



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:48 AM UTC

PDB ID : 8VZV / pdb_00008vzv
Title : Human TDO (hTDO) in complex with LM10
Authors : Ishigami, I.; Yeh, S.-R.; Lewis-Ballester, A.
Deposited on : 2024-02-12
Resolution : 2.29 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

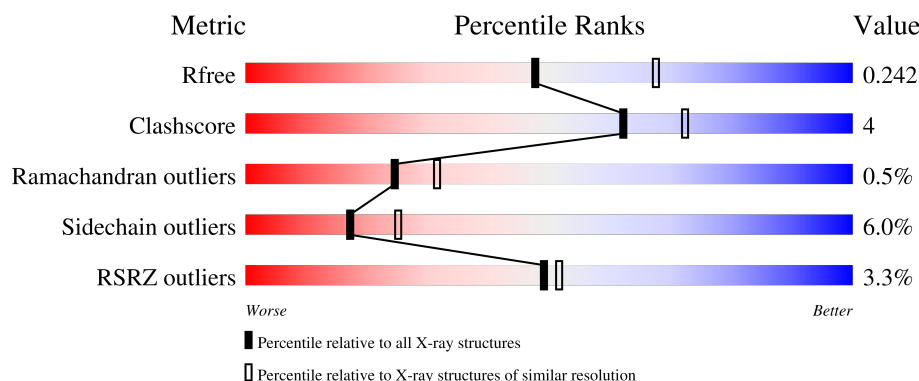
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	380	 3% 79% 10% • 9%
1	BBB	380	 4% 80% 9% • 9%
1	CCC	380	 3% 73% 10% • 14%
1	DDD	380	 2% 80% 9% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZIQ	BBB	402	-	X	-	-
3	ZIQ	DDD	402	-	X	-	-
4	A1AER	DDD	403	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11959 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	344	Total	C	N	O	S	0	0	0
			2915	1876	507	521	11			
1	BBB	344	Total	C	N	O	S	0	0	0
			2899	1866	503	519	11			
1	CCC	326	Total	C	N	O	S	0	0	0
			2761	1780	482	488	11			
1	DDD	343	Total	C	N	O	S	0	0	0
			2908	1869	509	519	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	17	MET	-	initiating methionine	UNP P48775
AAA	390	GLU	-	expression tag	UNP P48775
AAA	391	HIS	-	expression tag	UNP P48775
AAA	392	HIS	-	expression tag	UNP P48775
AAA	393	HIS	-	expression tag	UNP P48775
AAA	394	HIS	-	expression tag	UNP P48775
AAA	395	HIS	-	expression tag	UNP P48775
AAA	396	HIS	-	expression tag	UNP P48775
BBB	17	MET	-	initiating methionine	UNP P48775
BBB	390	GLU	-	expression tag	UNP P48775
BBB	391	HIS	-	expression tag	UNP P48775
BBB	392	HIS	-	expression tag	UNP P48775
BBB	393	HIS	-	expression tag	UNP P48775
BBB	394	HIS	-	expression tag	UNP P48775
BBB	395	HIS	-	expression tag	UNP P48775
BBB	396	HIS	-	expression tag	UNP P48775
CCC	17	MET	-	initiating methionine	UNP P48775
CCC	390	GLU	-	expression tag	UNP P48775
CCC	391	HIS	-	expression tag	UNP P48775
CCC	392	HIS	-	expression tag	UNP P48775
CCC	393	HIS	-	expression tag	UNP P48775

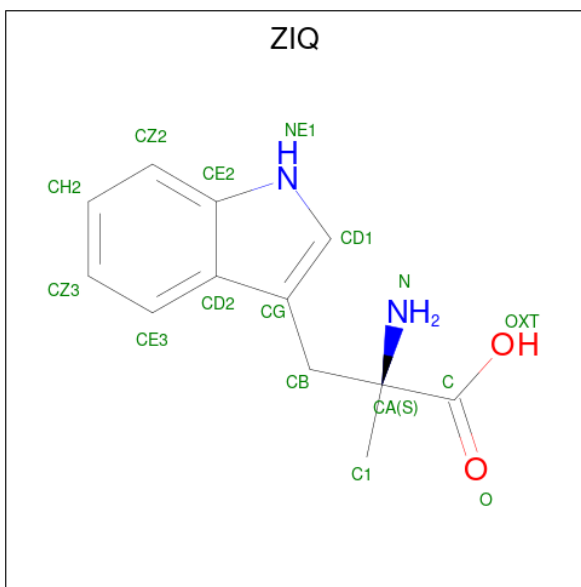
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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	394	HIS	-	expression tag	UNP P48775
CCC	395	HIS	-	expression tag	UNP P48775
CCC	396	HIS	-	expression tag	UNP P48775
DDD	17	MET	-	initiating methionine	UNP P48775
DDD	390	GLU	-	expression tag	UNP P48775
DDD	391	HIS	-	expression tag	UNP P48775
DDD	392	HIS	-	expression tag	UNP P48775
DDD	393	HIS	-	expression tag	UNP P48775
DDD	394	HIS	-	expression tag	UNP P48775
DDD	395	HIS	-	expression tag	UNP P48775
DDD	396	HIS	-	expression tag	UNP P48775

- # HEM

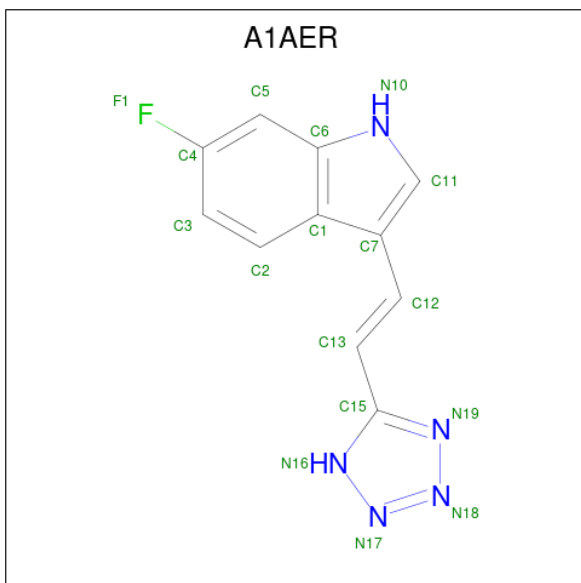
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	BBB	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	CCC	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	DDD	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			16	12	2	2		
3	BBB	1	Total	C	N	O	0	0
			16	12	2	2		
3	CCC	1	Total	C	N	O	0	0
			16	12	2	2		
3	DDD	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 4 is 6-fluoro-3-[(E)-2-(1H-tetrazol-5-yl)ethenyl]-1H-indole (CCD ID: A1AER) (formula: $C_{11}H_8FN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	F	N	0	0
			17	11	1	5		
4	BBB	1	Total	C	F	N	0	0
			17	11	1	5		
4	DDD	1	Total	C	F	N	0	0
			17	11	1	5		

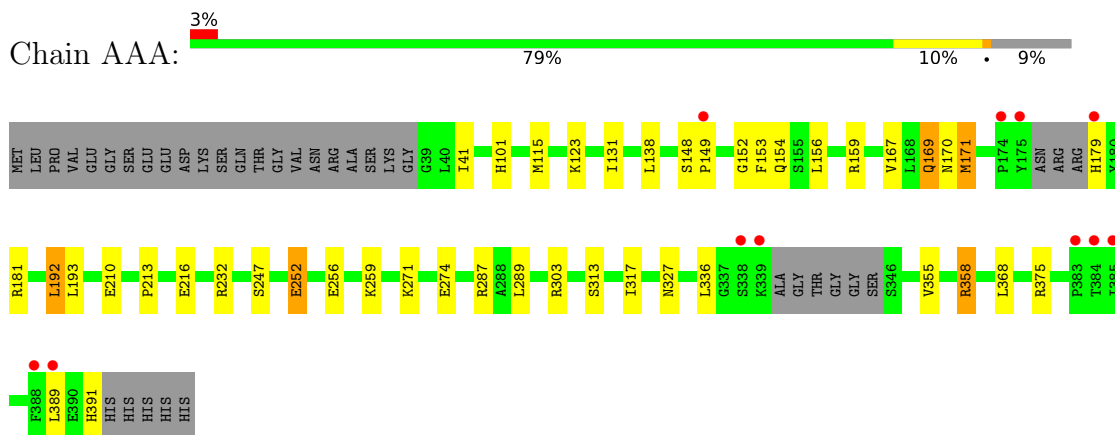
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	43	Total	O	0	0
			43	43		
5	BBB	60	Total	O	0	0
			60	60		
5	CCC	39	Total	O	0	0
			39	39		
5	DDD	47	Total	O	0	0
			47	47		

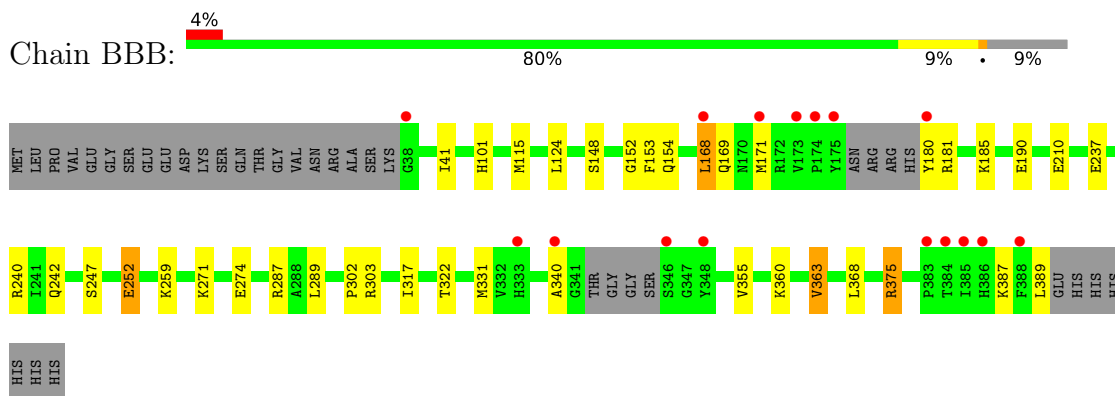
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

