



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:28 PM UTC

PDB ID : 7ZIC / pdb_00007zic
Title : Crystal structure of CYP125 from Mycobacterium tuberculosis in complex with an inhibitor
Authors : Snee, M.; Levy, C.; Kavanagh, M.
Deposited on : 2022-04-07
Resolution : 1.90 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

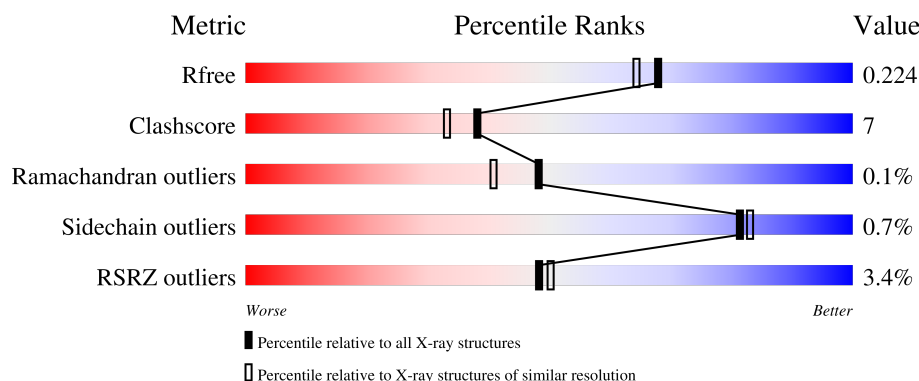
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	418	5% 89% 10% .
1	B	418	5% 82% 15% .
1	C	418	5% 84% 13% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20882 atoms, of which 9926 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 Steroid C26-monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	412	Total	C	H	N	O	S	16	32	0
			6812	2185	3396	588	624	19			
1	B	404	Total	C	H	N	O	S	0	15	0
			6383	2065	3140	558	604	16			
1	C	410	Total	C	H	N	O	S	0	18	0
			6536	2107	3217	575	618	19			

There are 6 discrepancies between the modelled and reference sequences:

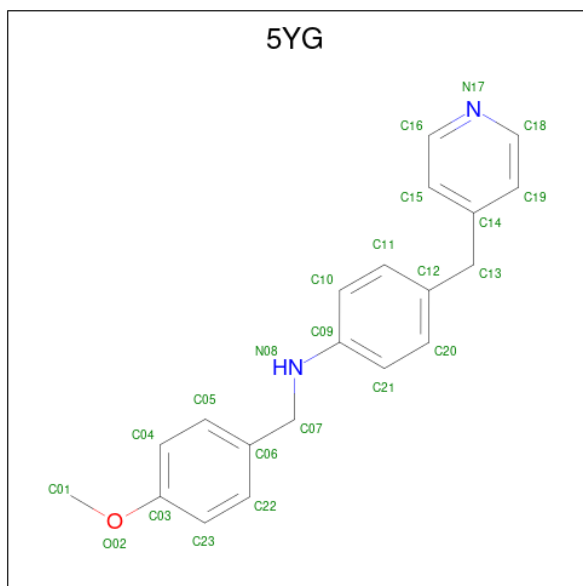
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	-	expression tag	UNP P9WPP1
A	17	GLY	-	expression tag	UNP P9WPP1
B	16	ASN	-	expression tag	UNP P9WPP1
B	17	GLY	-	expression tag	UNP P9WPP1
C	16	ASN	-	expression tag	UNP P9WPP1
C	17	GLY	-	expression tag	UNP P9WPP1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	3	3		

- Molecule 3 is {N}-[(4-methoxyphenyl)methyl]-4-(pyridin-4-ylmethyl)aniline (CCD ID: 5YG) (formula: C₂₀H₂₀N₂O) (labeled as "Ligand of Interest" by depositor).



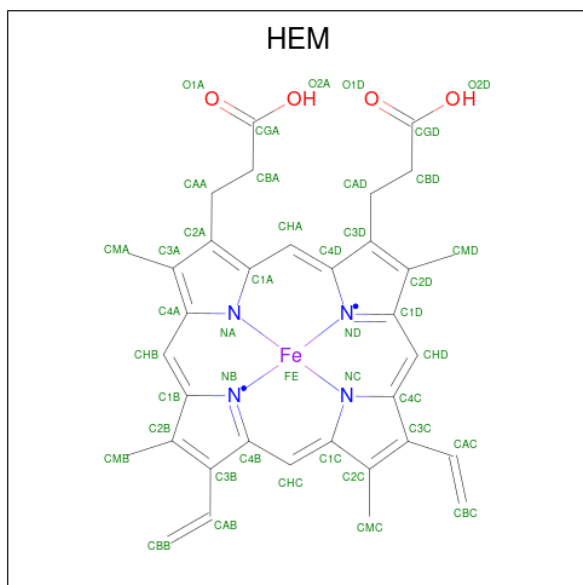
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	1
			86	40	40	4	2		
3	B	1	Total	C	H	N	O	0	0
			43	20	20	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			43	20	20	2	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

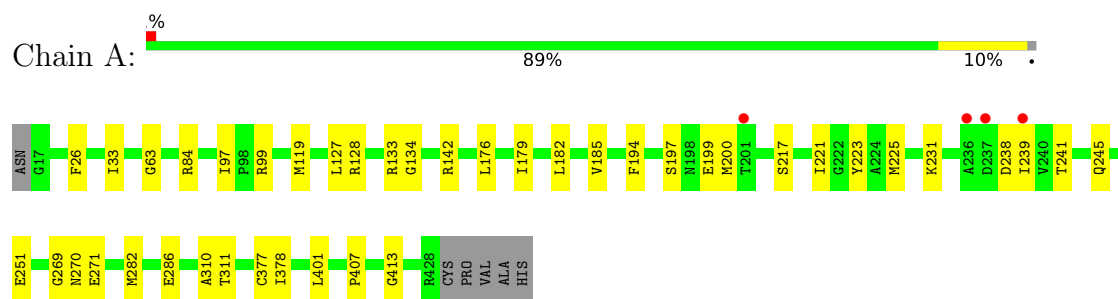
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	323	Total	O	0	0
			323	323		
7	B	186	Total	O	0	0
			186	186		
7	C	160	Total	O	0	0
			160	160		

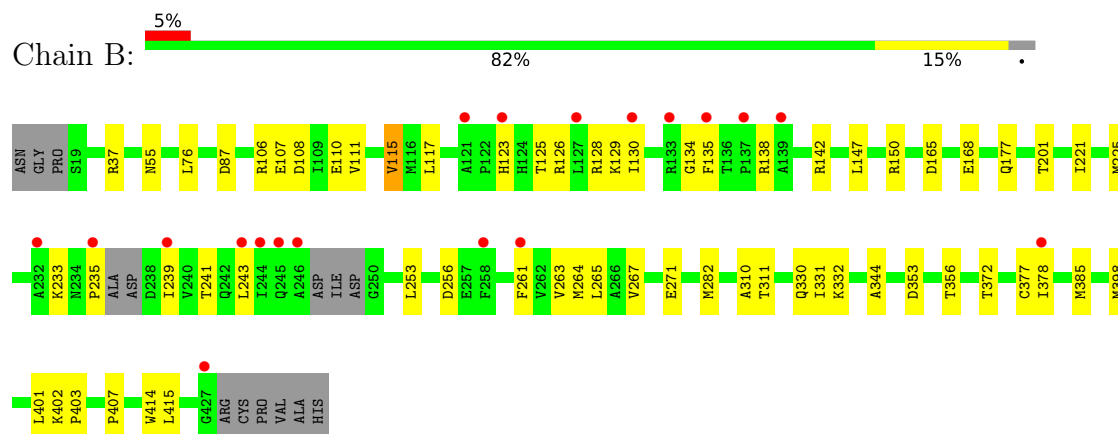
3 Residue-property plots

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.

