/166 (95%)	0.15	4 (2%)	58 48	57, 87, 113, 126	0
All	All	806/844 (95%)	0.11	32 (3%)	42 34	52, 75, 115, 186	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	30	ILE	5.2
3	C	45	VAL	5.0
2	B	39	VAL	4.4
3	C	44	LEU	4.2
1	A	256	GLY	3.9
1	A	157[A]	HIS	3.9
2	B	24	ILE	3.9
1	A	48	ASP	3.8
1	A	8	THR	3.4
1	A	6	SER	3.4
1	A	470	THR	3.1
1	A	7	GLU	3.0
3	C	162	LEU	2.9
2	B	29	GLN	2.7
2	B	26	GLY	2.6
1	A	5	ILE	2.6
2	B	28	THR	2.5
2	B	27	LEU	2.4
1	A	238	TYR	2.3
2	B	33	LEU	2.3
1	A	47	LEU	2.2
1	A	9	ALA	2.2
2	B	25	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	THR	2.2
1	A	152	LYS	2.1
2	B	35	PHE	2.1
2	B	86	TYR	2.1
1	A	229	LYS	2.1
3	C	105	THR	2.1
2	B	31	VAL	2.0
1	A	255	ALA	2.0
1	A	236	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

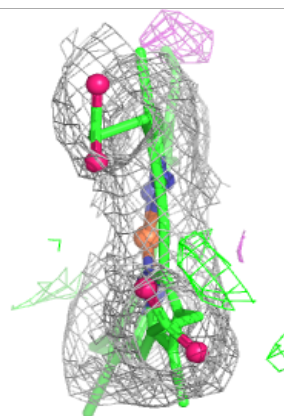
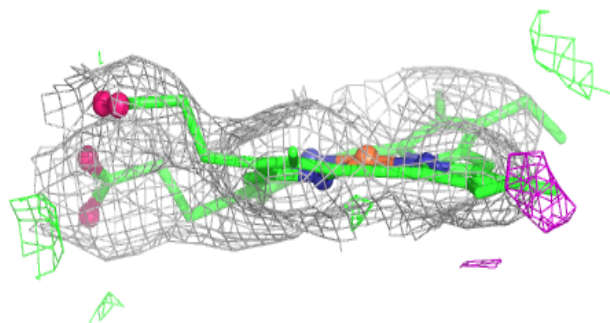
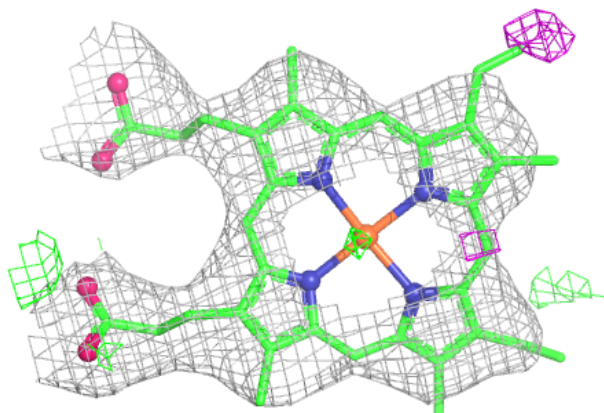
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SO4	A	508	5/5	0.67	0.23	130,130,130,131	0
7	PO4	A	509	5/5	0.76	0.10	113,115,117,127	0
6	CA	A	504	1/1	0.83	0.12	97,97,97,97	0
8	NA	A	507	1/1	0.88	0.14	71,71,71,71	0
7	PO4	A	505	5/5	0.89	0.10	74,84,93,94	0
6	CA	A	506	1/1	0.89	0.08	62,62,62,62	0
4	HEM	A	501	43/43	0.97	0.10	63,71,78,81	0
4	HEM	A	502	43/43	0.97	0.10	57,67,74,76	0
10	HEC	B	301	43/43	0.98	0.10	55,67,73,77	0
5	CU	A	503	1/1	0.99	0.03	72,72,72,72	0