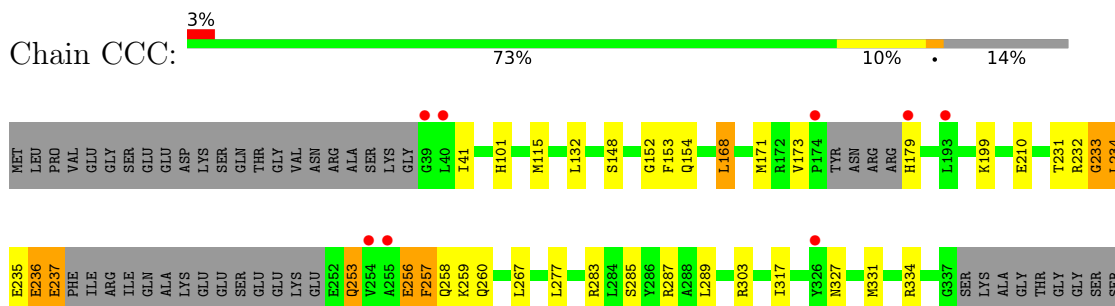
- Molecule 1: Tryptophan 2,3-dioxygenase

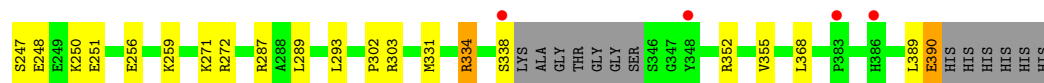


- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.43Å 152.92Å 87.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 30.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.29) 97.3 (30.00-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.238 0.207 , 0.242	Depositor DCC
R_{free} test set	4274 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11959	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZIQ, HEM, A1AER

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	AAA	1.03	1/2983 (0.0%)	1.41	1/4013 (0.0%)
1	BBB	1.02	0/2965	1.42	2/3988 (0.1%)
1	CCC	1.03	0/2826	1.38	0/3804
1	DDD	1.02	0/2975	1.40	2/4003 (0.0%)
All	All	1.02	1/11749 (0.0%)	1.41	5/15808 (0.0%)

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	DDD	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	213	PRO	C-O	-5.33	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	390	GLU	CA-C-O	5.89	130.81	120.80
1	BBB	252	GLU	CB-CA-C	5.50	121.80	110.31
1	BBB	363	VAL	CB-CA-C	-5.37	102.49	111.29
1	AAA	252	GLU	CB-CA-C	5.23	120.71	110.67
1	DDD	246	GLU	CB-CA-C	5.06	119.71	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	242	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2915	0	2897	21	0
1	BBB	2899	0	2888	19	0
1	CCC	2761	0	2746	31	0
1	DDD	2908	0	2890	24	0
2	AAA	43	0	30	5	0
2	BBB	43	0	30	4	0
2	CCC	43	0	30	3	0
2	DDD	43	0	30	3	0
3	AAA	16	0	0	0	0
3	BBB	16	0	0	0	0
3	CCC	16	0	0	0	0
3	DDD	16	0	0	0	0
4	AAA	17	0	0	3	0
4	BBB	17	0	0	1	0
4	DDD	17	0	0	1	0
5	AAA	43	0	0	2	0
5	BBB	60	0	0	2	0
5	CCC	39	0	0	2	0
5	DDD	47	0	0	2	0
All	All	11959	0	11541	96	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 4.

All (96) 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:AAA:391:HIS:C	1:DDD:390:GLU:C	2.14	1.15
1:DDD:115:MET:HA	1:DDD:115:MET:HE2	1.58	0.85
1:DDD:334:ARG:NH1	5:DDD:501:HOH:O	2.15	0.79
4:BBB:403:A1AER:N10	5:BBB:501:HOH:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:246:GLU:HB3	1:DDD:250:LYS:HD3	1.71	0.73
1:DDD:169:GLN:HG3	1:DDD:179:HIS:NE2	2.05	0.72
4:DDD:403:A1AER:N10	5:DDD:502:HOH:O	2.23	0.71
4:AAA:403:A1AER:N10	5:AAA:501:HOH:O	2.24	0.69
1:CCC:232:ARG:C	1:CCC:233:GLY:O	2.33	0.68
1:DDD:169:GLN:CG	1:DDD:179:HIS:NE2	2.61	0.64
2:AAA:401:HEM:HBC2	2:AAA:401:HEM:HHD	1.78	0.63
2:DDD:401:HEM:HBC2	2:DDD:401:HEM:HHD	1.80	0.63
1:AAA:41:ILE:HA	1:BBB:154:GLN:HE22	1.62	0.63
1:CCC:277:LEU:CD2	5:CCC:539:HOH:O	2.49	0.60
2:CCC:401:HEM:HMB1	2:CCC:401:HEM:HBB2	1.82	0.59
1:AAA:169:GLN:HG2	1:AAA:170:ASN:N	2.16	0.59
1:AAA:167:VAL:HG13	1:AAA:171:MET:HE2	1.84	0.58
1:CCC:235:GLU:C	1:CCC:237:GLU:H	2.11	0.58
2:BBB:401:HEM:HBC2	2:BBB:401:HEM:HHD	1.87	0.56
1:CCC:173:VAL:HG23	1:CCC:350:TYR:CE1	2.43	0.54
1:BBB:168:LEU:HB3	1:BBB:171:MET:HE3	1.88	0.54
1:AAA:154:GLN:HE22	1:BBB:41:ILE:HA	1.72	0.54
4:AAA:403:A1AER:C11	5:AAA:501:HOH:O	2.55	0.53
1:AAA:156:LEU:HD12	1:AAA:192:LEU:CD1	2.38	0.53
1:CCC:154:GLN:HE22	1:DDD:41:ILE:HA	1.74	0.53
1:CCC:231:THR:O	1:CCC:233:GLY:O	2.27	0.52
1:AAA:391:HIS:C	1:DDD:390:GLU:CA	2.83	0.52
1:CCC:334:ARG:HD2	5:CCC:530:HOH:O	2.09	0.52
2:CCC:401:HEM:HBB2	2:CCC:401:HEM:CMB	2.40	0.51
1:DDD:248:GLU:HA	1:DDD:248:GLU:OE1	2.08	0.51
1:DDD:303:ARG:HD3	1:DDD:389:LEU:HA	1.93	0.50
1:CCC:210:GLU:HG2	1:CCC:287:ARG:HB3	1.94	0.50
1:DDD:152:GLY:HA3	2:DDD:401:HEM:C1D	2.46	0.50
1:AAA:156:LEU:CD1	1:AAA:192:LEU:CD1	2.89	0.50
1:CCC:168:LEU:HD22	1:CCC:283:ARG:NH2	2.26	0.50
1:CCC:303:ARG:HD3	1:CCC:389:LEU:HA	1.93	0.49
1:CCC:234:LEU:O	1:CCC:237:GLU:N	2.45	0.49
1:BBB:302:PRO:HB3	1:CCC:391:HIS:CD2	2.47	0.49
1:BBB:210:GLU:HG2	1:BBB:287:ARG:HB3	1.94	0.49
2:AAA:401:HEM:HMB2	2:AAA:401:HEM:HBB2	1.96	0.48
1:BBB:303:ARG:HD3	1:BBB:389:LEU:HA	1.96	0.48
1:DDD:210:GLU:HG2	1:DDD:287:ARG:HB3	1.94	0.48
1:AAA:210:GLU:HG2	1:AAA:287:ARG:HB3	1.94	0.48
1:CCC:253:GLN:HA	1:CCC:253:GLN:OE1	2.11	0.48
1:CCC:256:GLU:HG3	1:CCC:257:PHE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:391:HIS:ND1	1:DDD:302:PRO:HB3	2.28	0.47
1:CCC:152:GLY:HA3	2:CCC:401:HEM:C1D	2.49	0.47
1:CCC:256:GLU:O	1:CCC:259:LYS:N	2.34	0.47
1:DDD:238:PHE:C	1:DDD:238:PHE:CD2	2.92	0.47
1:DDD:93:VAL:HG21	1:DDD:115:MET:HE3	1.96	0.47
1:BBB:303:ARG:HG3	1:CCC:391:HIS:HB2	1.96	0.47
1:CCC:115:MET:HE3	1:CCC:317:ILE:CD1	2.44	0.47
1:AAA:303:ARG:HD3	1:AAA:389:LEU:HA	1.97	0.46
1:AAA:152:GLY:HA3	2:AAA:401:HEM:C1D	2.50	0.46
1:BBB:168:LEU:HD22	1:BBB:168:LEU:HA	1.88	0.46
2:DDD:401:HEM:HMB1	2:DDD:401:HEM:HBB2	1.97	0.45
2:AAA:401:HEM:HBC2	2:AAA:401:HEM:CHD	2.45	0.45
1:AAA:171:MET:HE3	1:AAA:358:ARG:O	2.16	0.45
1:AAA:131:ILE:CD1	1:BBB:124:LEU:HD22	2.47	0.45
1:BBB:331:MET:HE2	1:BBB:331:MET:HB3	1.82	0.45
1:AAA:138:LEU:CD1	1:CCC:372:LEU:HD22	2.46	0.44
1:AAA:115:MET:HE3	1:AAA:317:ILE:CD1	2.47	0.44
1:CCC:168:LEU:HD12	1:CCC:168:LEU:HA	1.78	0.44
1:BBB:115:MET:HE3	1:BBB:317:ILE:CD1	2.47	0.44
1:CCC:331:MET:HE2	1:CCC:331:MET:HB3	1.83	0.44
1:BBB:237:GLU:HG3	1:BBB:240:ARG:NH2	2.33	0.44
1:AAA:336:LEU:HD11	4:AAA:403:A1AER:N16	2.33	0.44
1:BBB:355:VAL:HG12	1:BBB:355:VAL:O	2.18	0.44
1:CCC:41:ILE:HA	1:DDD:154:GLN:HE22	1.83	0.43
1:CCC:173:VAL:HG23	1:CCC:350:TYR:HE1	1.80	0.43
1:BBB:152:GLY:HA3	2:BBB:401:HEM:C1D	2.53	0.43
1:DDD:289:LEU:HD11	1:DDD:368:LEU:HD21	2.00	0.43
1:CCC:256:GLU:O	1:CCC:258:GLN:N	2.51	0.43
1:CCC:289:LEU:HD11	1:CCC:368:LEU:HD21	1.99	0.43
1:BBB:180:TYR:N	5:BBB:504:HOH:O	2.52	0.43
1:AAA:159:ARG:NH2	2:AAA:401:HEM:O1D	2.47	0.43
1:AAA:131:ILE:HD12	1:BBB:124:LEU:HD22	2.02	0.42
1:AAA:355:VAL:HG12	1:AAA:355:VAL:O	2.20	0.42
1:CCC:355:VAL:HG12	1:CCC:355:VAL:O	2.19	0.42
1:DDD:355:VAL:O	1:DDD:355:VAL:HG12	2.19	0.42
1:CCC:233:GLY:O	1:CCC:235:GLU:N	2.53	0.42
1:AAA:289:LEU:HD11	1:AAA:368:LEU:HD21	2.02	0.42
1:DDD:331:MET:HE2	1:DDD:331:MET:HB3	1.80	0.42
1:BBB:289:LEU:HD11	1:BBB:368:LEU:HD21	2.01	0.42
1:DDD:115:MET:HE2	1:DDD:115:MET:CA	2.40	0.42
1:BBB:322:THR:HG21	1:BBB:360:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:362:PHE:HB3	1:CCC:365:LEU:HD12	2.03	0.41
1:DDD:289:LEU:CD1	1:DDD:368:LEU:HD21	2.50	0.41
1:BBB:375:ARG:NH2	1:DDD:142:ASP:OD2	2.54	0.41
1:CCC:236:GLU:O	1:CCC:237:GLU:C	2.64	0.41
2:BBB:401:HEM:HMB1	2:BBB:401:HEM:HBB2	2.03	0.41
2:BBB:401:HEM:HHD	2:BBB:401:HEM:CBC	2.52	0.40
1:CCC:132:LEU:HD12	1:CCC:132:LEU:HA	1.87	0.40
1:DDD:191:LEU:HD12	1:DDD:191:LEU:HA	1.83	0.40
1:CCC:232:ARG:O	1:CCC:233:GLY:O	2.40	0.40
1:DDD:293:LEU:HD12	1:DDD:293:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	338/380 (89%)	329 (97%)	9 (3%)	0	100	100
1	BBB	338/380 (89%)	325 (96%)	12 (4%)	1 (0%)	36	46
1	CCC	318/380 (84%)	306 (96%)	7 (2%)	5 (2%)	7	7
1	DDD	337/380 (89%)	328 (97%)	9 (3%)	0	100	100
All	All	1331/1520 (88%)	1288 (97%)	37 (3%)	6 (0%)	24	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	340	ALA
1	CCC	257	PHE
1	CCC	233	GLY
1	CCC	234	LEU
1	CCC	236	GLU