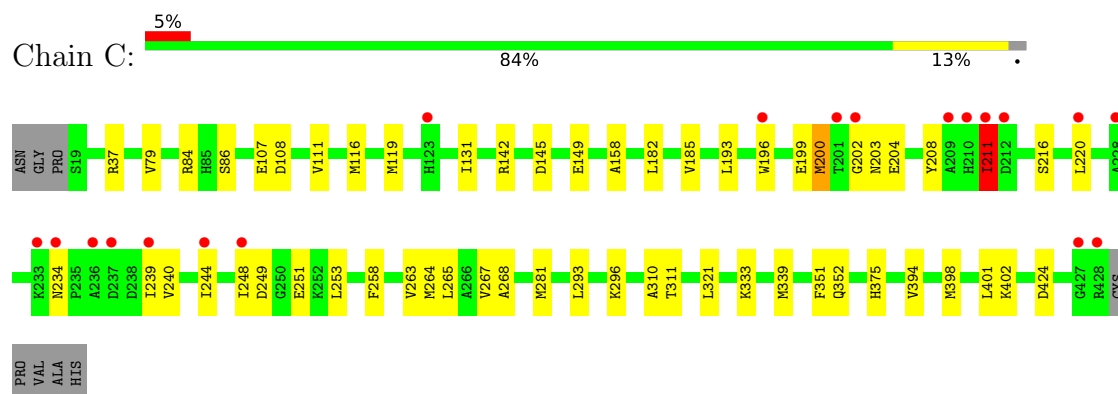
• Molecule 1: Steroid C26-monooxygenase



• Molecule 1: Steroid C26-monooxygenase



• Molecule 1: Steroid C26-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.23Å 68.68Å 144.47Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	72.06 – 1.90 72.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (72.06-1.90) 92.7 (72.06-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.224 0.189 , 0.224	Depositor DCC
R_{free} test set	5021 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20882	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: HEM, SO4, GOL, 5YG, CL

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	0.36	0/3589	0.51	0/4861
1	B	0.25	0/3373	0.39	0/4574
1	C	0.23	0/3453	0.39	0/4681
All	All	0.29	0/10415	0.44	0/14116

There are no bond length outliers.

There are no bond angle outliers.

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	3416	3396	3376	32	1
1	B	3243	3140	3131	51	1
1	C	3319	3217	3202	47	1
2	A	6	3	8	0	0
3	A	46	40	0	1	0
3	B	23	20	0	0	0
3	C	23	20	0	0	0
4	A	43	30	30	5	0
4	B	43	30	30	3	0
4	C	43	30	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	20	0	0	0	0
5	B	25	0	0	1	0
5	C	35	0	0	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	323	0	0	4	2
7	B	186	0	0	1	0
7	C	160	0	0	1	0
All	All	10956	9926	9807	136	3

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 7.