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

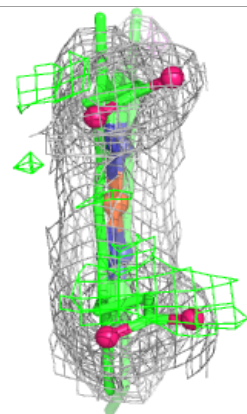
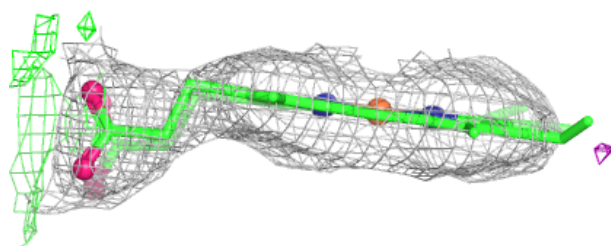
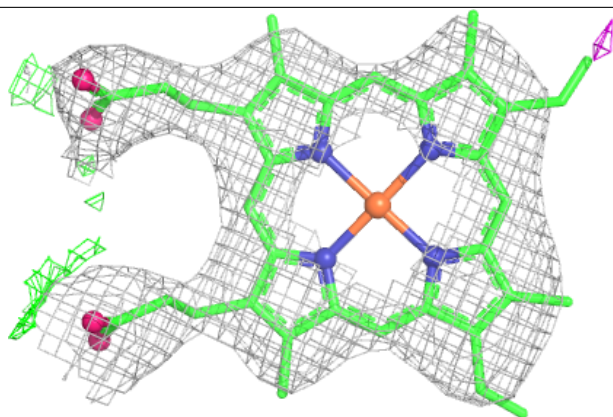
Electron density around HEM A 501:

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



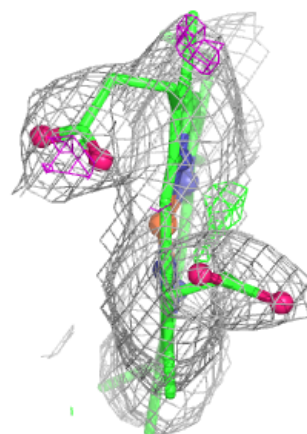
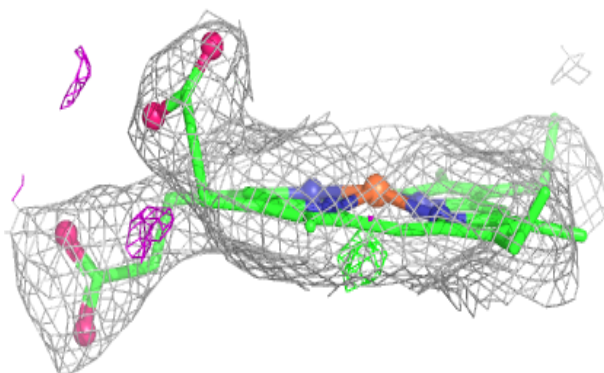
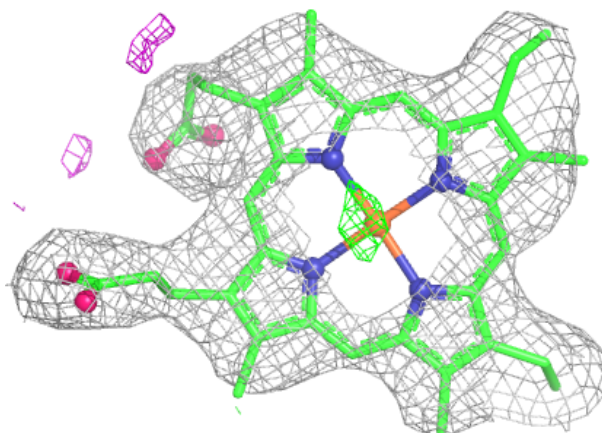
Electron density around HEM A 502:

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



Electron density around HEC B 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.