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Mol	Chain	Res	Type
1	CCC	285	SER

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	AAA	320/348 (92%)	297 (93%)	23 (7%)	13	18
1	BBB	317/348 (91%)	300 (95%)	17 (5%)	20	29
1	CCC	303/348 (87%)	287 (95%)	16 (5%)	20	30
1	DDD	319/348 (92%)	299 (94%)	20 (6%)	16	23
All	All	1259/1392 (90%)	1183 (94%)	76 (6%)	17	25

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	101	HIS
1	AAA	123	LYS
1	AAA	148	SER
1	AAA	149	PRO
1	AAA	153	PHE
1	AAA	169	GLN
1	AAA	171	MET
1	AAA	179	HIS
1	AAA	181	ARG
1	AAA	192	LEU
1	AAA	193	LEU
1	AAA	216	GLU
1	AAA	232	ARG
1	AAA	247	SER
1	AAA	252	GLU
1	AAA	256	GLU
1	AAA	259	LYS
1	AAA	271	LYS
1	AAA	274	GLU
1	AAA	313	SER

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Mol	Chain	Res	Type
1	AAA	327	ASN
1	AAA	358	ARG
1	AAA	375	ARG
1	BBB	101	HIS
1	BBB	148	SER
1	BBB	153	PHE
1	BBB	168	LEU
1	BBB	169	GLN
1	BBB	181	ARG
1	BBB	185	LYS
1	BBB	190	GLU
1	BBB	242	GLN
1	BBB	247	SER
1	BBB	252	GLU
1	BBB	259	LYS
1	BBB	271	LYS
1	BBB	274	GLU
1	BBB	363	VAL
1	BBB	375	ARG
1	BBB	387	LYS
1	CCC	101	HIS
1	CCC	148	SER
1	CCC	153	PHE
1	CCC	168	LEU
1	CCC	171	MET
1	CCC	179	HIS
1	CCC	199	LYS
1	CCC	237	GLU
1	CCC	253	GLN
1	CCC	256	GLU
1	CCC	260	GLN
1	CCC	267	LEU
1	CCC	327	ASN
1	CCC	358	ARG
1	CCC	387	LYS
1	CCC	389	LEU
1	DDD	101	HIS
1	DDD	148	SER
1	DDD	149	PRO
1	DDD	153	PHE
1	DDD	169	GLN
1	DDD	185	LYS

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Mol	Chain	Res	Type
1	DDD	191	LEU
1	DDD	193	LEU
1	DDD	238	PHE
1	DDD	242	GLN
1	DDD	246	GLU
1	DDD	247	SER
1	DDD	251	GLU
1	DDD	256	GLU
1	DDD	259	LYS
1	DDD	271	LYS
1	DDD	272	ARG
1	DDD	334	ARG
1	DDD	338	SER
1	DDD	352	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZIQ	BBB	402	-	14,17,17	3.75	8 (57%)	20,25,25	4.83	12 (60%)
2	HEM	BBB	401	1,5	50,50,50	1.70	12 (24%)	67,82,82	1.82	22 (32%)
2	HEM	CCC	401	1,5	50,50,50	1.63	10 (20%)	67,82,82	1.62	10 (14%)
3	ZIQ	AAA	402	-	14,17,17	3.97	4 (28%)	20,25,25	5.18	12 (60%)
3	ZIQ	DDD	402	-	14,17,17	3.71	8 (57%)	20,25,25	5.25	12 (60%)
4	A1AER	BBB	403	-	19,19,19	2.61	6 (31%)	25,26,26	4.21	13 (52%)
4	A1AER	AAA	403	-	19,19,19	2.57	6 (31%)	25,26,26	5.33	14 (56%)
4	A1AER	DDD	403	-	19,19,19	2.16	5 (26%)	25,26,26	4.76	15 (60%)
3	ZIQ	CCC	402	-	14,17,17	3.86	9 (64%)	20,25,25	4.98	11 (55%)
2	HEM	AAA	401	1,5	50,50,50	1.76	9 (18%)	67,82,82	1.85	21 (31%)
2	HEM	DDD	401	1,5	50,50,50	1.71	14 (28%)	67,82,82	1.60	14 (20%)