All (136) 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:182:LEU:HG	1:A:239:ILE:HD13	1.57	0.85
1:B:134:GLY:HA3	1:B:239:ILE:HD12	1.64	0.78
1:B:356[A]:THR:HG23	7:B:652:HOH:O	1.84	0.76
1:B:402:LYS:HE3	1:B:403:PRO:HD2	1.68	0.75
1:B:261:PHE:O	1:B:265:LEU:HD23	1.85	0.75
1:B:263:VAL:O	1:B:267[B]:VAL:HG12	1.86	0.75
1:C:234:ASN:O	1:C:234:ASN:ND2	2.27	0.67
4:C:502:HEM:HMC1	4:C:502:HEM:HBC2	1.76	0.67
1:C:158:ALA:HB3	1:C:398[B]:MET:HE1	1.78	0.66
4:B:502:HEM:HBC2	4:B:502:HEM:HMC2	1.79	0.65
1:C:248:ILE:HG23	1:C:249:ASP:OD1	1.97	0.64
1:C:185:VAL:HG21	1:C:193:LEU:HD22	1.80	0.64
1:A:176[B]:LEU:HD22	1:A:194[B]:PHE:CD1	2.33	0.63
1:C:281[B]:MET:HE2	1:C:401:LEU:HD21	1.81	0.63
1:B:134:GLY:CA	1:B:239:ILE:HD12	2.30	0.62
1:B:330:GLN:O	1:B:332:LYS:NZ	2.28	0.60
1:C:107:GLU:O	1:C:111:VAL:HG13	2.00	0.60
4:C:502:HEM:HBC2	4:C:502:HEM:CMC	2.34	0.58
1:C:239:ILE:HD12	1:C:239:ILE:N	2.20	0.57
4:A:1403:HEM:HMC1	4:A:1403:HEM:HBC2	1.87	0.56
1:C:84:ARG:NH2	5:C:506:SO4:O1	2.38	0.56
1:C:240:VAL:HG13	1:C:258:PHE:CZ	2.40	0.56
1:A:200[A]:MET:HE1	1:A:217:SER:HA	1.86	0.56
1:B:123[A]:HIS:CD2	1:B:126:ARG:HH21	2.24	0.56
1:B:261:PHE:CE1	1:B:265:LEU:HD21	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HG12	1:B:243:LEU:HD11	1.88	0.55
1:B:378:ILE:C	1:B:378:ILE:HD12	2.31	0.55
1:C:199:GLU:HG3	1:C:211[A]:ILE:HG23	1.89	0.54
1:B:37:ARG:HD2	1:C:37:ARG:HD2	1.89	0.54
1:B:201:THR:HB	1:B:271:GLU:OE1	2.08	0.54
1:B:107:GLU:H	1:B:107:GLU:CD	2.16	0.53
1:C:200[A]:MET:HE2	1:C:220:LEU:HD12	1.89	0.53
1:C:204:GLU:OE1	7:C:601:HOH:O	2.19	0.53
1:B:128:ARG:HB3	1:B:129:LYS:HE2	1.90	0.53
1:A:282:MET:HE3	1:A:407:PRO:HG3	1.90	0.52
1:A:99[B]:ARG:HG2	1:A:413:GLY:HA3	1.90	0.52
1:B:115:VAL:HG13	1:B:264[A]:MET:SD	2.49	0.52
1:B:147:LEU:HD12	1:B:385:MET:HE3	1.92	0.52
4:B:502:HEM:HBC2	4:B:502:HEM:CMC	2.39	0.52
1:A:271:GLU:HG3	7:A:1505:HOH:O	2.09	0.51
1:C:200[A]:MET:HE1	1:C:263:VAL:HG13	1.92	0.51
1:B:150:ARG:CD	1:B:177:GLN:HG3	2.42	0.50
4:A:1403:HEM:HBC2	4:A:1403:HEM:CMC	2.42	0.50
1:A:142:ARG:NH1	1:A:142:ARG:HG2	2.26	0.50
1:A:310:ALA:O	1:A:311:THR:C	2.55	0.50
1:B:108:ASP:O	1:B:111:VAL:HG12	2.11	0.50
1:C:281[A]:MET:HE3	1:C:394:VAL:HG11	1.95	0.49
1:A:133[B]:ARG:HH11	1:A:133[B]:ARG:HB2	1.77	0.49
1:B:138:ARG:O	1:B:142:ARG:HB2	2.12	0.49
1:C:251:GLU:HA	1:C:251:GLU:OE1	2.11	0.49
1:B:243:LEU:HB3	1:B:253:LEU:HD12	1.95	0.48
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.77	0.48
1:A:231:LYS:HE2	1:A:238:ASP:OD2	2.13	0.48
1:A:99[B]:ARG:HD2	7:A:1594:HOH:O	2.13	0.47
1:A:97[A]:ILE:HD11	3:A:1402[A]:5YG:C11	2.45	0.47
1:B:115:VAL:HG12	1:B:117:LEU:H	1.80	0.47
1:A:241:THR:O	1:A:245:GLN:HB2	2.15	0.47
1:A:269:GLY:HA2	4:A:1403:HEM:HMC3	1.97	0.47
1:A:377:CYS:HA	4:A:1403:HEM:CHA	2.45	0.47
1:B:310:ALA:O	1:B:311:THR:C	2.59	0.46
1:B:138:ARG:HH12	1:B:142:ARG:NH1	2.13	0.46
1:C:240:VAL:HG13	1:C:258:PHE:CE1	2.50	0.46
1:B:125:THR:O	1:B:129:LYS:HE3	2.16	0.46
1:B:239:ILE:CG1	1:B:243:LEU:HD11	2.46	0.46
1:B:239:ILE:O	1:B:243:LEU:HG	2.16	0.46
1:A:134[A]:GLY:O	1:A:239:ILE:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:LYS:NZ	1:C:424:ASP:OD2	2.47	0.45
1:C:182:LEU:O	1:C:239:ILE:HD13	2.15	0.45
1:C:108:ASP:O	1:C:111:VAL:HG22	2.17	0.45
1:C:265:LEU:CD1	4:C:502:HEM:HBC1	2.47	0.45
1:C:196:TRP:HE3	1:C:220:LEU:HD23	1.82	0.45
1:C:208:TYR:HB3	1:C:211[A]:ILE:HD12	1.98	0.45
1:C:239:ILE:HD12	1:C:239:ILE:H	1.82	0.45
1:C:394:VAL:HG22	1:C:398[A]:MET:HE3	1.99	0.45
1:C:116[A]:MET:HA	1:C:119:MET:SD	2.56	0.45
1:A:179[B]:ILE:HD11	1:A:269:GLY:HA3	1.98	0.44
1:B:372:THR:HG23	5:B:505:SO4:O4	2.17	0.44
1:B:135[A]:PHE:CD1	1:B:378:ILE:HD13	2.52	0.44
1:C:310:ALA:O	1:C:311:THR:C	2.60	0.44
1:C:351:PHE:O	1:C:352:GLN:HB2	2.17	0.44
1:B:106:ARG:O	1:B:110:GLU:HG3	2.18	0.44
1:B:331:ILE:N	1:B:331:ILE:HD13	2.33	0.44
1:B:125:THR:O	1:B:129:LYS:CE	2.66	0.44
1:B:353:ASP:O	1:B:356[A]:THR:OG1	2.35	0.44
1:A:119:MET:SD	1:A:127:LEU:HD12	2.58	0.43
1:C:79:VAL:HG22	1:C:339:MET:HB3	1.99	0.43
1:A:99[B]:ARG:HG3	7:A:1559:HOH:O	2.19	0.43
1:A:251:GLU:OE1	1:A:251:GLU:HA	2.18	0.43
1:B:130:ILE:HG21	1:B:253:LEU:HG	2.01	0.43
1:C:265:LEU:HD11	4:C:502:HEM:HBC1	1.99	0.43
1:C:281[B]:MET:CE	1:C:401:LEU:HD21	2.46	0.43
4:C:502:HEM:CMB	4:C:502:HEM:HBB2	2.49	0.43
1:B:150:ARG:HD2	1:B:177:GLN:HG3	2.00	0.43
1:B:225:MET:HE1	1:B:256:ASP:HA	2.00	0.43
1:C:200[A]:MET:HE3	1:C:267:VAL:CG2	2.48	0.43
1:A:176[A]:LEU:HB3	1:A:194[A]:PHE:CE1	2.54	0.43
1:C:264[A]:MET:SD	4:C:502:HEM:HMD3	2.59	0.43
1:C:264[B]:MET:HE2	4:C:502:HEM:HMD3	2.00	0.43
1:C:375:HIS:HD2	4:C:502:HEM:O1D	2.02	0.43
1:B:128:ARG:NH2	1:B:378:ILE:HG22	2.33	0.42
1:B:165:ASP:OD2	1:B:168:GLU:HG3	2.19	0.42
1:C:131:ILE:CD1	1:C:253:LEU:HD21	2.49	0.42
1:B:233:LYS:C	1:B:235:PRO:HD2	2.44	0.42
1:C:202:GLY:O	1:C:208:TYR:HB2	2.20	0.42
1:A:128:ARG:CZ	1:A:378[A]:ILE:HG22	2.49	0.42
1:C:145:ASP:O	1:C:149:GLU:HG2	2.19	0.42
1:C:264[B]:MET:HE3	1:C:268:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:HG21	1:B:253:LEU:CD2	2.50	0.42
1:C:203:ASN:OD1	1:C:211[A]:ILE:HG22	2.20	0.42
1:A:377:CYS:HB2	4:A:1403:HEM:C1A	2.55	0.42
1:B:377:CYS:HA	4:B:502:HEM:CHA	2.50	0.42
1:C:199:GLU:O	1:C:211[A]:ILE:CG2	2.69	0.41
1:C:244:ILE:HG13	1:C:244:ILE:O	2.20	0.41
1:B:125:THR:O	1:B:129:LYS:HG2	2.20	0.41
1:B:221:ILE:HG13	1:B:263:VAL:HG21	2.01	0.41
1:A:197[A]:SER:OG	1:A:270:ASN:ND2	2.53	0.41
1:A:84[A]:ARG:HG3	7:A:1589:HOH:O	2.20	0.41
1:B:76:LEU:HA	1:B:344:ALA:HB1	2.02	0.41
1:B:235:PRO:HB3	1:B:241:THR:HG21	2.02	0.41
1:A:63:GLY:HA3	1:A:99[A]:ARG:HD2	2.02	0.41
1:B:414:TRP:CZ3	1:B:415[A]:LEU:HG	2.56	0.41
1:C:131:ILE:HD13	1:C:253:LEU:HD21	2.03	0.41
1:A:221:ILE:O	1:A:225:MET:HG3	2.22	0.40
1:A:26:PHE:CZ	1:A:33:ILE:HD13	2.57	0.40
1:B:282:MET:HE3	1:B:407:PRO:HG3	2.03	0.40
1:C:199:GLU:O	1:C:211[A]:ILE:HG23	2.21	0.40
1:C:321:LEU:O	1:C:333:LYS:HD2	2.22	0.40
1:C:293:LEU:HA	1:C:296:LYS:NZ	2.37	0.40
1:C:199:GLU:HG2	1:C:216:SER:OG	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1734:HOH:O	7:A:1734:HOH:O[2_556]	1.98	0.22
1:A:199:GLU:OE1	7:A:1772:HOH:O[4_546]	2.16	0.04
1:B:168:GLU:OE2	1:C:142:ARG:NH2[4_555]	2.16	0.04

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	442/418 (106%)	435 (98%)	7 (2%)	0	100	100
1	B	413/418 (99%)	401 (97%)	12 (3%)	0	100	100
1	C	426/418 (102%)	412 (97%)	12 (3%)	2 (0%)	25	17
All	All	1281/1254 (102%)	1248 (97%)	31 (2%)	2 (0%)	48	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	211[A]	ILE
1	C	211[B]	ILE

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	367/341 (108%)	365 (100%)	2 (0%)	86	88
1	B	341/341 (100%)	337 (99%)	4 (1%)	67	68
1	C	350/341 (103%)	345 (99%)	5 (1%)	62	62
All	All	1058/1023 (103%)	1047 (99%)	11 (1%)	81	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286[A]	GLU
1	A	286[B]	GLU
1	B	55	ASN
1	B	115	VAL
1	B	398[A]	MET
1	B	398[B]	MET
1	C	86	SER
1	C	200[A]	MET
1	C	200[B]	MET

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Mol	Chain	Res	Type
1	C	211[A]	ILE
1	C	211[B]	ILE