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	ZIQ	BBB	402	-	-	2/11/11/11	0/2/2/2
2	HEM	BBB	401	1,5	-	2/14/54/54	-
2	HEM	CCC	401	1,5	-	2/14/54/54	-
3	ZIQ	AAA	402	-	-	4/11/11/11	0/2/2/2
3	ZIQ	DDD	402	-	-	4/11/11/11	0/2/2/2
4	A1AER	BBB	403	-	-	2/5/5/5	0/3/3/3
4	A1AER	AAA	403	-	-	1/5/5/5	0/3/3/3
4	A1AER	DDD	403	-	-	2/5/5/5	0/3/3/3
3	ZIQ	CCC	402	-	-	0/11/11/11	0/2/2/2
2	HEM	AAA	401	1,5	-	4/14/54/54	-
2	HEM	DDD	401	1,5	-	3/14/54/54	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	ZIQ	CE3-CD2	-10.72	1.23	1.39
3	CCC	402	ZIQ	CE3-CD2	-9.49	1.25	1.39
3	DDD	402	ZIQ	CE3-CD2	-8.47	1.27	1.39
3	BBB	402	ZIQ	CE3-CD2	-8.35	1.27	1.39
3	AAA	402	ZIQ	CZ3-CE3	-7.75	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	402	ZIQ	CZ3-CE3	-7.56	1.26	1.38
3	CCC	402	ZIQ	CZ3-CE3	-7.31	1.26	1.38
3	BBB	402	ZIQ	CD2-CE2	7.04	1.50	1.41
4	BBB	403	A1AER	C1-C6	6.49	1.49	1.41
4	AAA	403	A1AER	N17-N18	6.18	1.42	1.30
4	BBB	403	A1AER	N17-N18	5.96	1.41	1.30
4	DDD	403	A1AER	N17-N18	5.92	1.41	1.30
3	BBB	402	ZIQ	CZ3-CE3	-5.23	1.30	1.38
2	AAA	401	HEM	C1C-C2C	-5.11	1.35	1.45
4	AAA	403	A1AER	C1-C6	5.11	1.47	1.41
3	CCC	402	ZIQ	CD2-CE2	4.75	1.47	1.41
2	CCC	401	HEM	FE-NB	4.73	2.09	1.94
2	AAA	401	HEM	FE-NB	4.72	2.09	1.94
2	BBB	401	HEM	FE-NB	4.56	2.08	1.94
4	AAA	403	A1AER	C15-N16	-4.51	1.29	1.34
3	DDD	402	ZIQ	CD2-CE2	4.39	1.46	1.41
2	DDD	401	HEM	FE-NC	4.32	2.09	1.95
2	CCC	401	HEM	FE-NC	4.24	2.09	1.95
4	AAA	403	A1AER	N16-N17	4.24	1.40	1.35
4	DDD	403	A1AER	C1-C6	4.17	1.46	1.41
2	AAA	401	HEM	FE-NC	4.14	2.08	1.95
2	BBB	401	HEM	C4D-ND	-3.95	1.33	1.40
2	DDD	401	HEM	FE-NB	3.91	2.06	1.94
4	BBB	403	A1AER	N16-N17	3.86	1.39	1.35
2	BBB	401	HEM	FE-NC	3.69	2.07	1.95
4	BBB	403	A1AER	C15-N16	-3.68	1.30	1.34
2	AAA	401	HEM	C3C-C4C	-3.66	1.39	1.46
4	DDD	403	A1AER	C15-N16	-3.62	1.30	1.34
3	AAA	402	ZIQ	CD2-CE2	3.55	1.45	1.41
3	AAA	402	ZIQ	CD1-CG	3.51	1.42	1.36
4	BBB	403	A1AER	N19-N18	3.51	1.41	1.36
2	BBB	401	HEM	C1C-C2C	-3.48	1.38	1.45
2	CCC	401	HEM	C4B-NB	-3.45	1.32	1.38
2	CCC	401	HEM	C1B-NB	-3.44	1.34	1.40
3	BBB	402	ZIQ	CD1-CG	3.36	1.41	1.36
2	DDD	401	HEM	C1C-C2C	-3.32	1.38	1.45
3	BBB	402	ZIQ	CH2-CZ3	3.32	1.45	1.38
3	CCC	402	ZIQ	CD1-CG	3.11	1.41	1.36
2	DDD	401	HEM	C1B-NB	-3.11	1.34	1.40
3	DDD	402	ZIQ	CE2-NE1	-3.03	1.32	1.37
4	AAA	403	A1AER	N19-N18	3.01	1.40	1.36
2	BBB	401	HEM	CBD-CGD	2.98	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	HEM	C3B-C4B	2.97	1.50	1.44
2	CCC	401	HEM	C4D-ND	-2.97	1.35	1.40
2	AAA	401	HEM	C1C-NC	-2.94	1.34	1.39
2	AAA	401	HEM	C4D-ND	-2.91	1.35	1.40
2	AAA	401	HEM	C4B-NB	-2.90	1.33	1.38
3	DDD	402	ZIQ	CB-CA	-2.87	1.51	1.55
2	DDD	401	HEM	C3C-C4C	-2.81	1.41	1.46
2	AAA	401	HEM	C1B-NB	-2.73	1.35	1.40
2	BBB	401	HEM	C4B-NB	-2.63	1.33	1.38
3	CCC	402	ZIQ	CH2-CZ2	2.60	1.43	1.38
2	DDD	401	HEM	FE-ND	-2.60	1.86	1.94
2	DDD	401	HEM	C1C-NC	-2.57	1.34	1.39
2	CCC	401	HEM	C1C-C2C	-2.52	1.40	1.45
2	BBB	401	HEM	C1C-NC	-2.52	1.34	1.39
2	BBB	401	HEM	C3C-C4C	-2.51	1.41	1.46
3	DDD	402	ZIQ	CD2-CG	2.49	1.48	1.44
2	DDD	401	HEM	C4B-NB	-2.49	1.34	1.38
2	BBB	401	HEM	C3B-C4B	2.46	1.49	1.44
4	DDD	403	A1AER	N16-N17	2.43	1.38	1.35
3	DDD	402	ZIQ	CH2-CZ2	2.41	1.43	1.38
2	DDD	401	HEM	C4D-ND	-2.40	1.36	1.40
3	BBB	402	ZIQ	CZ2-CE2	2.40	1.43	1.39
2	CCC	401	HEM	C3C-C4C	-2.40	1.41	1.46
3	CCC	402	ZIQ	CD2-CG	2.39	1.47	1.44
3	BBB	402	ZIQ	CD1-NE1	2.31	1.40	1.37
4	DDD	403	A1AER	N19-N18	2.30	1.39	1.36
2	BBB	401	HEM	CBA-CGA	2.29	1.55	1.50
2	CCC	401	HEM	C1C-NC	-2.27	1.35	1.39
2	CCC	401	HEM	C4D-C3D	2.24	1.48	1.45
3	DDD	402	ZIQ	O-C	2.20	1.29	1.22
3	CCC	402	ZIQ	CE2-NE1	-2.19	1.34	1.37
3	CCC	402	ZIQ	CH2-CZ3	2.18	1.43	1.38
3	BBB	402	ZIQ	CH2-CZ2	2.18	1.42	1.38
2	CCC	401	HEM	C3B-C4B	2.17	1.49	1.44
2	DDD	401	HEM	C1A-C2A	-2.17	1.40	1.44
2	DDD	401	HEM	C4A-NA	-2.09	1.35	1.39
4	BBB	403	A1AER	F1-C4	-2.08	1.31	1.36
2	BBB	401	HEM	C1D-ND	-2.07	1.34	1.38
2	BBB	401	HEM	CBD-CAD	2.04	1.59	1.51
3	CCC	402	ZIQ	CB-CA	-2.03	1.52	1.55
2	AAA	401	HEM	C1D-ND	-2.03	1.34	1.38
2	DDD	401	HEM	C1D-C2D	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	403	A1AER	C5-C4	2.02	1.41	1.37
2	DDD	401	HEM	C1D-ND	-2.00	1.34	1.38

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	403	A1AER	C1-C7-C11	14.49	114.08	106.12
3	AAA	402	ZIQ	CZ3-CE3-CD2	14.05	145.18	119.80
3	DDD	402	ZIQ	CZ3-CE3-CD2	13.92	144.94	119.80
3	CCC	402	ZIQ	CZ3-CE3-CD2	13.67	144.50	119.80
3	BBB	402	ZIQ	CZ3-CE3-CD2	12.94	143.18	119.80
4	DDD	403	A1AER	C1-C7-C11	11.66	112.53	106.12
4	AAA	403	A1AER	C5-C6-C1	-11.50	113.34	122.52
4	AAA	403	A1AER	C6-C1-C7	-10.34	99.52	106.53
3	AAA	402	ZIQ	CH2-CZ3-CE3	-10.28	107.55	120.24
3	DDD	402	ZIQ	CH2-CZ3-CE3	-10.16	107.71	120.24
4	DDD	403	A1AER	C5-C6-C1	-9.87	114.64	122.52
4	BBB	403	A1AER	C5-C6-C1	-9.63	114.84	122.52
4	BBB	403	A1AER	C1-C7-C11	9.55	111.36	106.12
3	CCC	402	ZIQ	CE3-CD2-CE2	-9.45	109.05	118.84
3	BBB	402	ZIQ	CH2-CZ3-CE3	-9.21	108.87	120.24
3	BBB	402	ZIQ	CE3-CD2-CE2	-8.90	109.61	118.84
3	CCC	402	ZIQ	CH2-CZ3-CE3	-8.81	109.37	120.24
3	DDD	402	ZIQ	CE3-CD2-CE2	-8.67	109.86	118.84
4	BBB	403	A1AER	C6-C1-C7	-8.37	100.85	106.53
4	DDD	403	A1AER	C7-C11-N10	-8.05	106.09	110.20
4	DDD	403	A1AER	C6-C1-C7	-8.00	101.11	106.53
4	AAA	403	A1AER	C7-C11-N10	-7.99	106.12	110.20
3	AAA	402	ZIQ	CE3-CD2-CE2	-7.85	110.71	118.84
4	AAA	403	A1AER	C2-C1-C6	7.50	126.61	118.84
3	AAA	402	ZIQ	CZ2-CE2-CD2	-7.35	115.07	122.19
4	DDD	403	A1AER	C2-C1-C6	6.67	125.75	118.84
4	DDD	403	A1AER	N16-C15-N19	6.53	117.16	108.92
4	BBB	403	A1AER	C13-C12-C7	-6.39	116.81	127.28
3	DDD	402	ZIQ	CZ2-CE2-CD2	-6.05	116.33	122.19
4	AAA	403	A1AER	N16-C15-N19	5.94	116.41	108.92
4	BBB	403	A1AER	C2-C1-C6	5.73	124.77	118.84
3	DDD	402	ZIQ	CZ2-CE2-NE1	5.62	139.74	130.74
4	BBB	403	A1AER	N16-C15-N19	5.57	115.94	108.92
4	DDD	403	A1AER	C13-C15-N19	-5.40	119.17	125.94
3	DDD	402	ZIQ	CD2-CG-CD1	-5.06	100.98	106.16
3	AAA	402	ZIQ	CZ2-CE2-NE1	5.02	138.77	130.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	402	ZIQ	CD2-CG-CD1	-4.96	101.08	106.16
3	BBB	402	ZIQ	CZ2-CE2-CD2	-4.78	117.56	122.19
3	CCC	402	ZIQ	CE3-CD2-CG	4.66	140.80	133.85
3	CCC	402	ZIQ	CZ2-CE2-NE1	4.63	138.16	130.74
3	CCC	402	ZIQ	CZ2-CE2-CD2	-4.59	117.75	122.19
3	BBB	402	ZIQ	CD2-CG-CD1	-4.54	101.51	106.16
2	BBB	401	HEM	CHC-C4B-NB	4.49	129.26	124.42
2	AAA	401	HEM	CHC-C4B-NB	4.49	129.26	124.42
4	AAA	403	A1AER	C13-C12-C7	-4.48	119.93	127.28
4	BBB	403	A1AER	C7-C11-N10	-4.47	107.91	110.20
3	BBB	402	ZIQ	CZ2-CE2-NE1	4.47	137.89	130.74
3	CCC	402	ZIQ	CD2-CG-CD1	-4.45	101.61	106.16
3	DDD	402	ZIQ	CD2-CE2-NE1	-4.31	103.93	107.52
2	CCC	401	HEM	CHD-C1D-ND	4.30	129.06	124.42
4	AAA	403	A1AER	C1-C7-C12	-4.24	117.05	129.88
4	DDD	403	A1AER	C15-N19-N18	-4.23	101.84	105.36
3	CCC	402	ZIQ	CE2-NE1-CD1	4.16	112.78	109.08
3	CCC	402	ZIQ	CD2-CE2-NE1	-4.12	104.09	107.52
3	BBB	402	ZIQ	CE3-CD2-CG	4.12	139.99	133.85
2	AAA	401	HEM	CBD-CAD-C3D	-4.12	101.15	112.53
4	DDD	403	A1AER	C13-C12-C7	-4.04	120.66	127.28
3	DDD	402	ZIQ	CE3-CD2-CG	3.96	139.75	133.85
2	DDD	401	HEM	CHD-C1D-ND	3.93	128.66	124.42
2	DDD	401	HEM	CBD-CAD-C3D	-3.93	101.66	112.53
2	BBB	401	HEM	CHD-C1D-ND	3.88	128.60	124.42
3	DDD	402	ZIQ	CE2-NE1-CD1	3.88	112.53	109.08
2	DDD	401	HEM	CHC-C4B-NB	3.86	128.58	124.42
2	CCC	401	HEM	CHC-C4B-NB	3.82	128.54	124.42
2	CCC	401	HEM	CBD-CAD-C3D	-3.80	102.02	112.53
2	BBB	401	HEM	CHD-C1D-C2D	-3.80	119.03	125.03
4	AAA	403	A1AER	C13-C15-N19	-3.77	121.21	125.94
4	DDD	403	A1AER	C1-C7-C12	-3.67	118.76	129.88
4	BBB	403	A1AER	C13-C15-N19	-3.67	121.33	125.94
2	AAA	401	HEM	C1B-NB-C4B	3.65	109.53	105.21
4	AAA	403	A1AER	C1-C6-N10	3.64	110.56	107.52
2	BBB	401	HEM	CBD-CAD-C3D	-3.60	102.59	112.53
3	BBB	402	ZIQ	CD2-CE2-NE1	-3.58	104.54	107.52
2	AAA	401	HEM	CHA-C4D-ND	3.55	128.76	124.37
2	AAA	401	HEM	CHD-C1D-ND	3.52	128.21	124.42
3	AAA	402	ZIQ	CB-CG-CD1	3.42	133.62	127.37
2	CCC	401	HEM	CHD-C1D-C2D	-3.40	119.65	125.03
3	DDD	402	ZIQ	CB-CA-C	-3.32	104.53	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	402	ZIQ	CE3-CD2-CG	3.29	138.76	133.85
2	DDD	401	HEM	CHA-C4D-ND	3.25	128.38	124.37
3	AAA	402	ZIQ	CE2-CD2-CG	3.24	110.44	107.17
3	DDD	402	ZIQ	CE2-CD2-CG	3.19	110.39	107.17
3	BBB	402	ZIQ	CE2-CD2-CG	3.19	110.39	107.17
2	AAA	401	HEM	CHB-C1B-NB	3.17	128.29	124.37
3	AAA	402	ZIQ	CG-CD1-NE1	3.16	113.78	110.31
2	AAA	401	HEM	C4B-C3B-C2B	-3.15	104.39	107.28
2	BBB	401	HEM	C1B-NB-C4B	3.13	108.92	105.21
4	BBB	403	A1AER	C15-N19-N18	-3.11	102.77	105.36
3	AAA	402	ZIQ	CB-CA-C	-3.09	104.85	109.10
2	BBB	401	HEM	O2D-CGD-O1D	-3.03	115.54	123.33
4	BBB	403	A1AER	C1-C7-C12	-2.95	120.95	129.88
3	CCC	402	ZIQ	CE2-CD2-CG	2.95	110.15	107.17
2	CCC	401	HEM	CAD-C3D-C4D	2.91	129.78	124.70
4	DDD	403	A1AER	C5-C6-N10	2.91	136.12	131.62
4	AAA	403	A1AER	C5-C6-N10	2.89	136.10	131.62
2	DDD	401	HEM	CHA-C4D-C3D	-2.83	120.01	125.23
2	BBB	401	HEM	O2D-CGD-CBD	2.82	122.90	114.00
4	DDD	403	A1AER	C3-C2-C1	-2.81	116.22	120.86
3	BBB	402	ZIQ	O-C-CA	-2.80	117.77	122.78
3	DDD	402	ZIQ	CB-CG-CD1	2.77	132.43	127.37
2	AAA	401	HEM	CHA-C4D-C3D	-2.74	120.17	125.23
2	CCC	401	HEM	O2D-CGD-CBD	2.72	122.61	114.00
2	DDD	401	HEM	C1A-CHA-C4D	-2.71	119.86	126.25
3	AAA	402	ZIQ	O-C-CA	-2.70	117.94	122.78
2	AAA	401	HEM	CHD-C4C-NC	2.68	127.38	124.45
2	AAA	401	HEM	C1A-CHA-C4D	-2.66	119.99	126.25
4	AAA	403	A1AER	C15-N19-N18	-2.62	103.18	105.36
4	AAA	403	A1AER	C3-C2-C1	-2.60	116.57	120.86
2	AAA	401	HEM	CHA-C1A-NA	2.60	128.57	123.86
4	BBB	403	A1AER	C5-C6-N10	2.57	135.59	131.62
2	AAA	401	HEM	CHD-C1D-C2D	-2.56	120.98	125.03
2	BBB	401	HEM	C4A-CHB-C1B	-2.53	120.29	126.25
3	BBB	402	ZIQ	CG-CD1-NE1	2.52	113.07	110.31
2	DDD	401	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
2	BBB	401	HEM	C4A-C3A-C2A	2.50	109.68	106.82
2	DDD	401	HEM	C1B-NB-C4B	2.49	108.16	105.21
2	BBB	401	HEM	CHB-C4A-NA	2.48	128.36	123.86
2	AAA	401	HEM	CAC-C3C-C4C	2.47	130.72	124.82
2	AAA	401	HEM	C4C-NC-C1C	2.46	109.84	105.82
4	BBB	403	A1AER	C1-C6-N10	2.46	109.57	107.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	HEM	CHC-C1C-NC	2.45	127.12	124.45
2	DDD	401	HEM	CAC-C3C-C4C	2.43	130.62	124.82
2	DDD	401	HEM	C4B-C3B-C2B	-2.39	105.08	107.28
2	BBB	401	HEM	O2A-CGA-O1A	-2.38	117.22	123.33
2	BBB	401	HEM	CAA-CBA-CGA	2.37	119.96	113.67
4	AAA	403	A1AER	C11-C7-C12	2.36	128.85	123.33
2	CCC	401	HEM	C2A-C1A-NA	-2.36	107.53	110.15
3	CCC	402	ZIQ	C1-CA-CB	-2.36	107.52	110.82
2	CCC	401	HEM	CHB-C1B-NB	2.35	127.27	124.37
2	BBB	401	HEM	CAD-C3D-C4D	2.34	128.78	124.70
2	BBB	401	HEM	O2A-CGA-CBA	2.33	121.36	114.00
2	BBB	401	HEM	CHB-C1B-NB	2.30	127.22	124.37
2	BBB	401	HEM	CHA-C4D-ND	2.29	127.20	124.37
4	DDD	403	A1AER	C11-C7-C12	2.28	128.65	123.33
2	AAA	401	HEM	O2D-CGD-CBD	2.28	121.19	114.00
4	BBB	403	A1AER	C3-C2-C1	-2.27	117.11	120.86
4	DDD	403	A1AER	C6-N10-C11	2.20	111.03	109.08
3	BBB	402	ZIQ	C1-CA-CB	-2.19	107.75	110.82
2	AAA	401	HEM	C2A-C1A-NA	-2.18	107.73	110.15
2	BBB	401	HEM	CAD-CBD-CGD	2.17	119.42	113.67
2	CCC	401	HEM	C4B-C3B-C2B	-2.16	105.29	107.28
2	CCC	401	HEM	CBA-CAA-C2A	-2.16	106.55	112.53
2	DDD	401	HEM	CAA-CBA-CGA	-2.15	107.97	113.67
2	AAA	401	HEM	C3B-C2B-C1B	2.14	108.02	106.41
2	BBB	401	HEM	CHA-C1A-NA	2.13	127.73	123.86
2	DDD	401	HEM	CHB-C1B-NB	2.13	127.00	124.37
2	DDD	401	HEM	CBA-CAA-C2A	-2.12	106.68	112.53
2	AAA	401	HEM	CMD-C2D-C1D	2.11	128.33	125.03
2	BBB	401	HEM	CHA-C4D-C3D	-2.11	121.34	125.23
4	DDD	403	A1AER	C1-C6-N10	2.06	109.24	107.52
2	AAA	401	HEM	CAC-C3C-C2C	-2.05	121.75	128.43
2	DDD	401	HEM	O2D-CGD-CBD	2.05	120.49	114.00
2	BBB	401	HEM	C3A-C4A-NA	-2.04	106.87	110.14
2	BBB	401	HEM	C2D-C1D-ND	2.04	112.26	109.90
2	AAA	401	HEM	CAD-CBD-CGD	2.02	119.01	113.67
2	BBB	401	HEM	CAA-C2A-C1A	2.01	128.86	124.94

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	ZIQ	OXT-C-CA-C1

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Mol	Chain	Res	Type	Atoms
3	DDD	402	ZIQ	O-C-CA-C1
3	DDD	402	ZIQ	OXT-C-CA-C1
4	DDD	403	A1AER	C12-C13-C15-N16
3	AAA	402	ZIQ	O-C-CA-C1
3	DDD	402	ZIQ	O-C-CA-CB
3	DDD	402	ZIQ	OXT-C-CA-CB
2	DDD	401	HEM	C4C-C3C-CAC-CBC
4	BBB	403	A1AER	C12-C13-C15-N16
4	AAA	403	A1AER	C13-C12-C7-C11
2	AAA	401	HEM	C2A-CAA-CBA-CGA
3	AAA	402	ZIQ	OXT-C-CA-CB
2	DDD	401	HEM	CAA-CBA-CGA-O2A
2	BBB	401	HEM	CAA-CBA-CGA-O1A
2	BBB	401	HEM	CAA-CBA-CGA-O2A
2	CCC	401	HEM	CAA-CBA-CGA-O1A
2	AAA	401	HEM	CAA-CBA-CGA-O1A
2	DDD	401	HEM	CAA-CBA-CGA-O1A
2	CCC	401	HEM	CAA-CBA-CGA-O2A
2	AAA	401	HEM	CAA-CBA-CGA-O2A
3	BBB	402	ZIQ	O-C-CA-C1
3	BBB	402	ZIQ	OXT-C-CA-C1
2	AAA	401	HEM	C4C-C3C-CAC-CBC
4	BBB	403	A1AER	C12-C13-C15-N19
4	DDD	403	A1AER	C12-C13-C15-N19
3	AAA	402	ZIQ	O-C-CA-CB