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

Mol	Chain	Res	Type
1	A	330	GLN
1	A	352	GLN
1	C	187	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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	B	502	3,1	42,50,50	1.45	6 (14%)	46,82,82	1.43	8 (17%)
5	SO4	A	1406	-	4,4,4	0.28	0	6,6,6	0.13	0
4	HEM	C	502	3,1	42,50,50	1.42	6 (14%)	46,82,82	1.49	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1405	-	4,4,4	0.19	0	6,6,6	0.10	0
5	SO4	B	507	-	4,4,4	0.28	0	6,6,6	0.19	0
5	SO4	A	1404	-	4,4,4	0.24	0	6,6,6	0.17	0
3	5YG	A	1402[A]	4	25,25,25	0.65	1 (4%)	32,32,32	0.72	0
5	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.17	0
5	SO4	C	503	-	4,4,4	0.21	0	6,6,6	0.14	0
5	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	B	506	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	C	509	-	4,4,4	0.26	0	6,6,6	0.12	0
3	5YG	C	501	4	25,25,25	0.62	1 (4%)	32,32,32	0.91	0
5	SO4	C	508	-	4,4,4	0.22	0	6,6,6	0.08	0
3	5YG	A	1402[B]	4	25,25,25	0.68	1 (4%)	32,32,32	0.66	0
5	SO4	A	1407	-	4,4,4	0.30	0	6,6,6	0.14	0
5	SO4	C	505	-	4,4,4	0.21	0	6,6,6	0.21	0
5	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.16	0
4	HEM	A	1403	3,1	42,50,50	1.56	7 (16%)	46,82,82	1.31	6 (13%)
2	GOL	A	1401	-	5,5,5	1.26	1 (20%)	5,5,5	0.96	0
3	5YG	B	501	4	25,25,25	0.62	1 (4%)	32,32,32	0.97	1 (3%)
5	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.06	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
3	5YG	C	501	4	-	3/11/11/11	0/3/3/3
4	HEM	B	502	3,1	-	0/12/54/54	-
3	5YG	A	1402[B]	4	-	4/11/11/11	0/3/3/3
4	HEM	A	1403	3,1	-	2/12/54/54	-
2	GOL	A	1401	-	-	0/4/4/4	-
3	5YG	B	501	4	-	2/11/11/11	0/3/3/3
4	HEM	C	502	3,1	-	3/12/54/54	-
3	5YG	A	1402[A]	4	-	4/11/11/11	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1403	HEM	C3C-C2C	-4.12	1.34	1.40
4	C	502	HEM	C3C-C2C	-4.10	1.34	1.40
4	B	502	HEM	C3C-C2C	-3.83	1.35	1.40
4	A	1403	HEM	C3C-CAC	3.63	1.55	1.47
4	B	502	HEM	C3C-CAC	2.96	1.54	1.47
4	C	502	HEM	C3C-CAC	2.96	1.54	1.47
4	C	502	HEM	CAB-C3B	2.91	1.55	1.47
4	A	1403	HEM	C3C-C4C	2.71	1.45	1.41
3	A	1402[B]	5YG	C09-N08	2.58	1.46	1.38
4	B	502	HEM	C3C-C4C	2.57	1.45	1.41
4	A	1403	HEM	CMD-C2D	2.56	1.56	1.50
3	A	1402[A]	5YG	C09-N08	2.51	1.45	1.38
3	B	501	5YG	C09-N08	2.38	1.45	1.38
4	B	502	HEM	CAB-C3B	2.38	1.53	1.47
4	A	1403	HEM	C1A-NA	2.33	1.41	1.36
4	C	502	HEM	C3C-C4C	2.23	1.44	1.41
3	C	501	5YG	C09-N08	2.23	1.45	1.38
2	A	1401	GOL	O2-C2	-2.22	1.36	1.43
4	A	1403	HEM	C4A-NA	2.22	1.40	1.36
4	A	1403	HEM	CAB-C3B	2.22	1.53	1.47
4	C	502	HEM	CMB-C2B	2.06	1.55	1.50
4	C	502	HEM	CMD-C2D	2.03	1.54	1.50
4	B	502	HEM	CMB-C2B	2.03	1.54	1.50
4	B	502	HEM	CMD-C2D	2.02	1.54	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	HEM	C4D-ND-C1D	3.49	109.34	105.21
4	C	502	HEM	CAA-CBA-CGA	-3.05	105.61	113.83
4	A	1403	HEM	CBA-CAA-C2A	3.02	117.61	112.54
4	B	502	HEM	C4C-CHD-C1D	3.01	126.53	122.56
4	B	502	HEM	C3D-C4D-ND	-2.94	106.94	110.17
4	A	1403	HEM	CMC-C2C-C3C	2.62	129.92	124.68
4	C	502	HEM	CMA-C3A-C4A	-2.62	124.62	128.46
4	C	502	HEM	C1B-NB-C4B	2.49	108.16	105.21
4	A	1403	HEM	C2C-C3C-C4C	2.41	108.58	106.90
4	C	502	HEM	C3B-C2B-C1B	2.39	108.20	106.41
4	C	502	HEM	C4C-CHD-C1D	2.36	125.67	122.56
4	B	502	HEM	CMC-C2C-C3C	2.31	129.29	124.68
4	A	1403	HEM	C3B-C4B-NB	-2.27	107.84	109.47
4	C	502	HEM	C4B-CHC-C1C	2.25	125.52	122.56
4	B	502	HEM	C4B-CHC-C1C	2.22	125.49	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	HEM	C4A-C3A-C2A	2.20	108.53	107.00
4	B	502	HEM	C1B-NB-C4B	2.20	107.82	105.21
3	B	501	5YG	C01-O02-C03	-2.17	112.85	117.50
4	A	1403	HEM	CAA-CBA-CGA	-2.17	108.00	113.83
4	C	502	HEM	C4D-ND-C1D	2.14	107.74	105.21
4	C	502	HEM	CMC-C2C-C3C	2.09	128.85	124.68
4	B	502	HEM	CMA-C3A-C4A	-2.08	125.41	128.46
4	B	502	HEM	C2D-C1D-ND	-2.05	107.54	109.90
4	A	1403	HEM	C1B-NB-C4B	2.01	107.58	105.21

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1403	HEM	C1A-C2A-CAA-CBA
4	A	1403	HEM	C3A-C2A-CAA-CBA
4	C	502	HEM	C3A-C2A-CAA-CBA
3	C	501	5YG	C04-C03-O02-C01
3	C	501	5YG	C23-C03-O02-C01
3	B	501	5YG	C04-C03-O02-C01
3	A	1402[A]	5YG	C04-C03-O02-C01
3	A	1402[A]	5YG	C23-C03-O02-C01
3	B	501	5YG	C23-C03-O02-C01
3	A	1402[B]	5YG	C04-C03-O02-C01
3	A	1402[B]	5YG	C23-C03-O02-C01
3	A	1402[A]	5YG	C21-C09-N08-C07
3	A	1402[A]	5YG	C10-C09-N08-C07
3	A	1402[B]	5YG	C21-C09-N08-C07
4	C	502	HEM	C1A-C2A-CAA-CBA
3	A	1402[B]	5YG	C10-C09-N08-C07
3	C	501	5YG	C10-C09-N08-C07
4	C	502	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

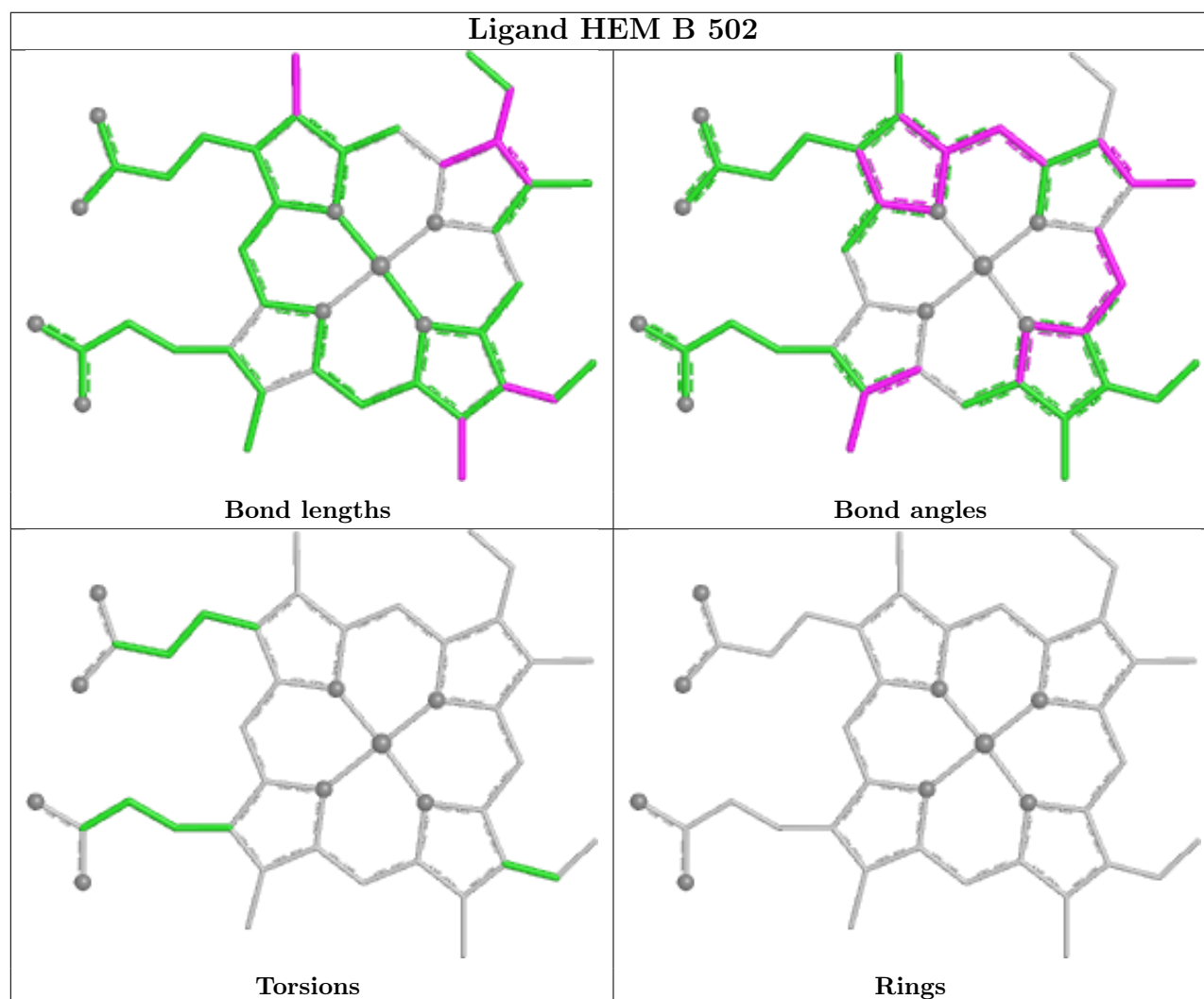
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	HEM	3	0
4	C	502	HEM	8	0
3	A	1402[A]	5YG	1	0
5	C	506	SO4	1	0