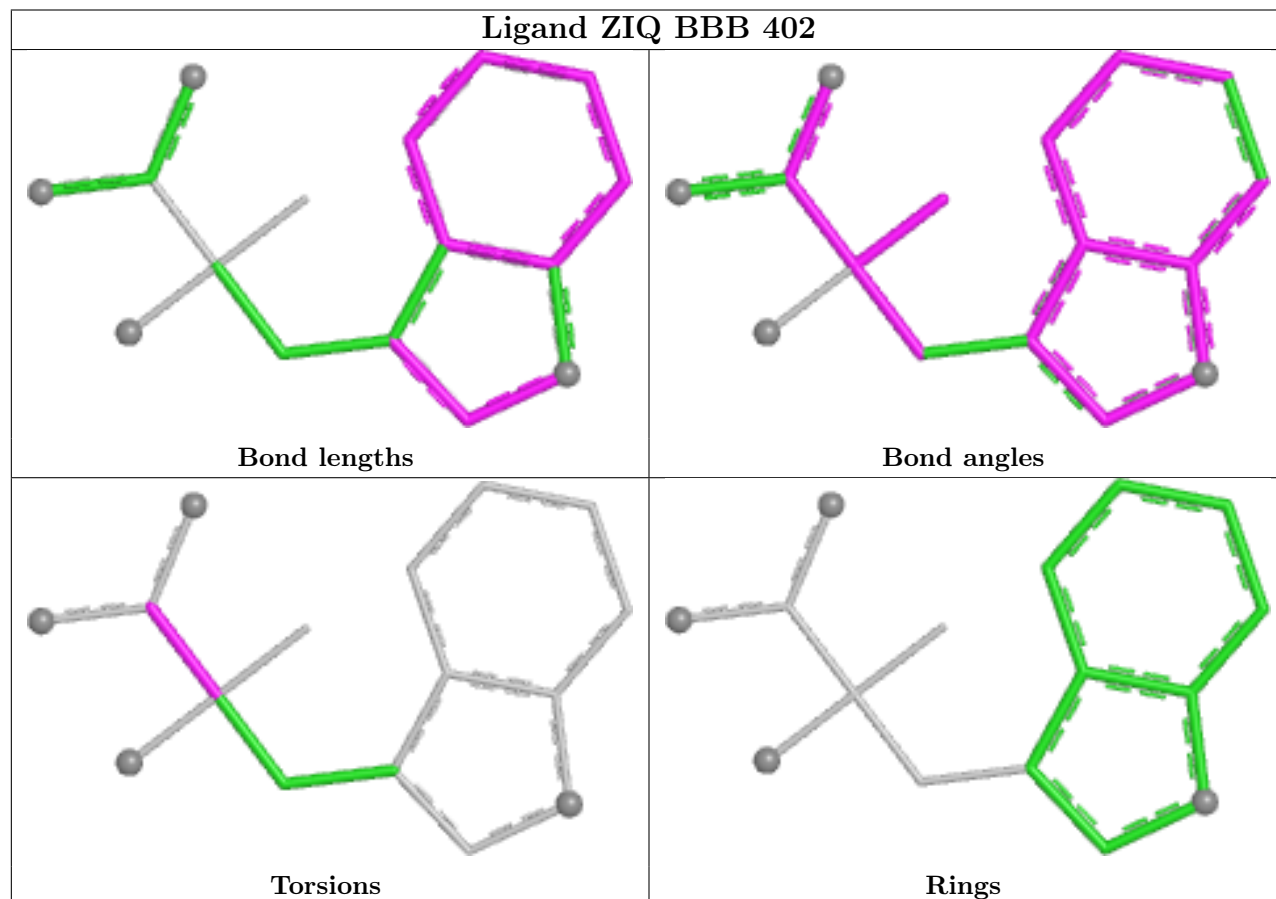
There are no ring outliers.

7 monomers are involved in 20 short contacts:

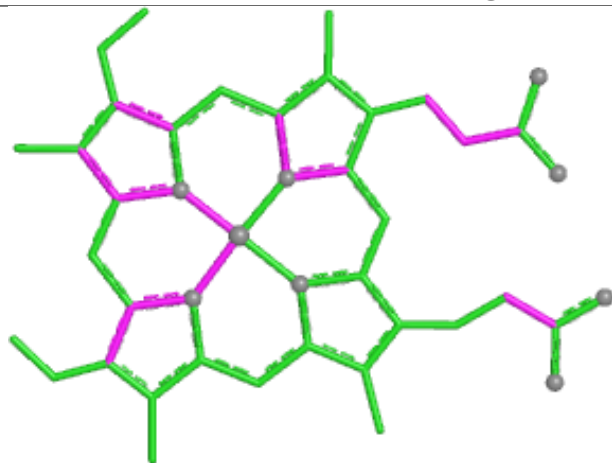
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	401	HEM	4	0
2	CCC	401	HEM	3	0
4	BBB	403	A1AER	1	0
4	AAA	403	A1AER	3	0
4	DDD	403	A1AER	1	0
2	AAA	401	HEM	5	0
2	DDD	401	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

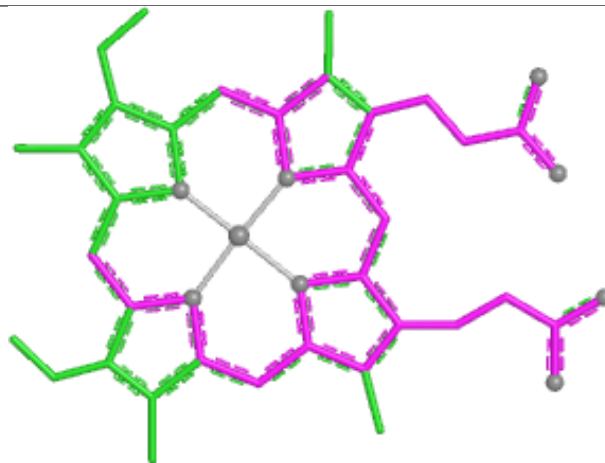
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



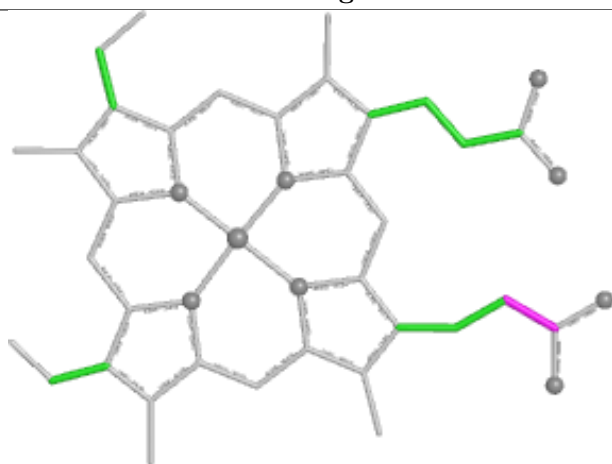
Ligand HEM BBB 401



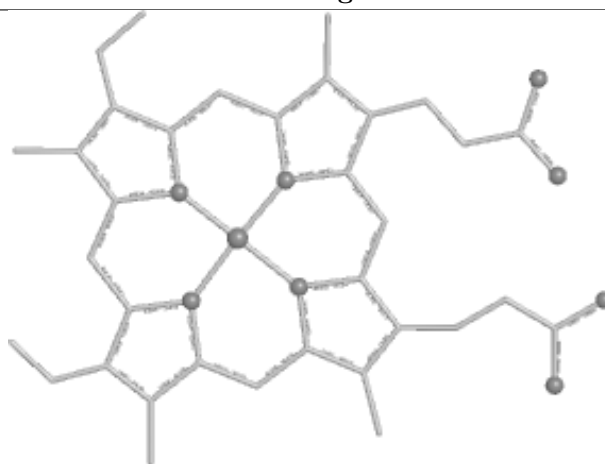
Bond lengths



Bond angles

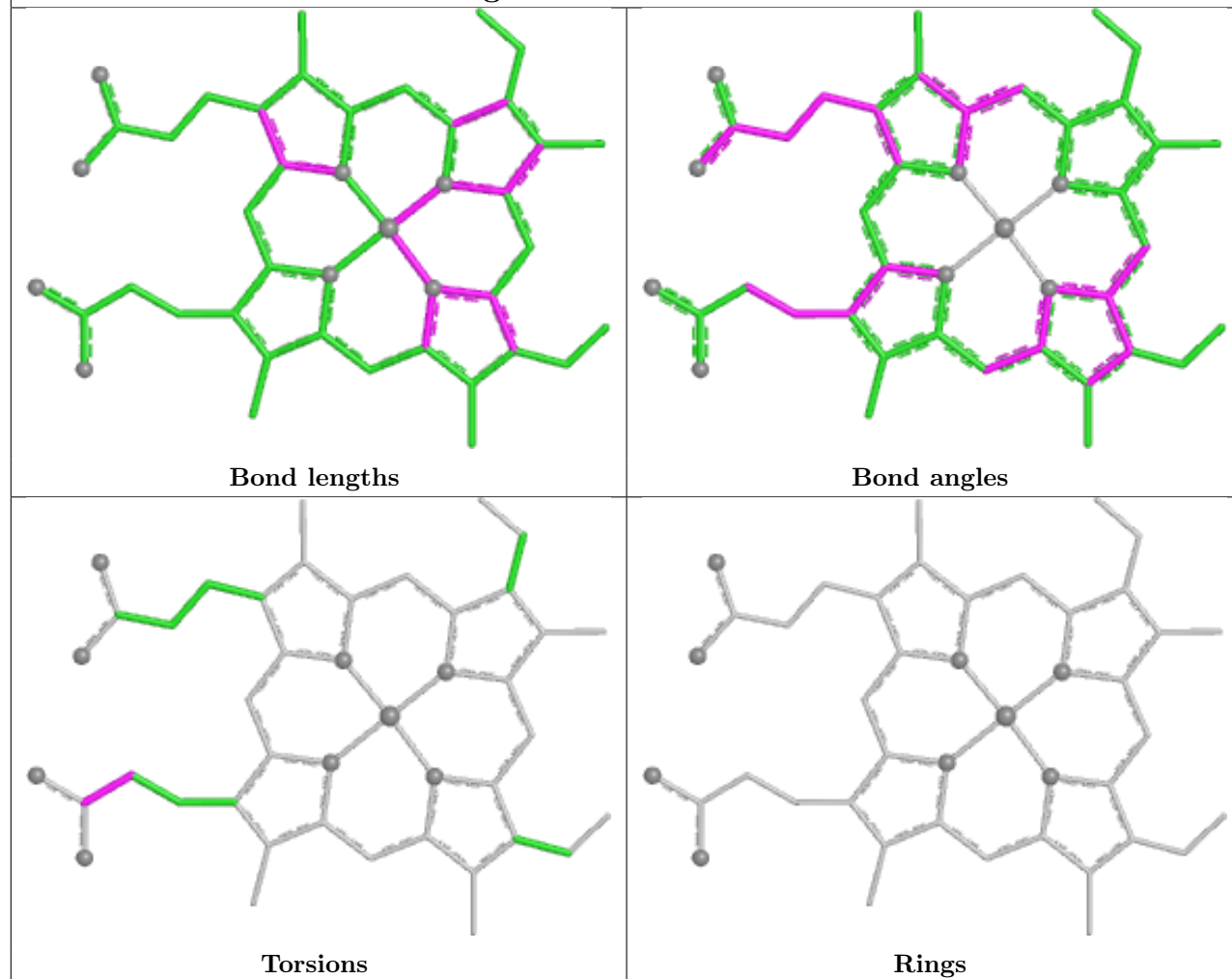


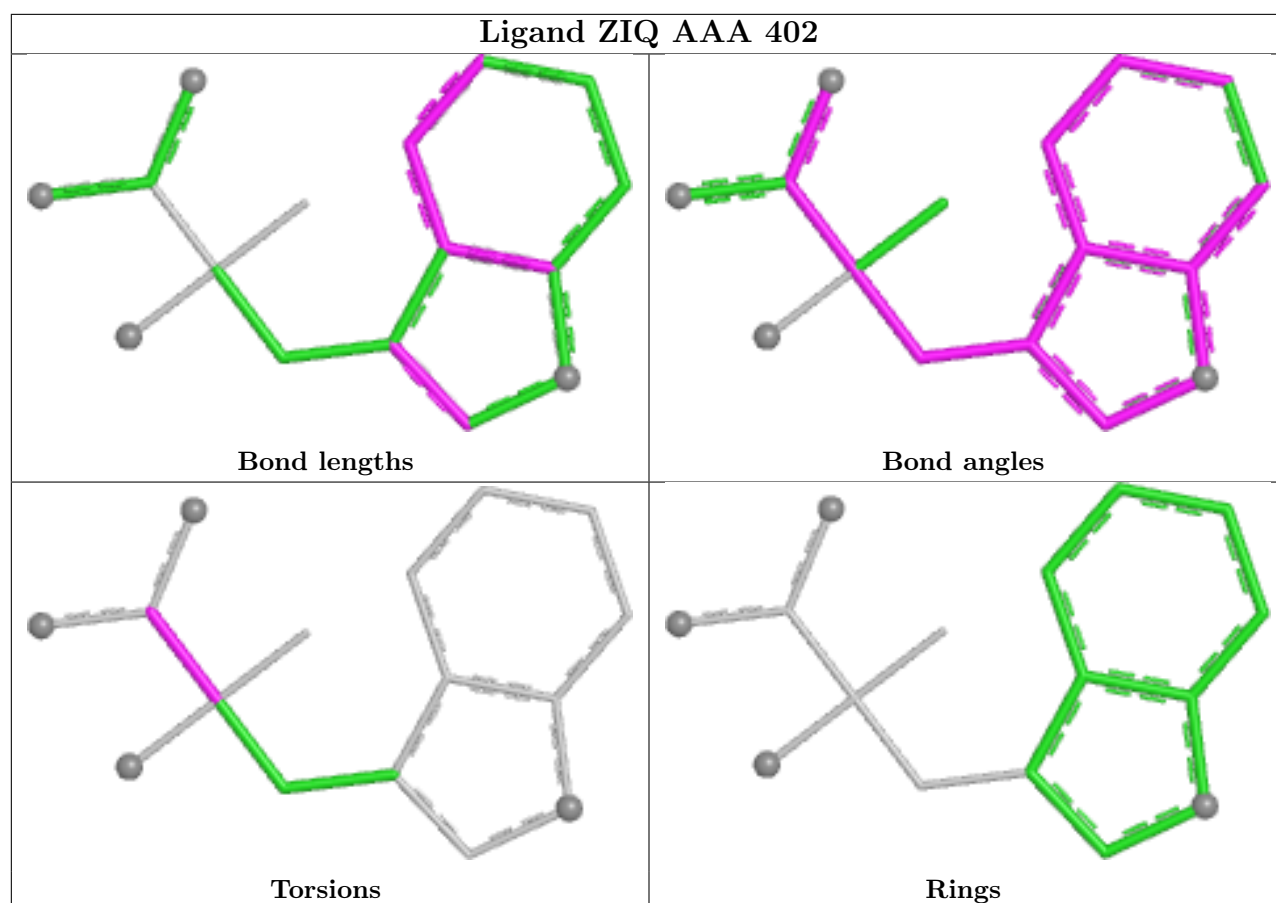
Torsions



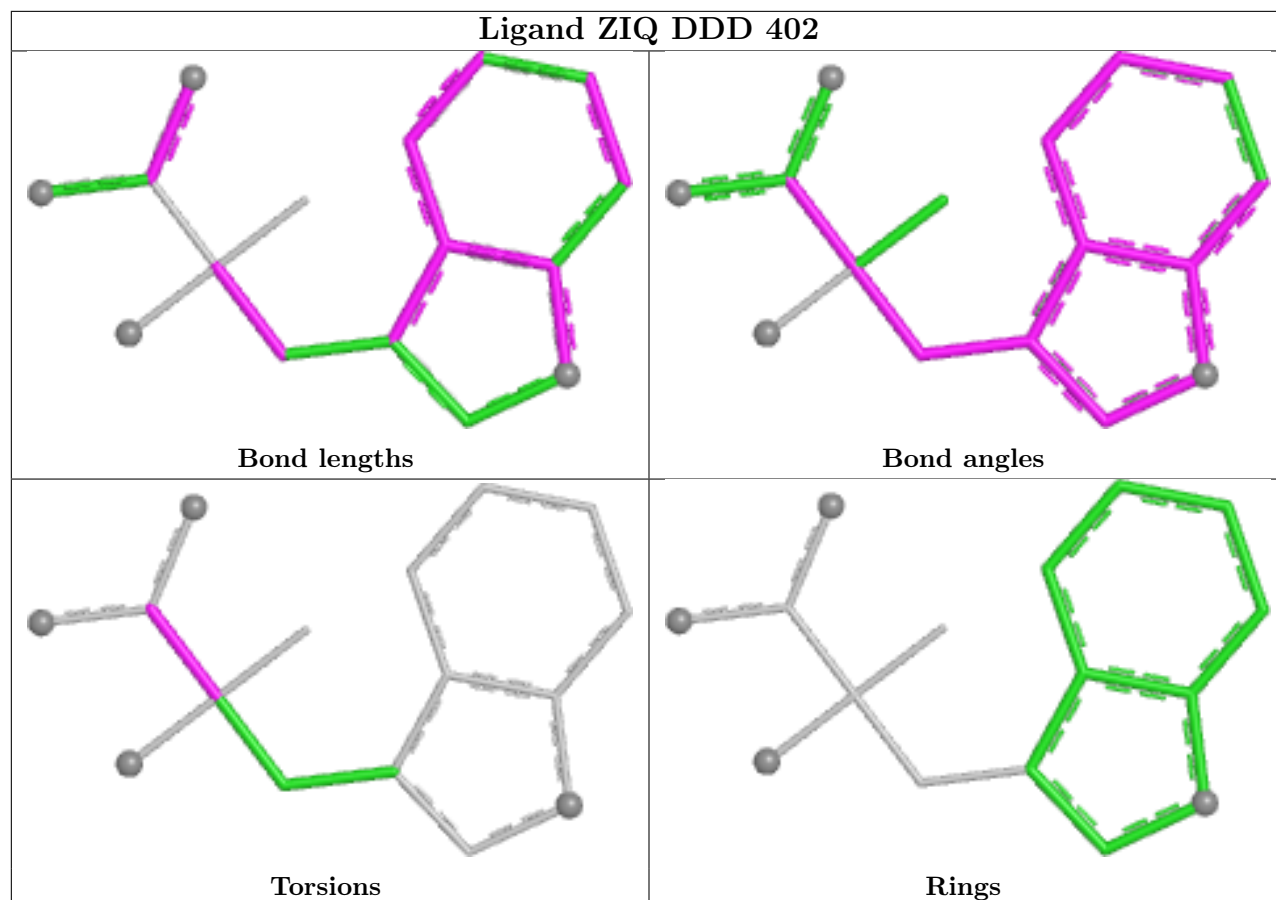