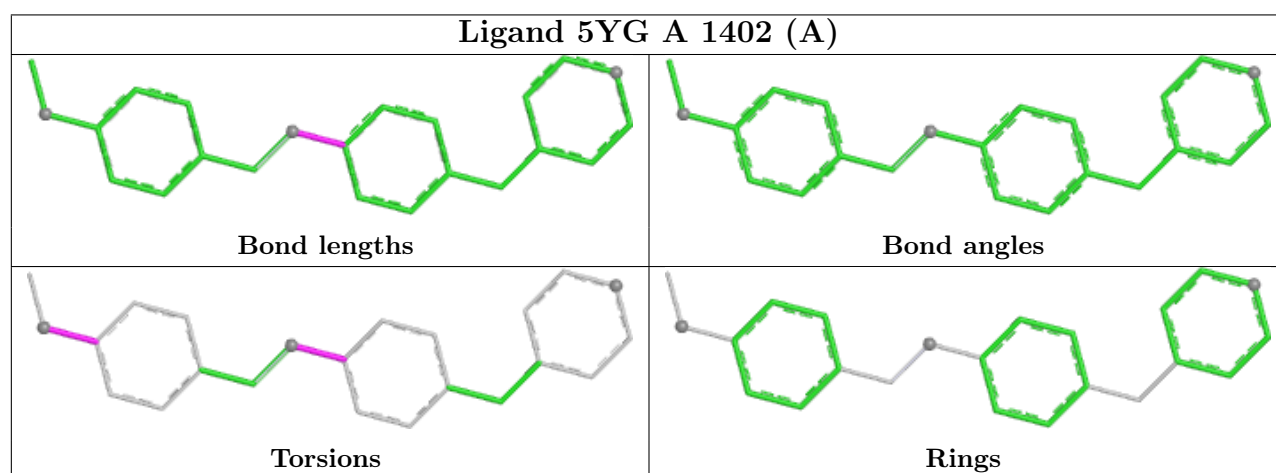
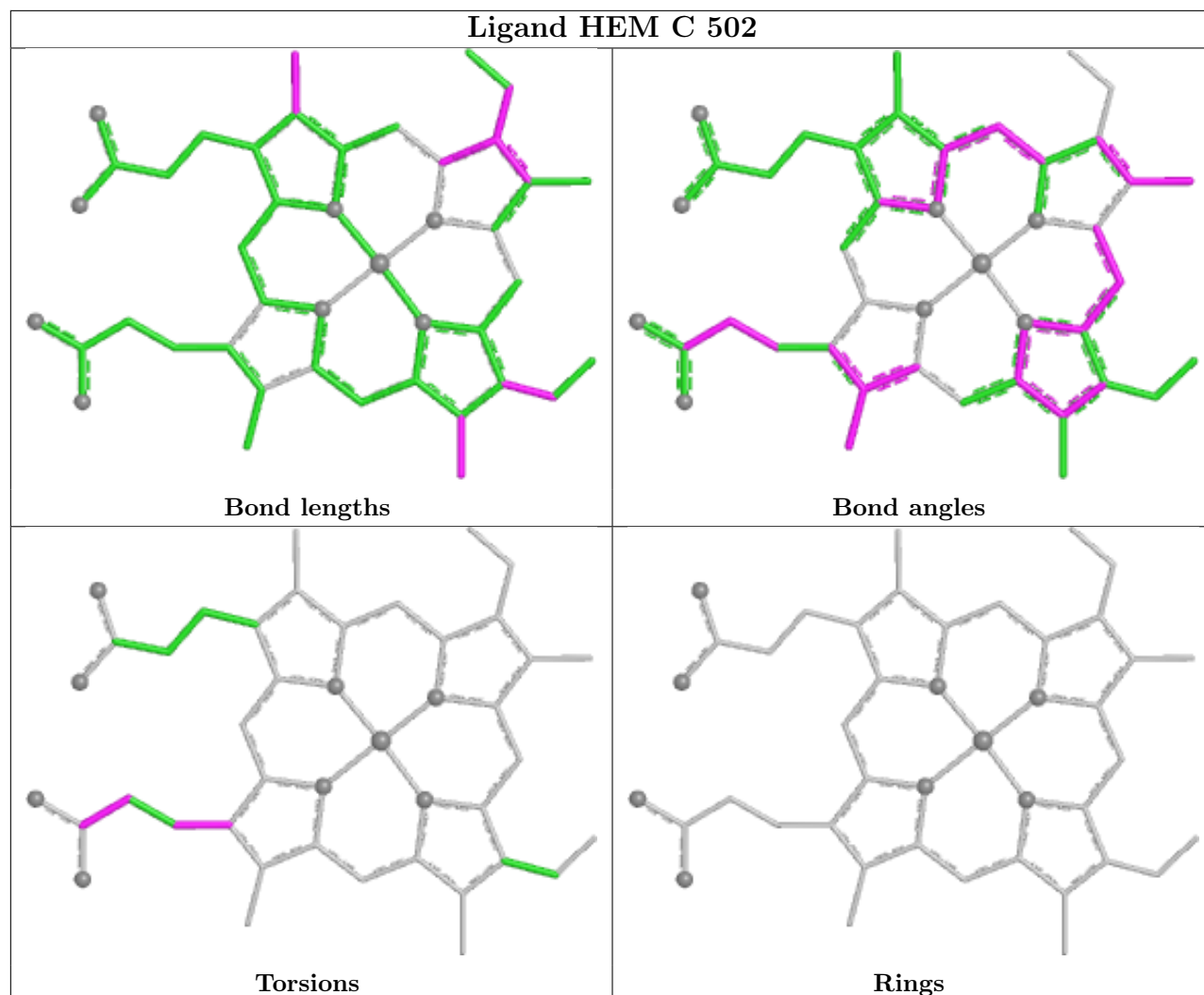
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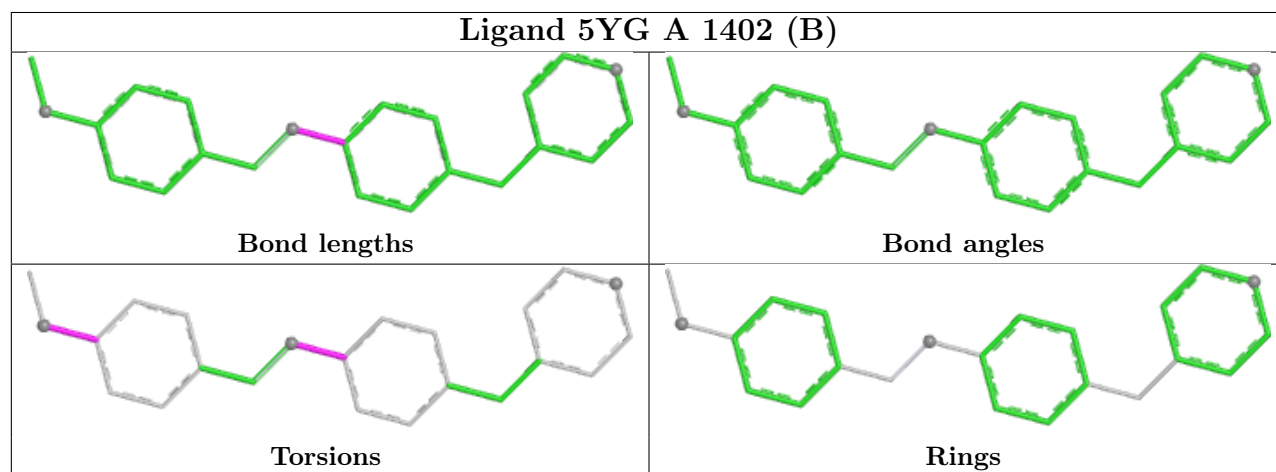
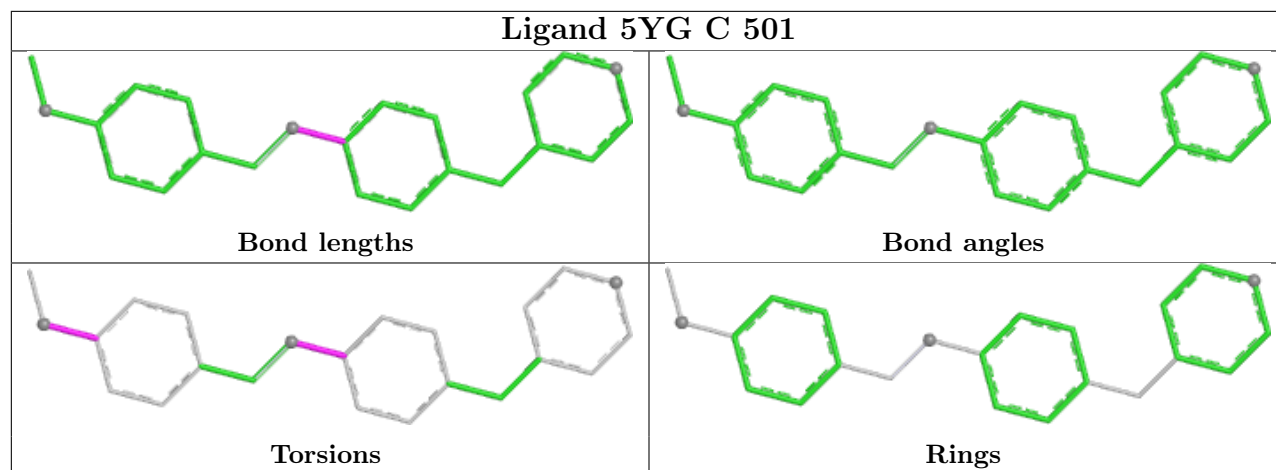
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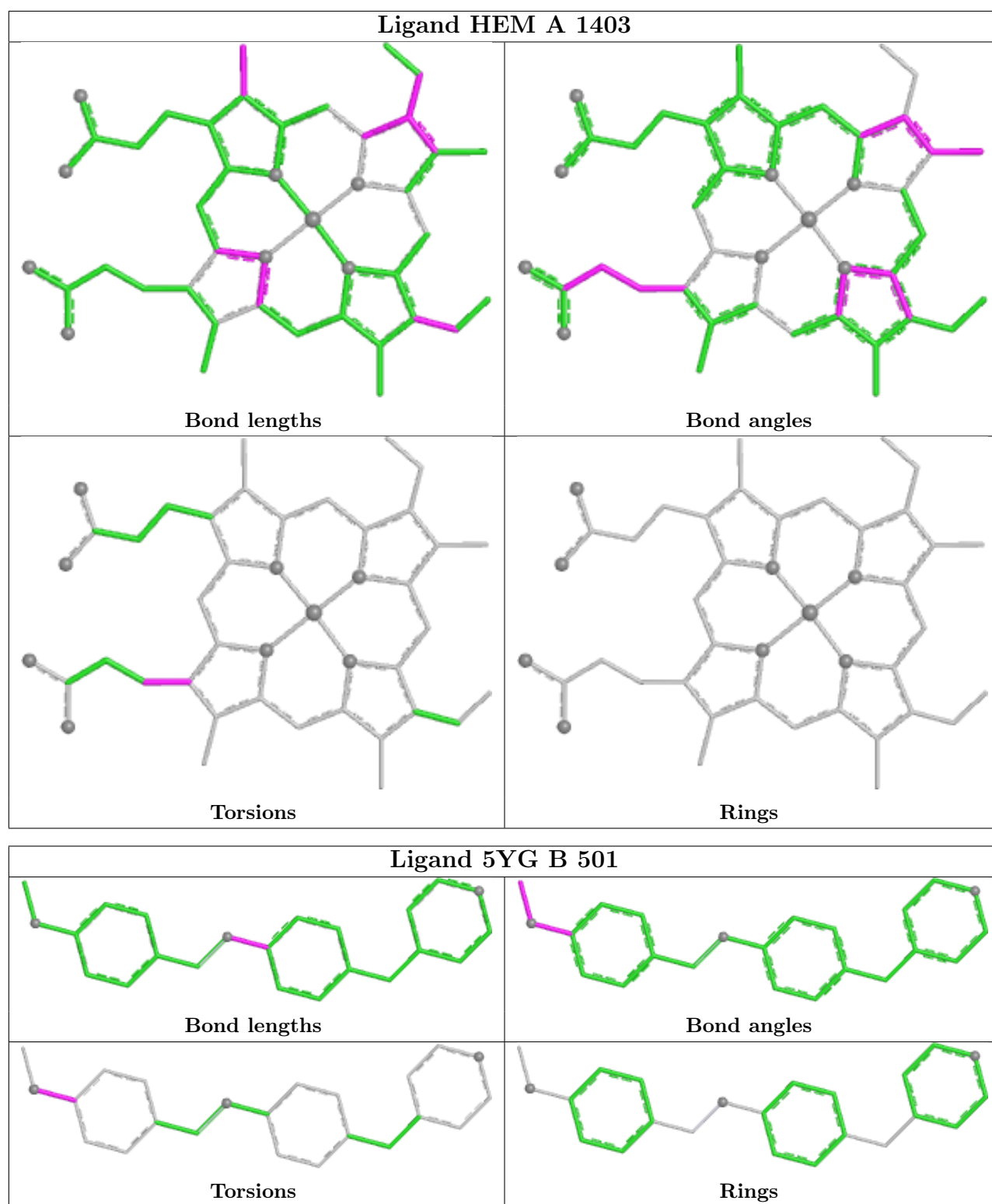
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1403	HEM	5	0
5	B	505	SO4	1	0

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 ⓘ

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	412/418 (98%)	-0.23	4 (0%) 79 81	12, 32, 59, 85	30 (7%)
1	B	404/418 (96%)	0.38	19 (4%) 37 38	20, 52, 87, 101	14 (3%)
1	C	410/418 (98%)	0.36	19 (4%) 38 39	21, 52, 81, 93	17 (4%)
All	All	1226/1254 (97%)	0.17	42 (3%) 48 50	12, 45, 80, 101	61 (4%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135[A]	PHE	6.3
1	C	211[A]	ILE	5.6
1	C	236	ALA	4.2
1	B	133	ARG	4.1
1	B	235	PRO	3.8
1	B	245	GLN	3.6
1	B	139	ALA	3.5
1	A	237	ASP	3.4
1	A	236	ALA	3.3
1	C	428	ARG	3.2
1	C	210[A]	HIS	3.1
1	C	239	ILE	2.9
1	B	123[A]	HIS	2.8
1	C	202	GLY	2.7
1	C	244	ILE	2.6
1	B	246	ALA	2.6
1	C	220	LEU	2.5
1	C	233	LYS	2.5
1	B	427	GLY	2.5
1	B	239	ILE	2.4
1	B	378	ILE	2.4
1	B	127	LEU	2.4
1	B	258	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	137	PRO	2.3
1	B	121	ALA	2.3
1	B	261	PHE	2.3
1	B	130	ILE	2.3
1	C	209[A]	ALA	2.2
1	C	212[A]	ASP	2.2
1	C	237	ASP	2.2
1	A	201	THR	2.2
1	A	239	ILE	2.2
1	B	243	LEU	2.1
1	C	427	GLY	2.1
1	C	123[A]	HIS	2.1
1	B	232	ALA	2.1
1	C	196	TRP	2.1
1	C	248	ILE	2.1
1	C	201	THR	2.1
1	C	228	ALA	2.0
1	B	244	ILE	2.0
1	C	234	ASN	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
5	SO4	B	506	5/5	0.60	0.12	85,90,98,104	0
5	SO4	C	507	5/5	0.66	0.12	66,68,71,81	5
5	SO4	C	506	5/5	0.70	0.11	85,91,96,101	5
5	SO4	C	508	5/5	0.73	0.13	67,79,87,88	5

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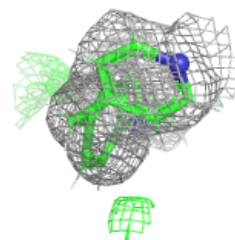
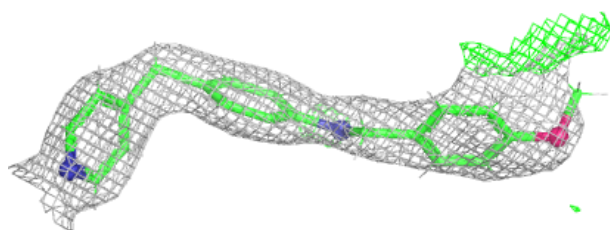
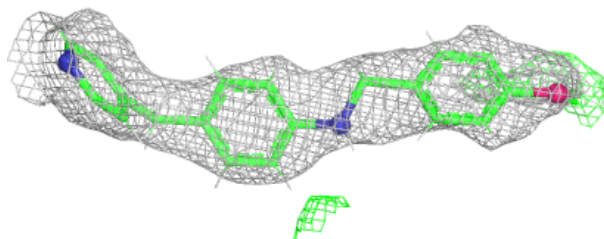
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	1401	6/6	0.77	0.14	43,52,60,68	0
5	SO4	C	509	5/5	0.77	0.12	66,70,78,80	0
5	SO4	C	504	5/5	0.78	0.10	48,51,57,68	5
5	SO4	A	1405	5/5	0.83	0.10	33,40,52,57	5
5	SO4	C	503	5/5	0.84	0.10	55,64,68,72	0
3	5YG	B	501	23/23	0.84	0.14	40,56,81,94	0
5	SO4	B	507	5/5	0.84	0.15	46,57,61,63	0
5	SO4	A	1404	5/5	0.85	0.13	50,53,57,63	5
5	SO4	B	505	5/5	0.86	0.19	48,51,62,63	5
5	SO4	A	1406	5/5	0.87	0.14	45,46,49,49	5
5	SO4	A	1407	5/5	0.88	0.11	47,48,51,63	0
3	5YG	A	1402[A]	23/23	0.88	0.17	21,33,49,51	43
3	5YG	A	1402[B]	23/23	0.88	0.17	21,33,49,52	43
5	SO4	C	505	5/5	0.88	0.09	52,57,62,67	5
3	5YG	C	501	23/23	0.89	0.13	41,58,83,86	0
6	CL	A	1408	1/1	0.89	0.14	65,65,65,65	0
5	SO4	B	504	5/5	0.90	0.09	40,43,49,50	5
5	SO4	B	503	5/5	0.92	0.09	65,67,69,70	5
6	CL	C	510	1/1	0.93	0.12	72,72,72,72	0
4	HEM	B	502	43/43	0.97	0.09	34,45,63,68	0
4	HEM	C	502	43/43	0.97	0.08	37,48,63,64	0
4	HEM	A	1403	43/43	0.98	0.06	17,24,32,40	0

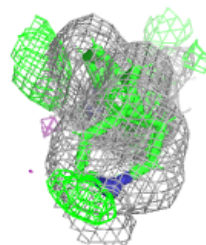
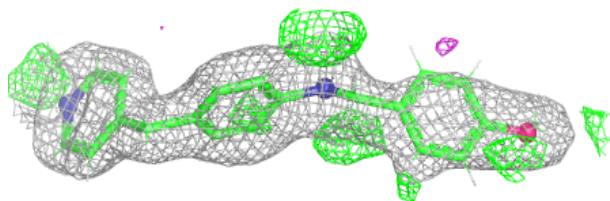
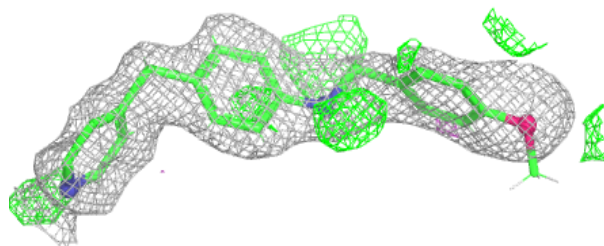
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5YG B 501:

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

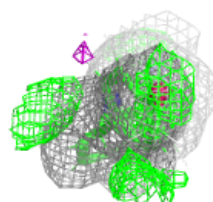
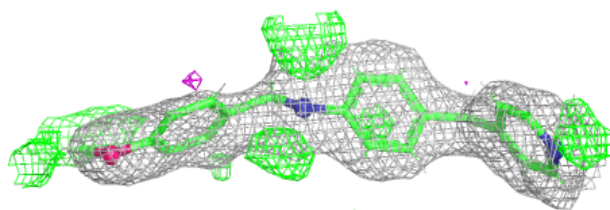
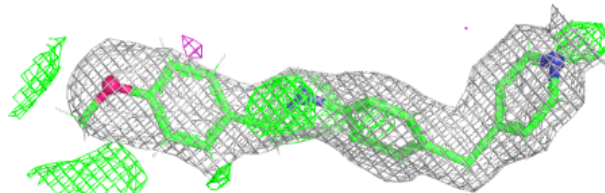
**Electron density around 5YG A 1402 (A):**

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

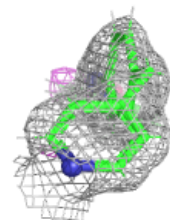
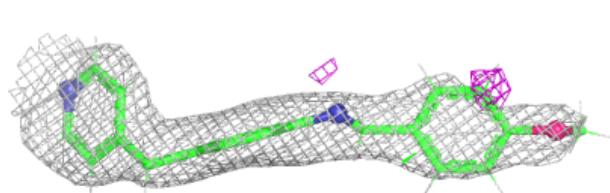
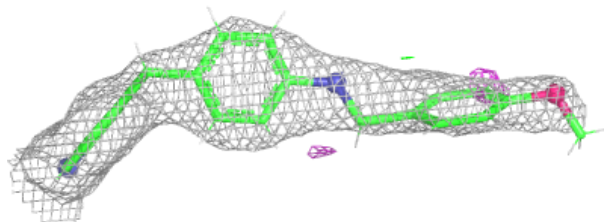


Electron density around 5YG A 1402 (B):

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

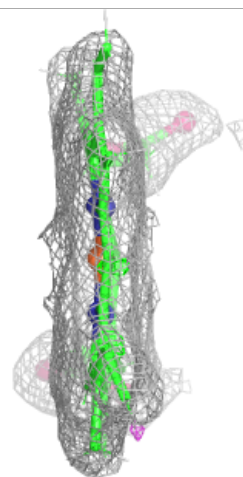
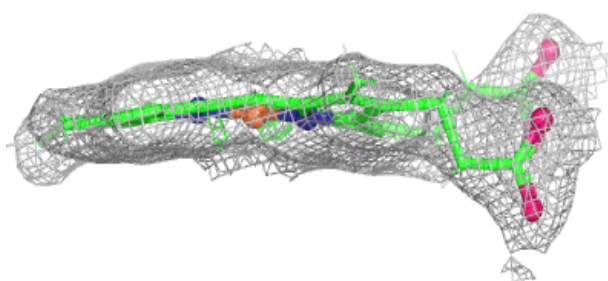
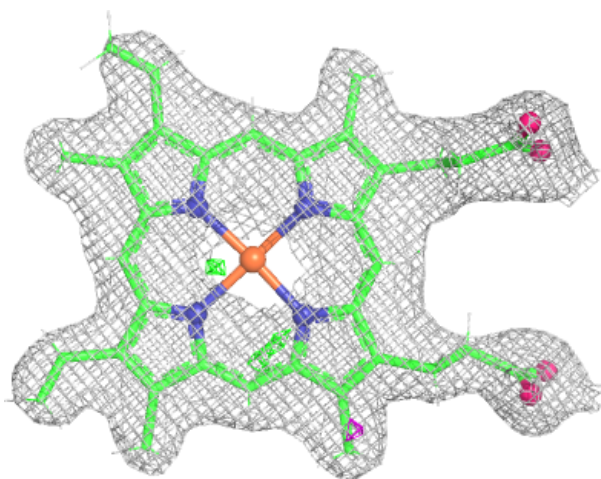
**Electron density around 5YG C 501:**

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



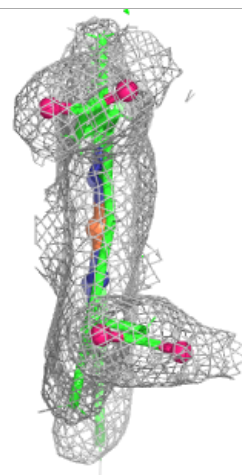
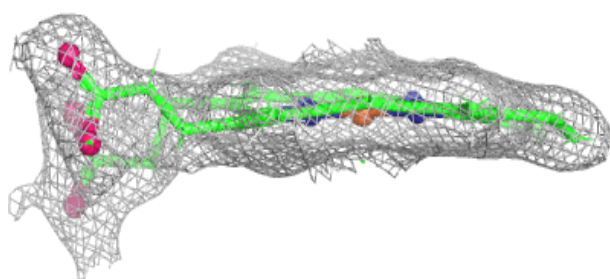
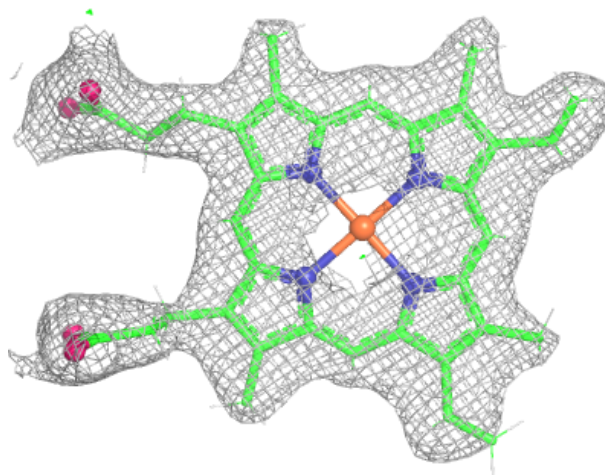
Electron density around HEM B 502:

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



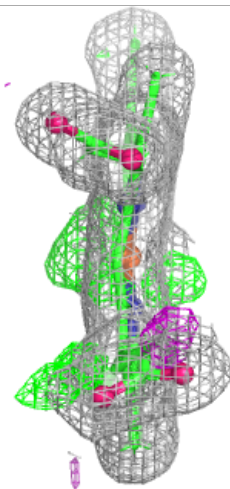
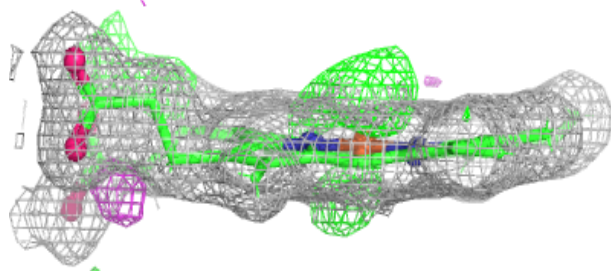
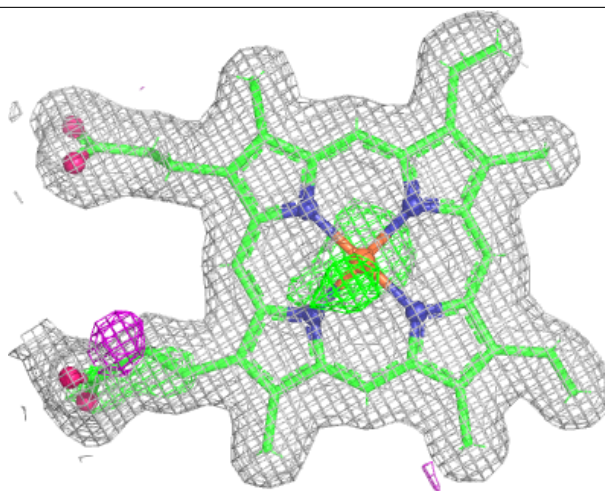
Electron density around HEM C 502:

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



Electron density around HEM A 1403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.