Rings

Ligand HEM CCC 401

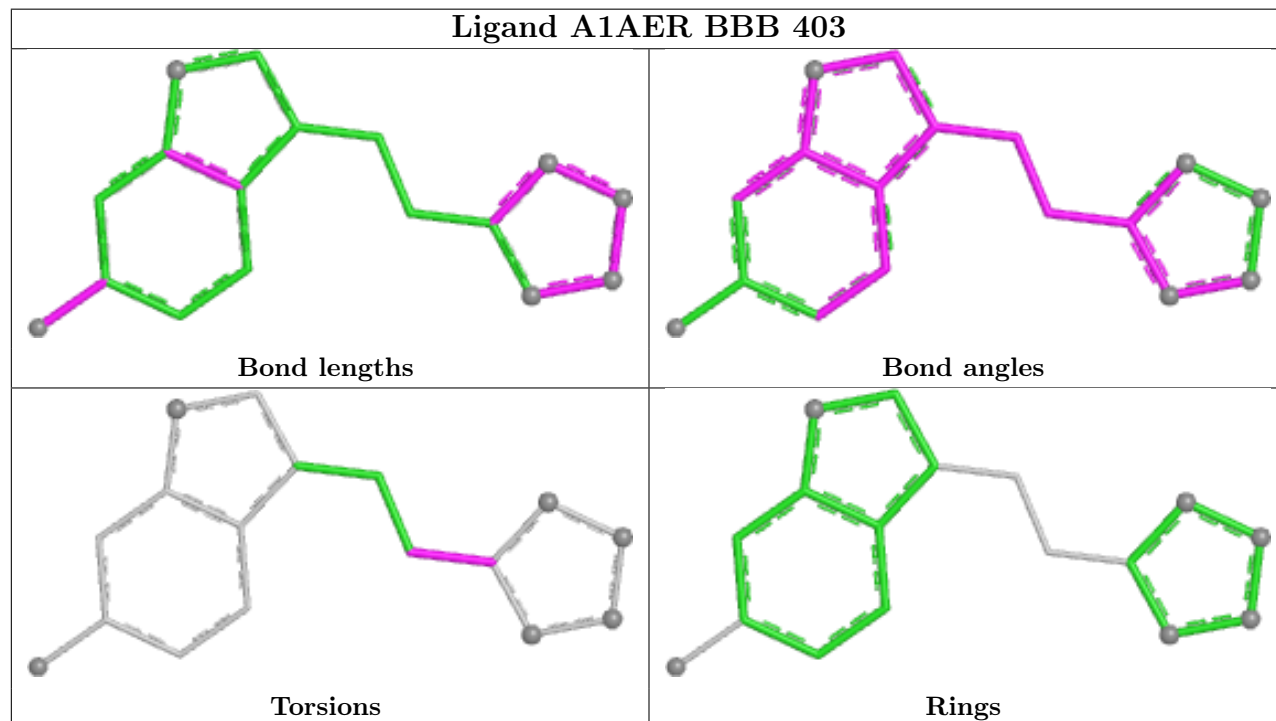




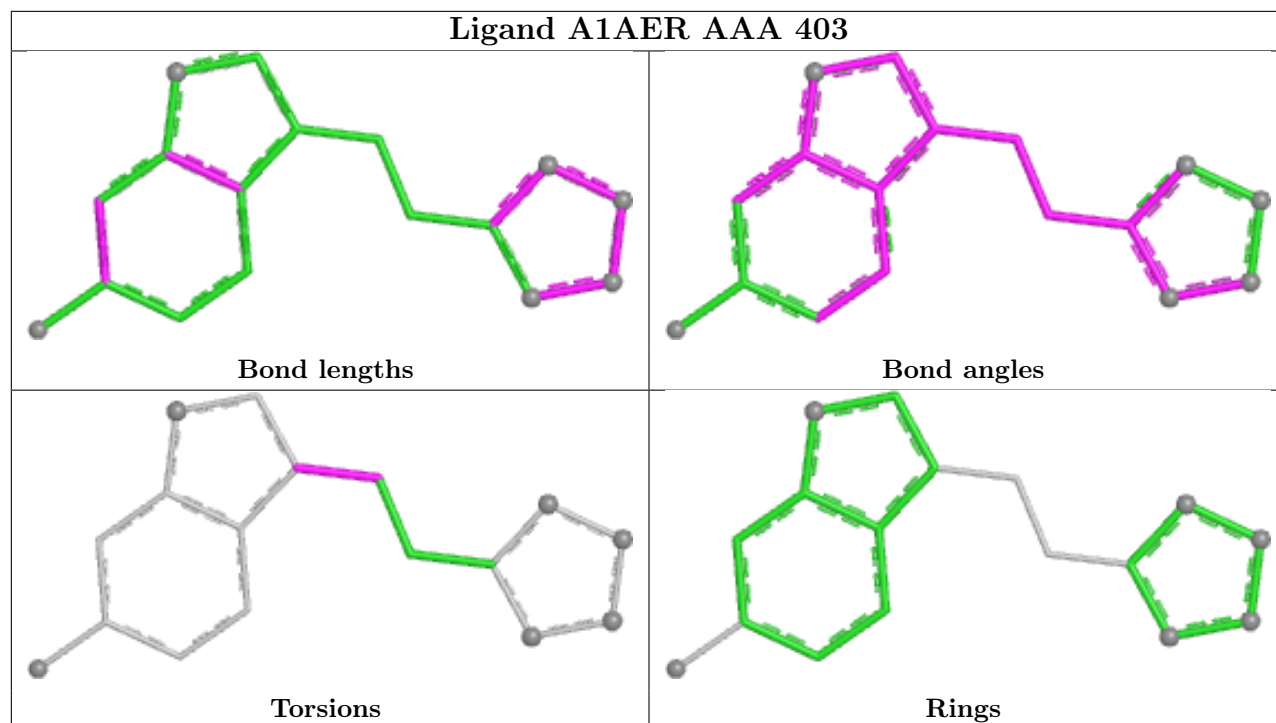
Ligand ZIQ DDD 402



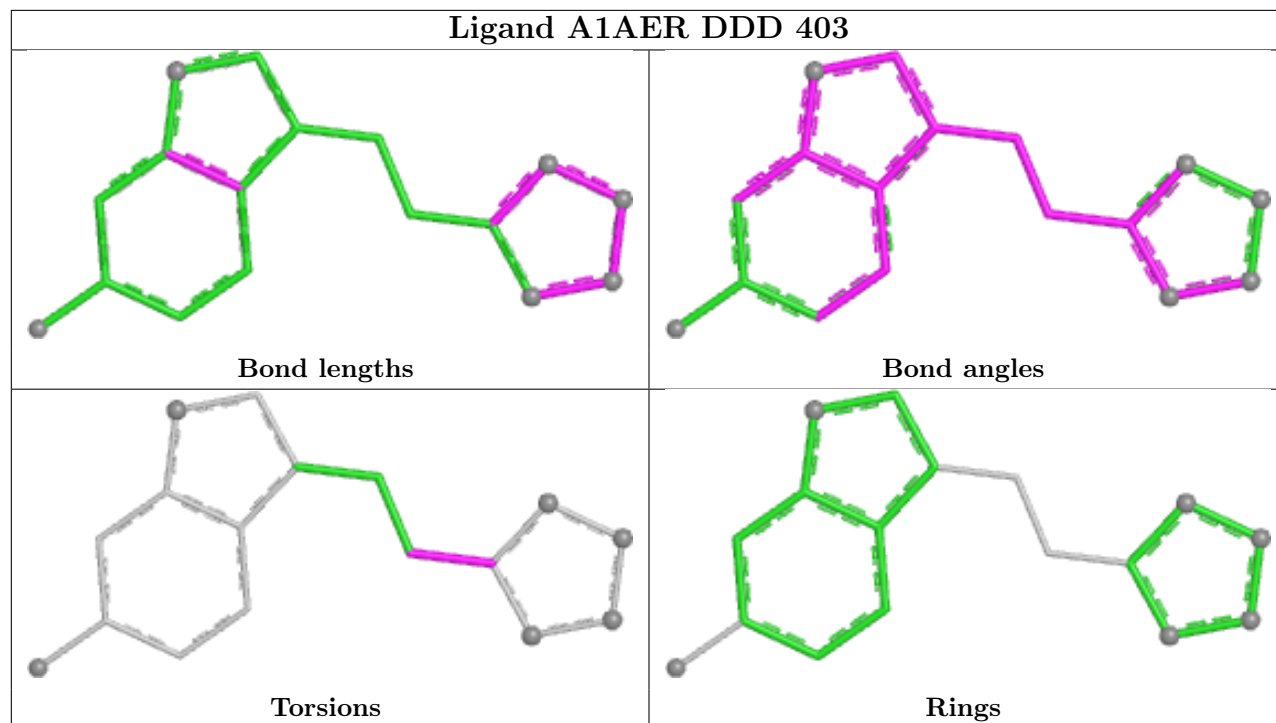
Ligand A1AER BBB 403



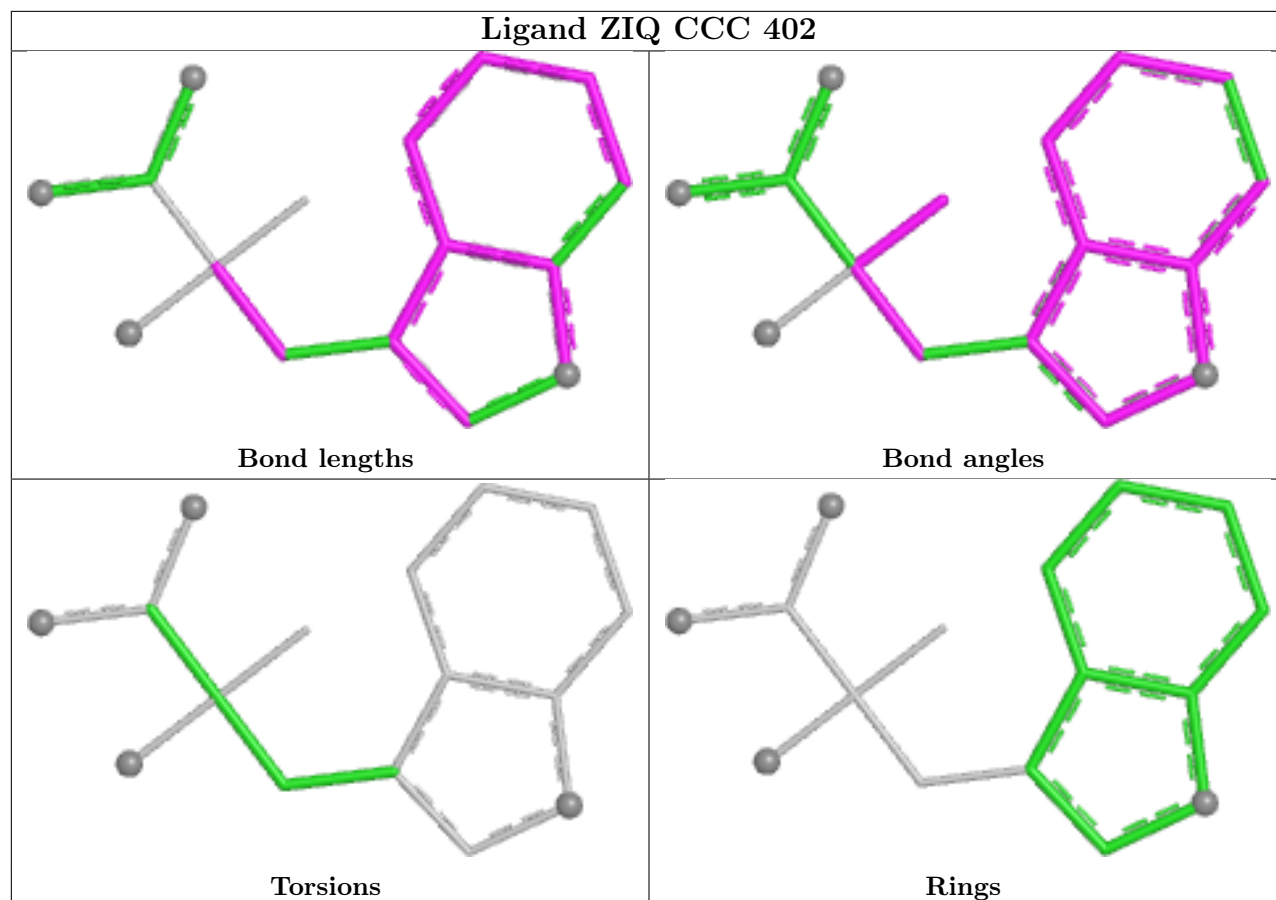
Ligand A1AER AAA 403



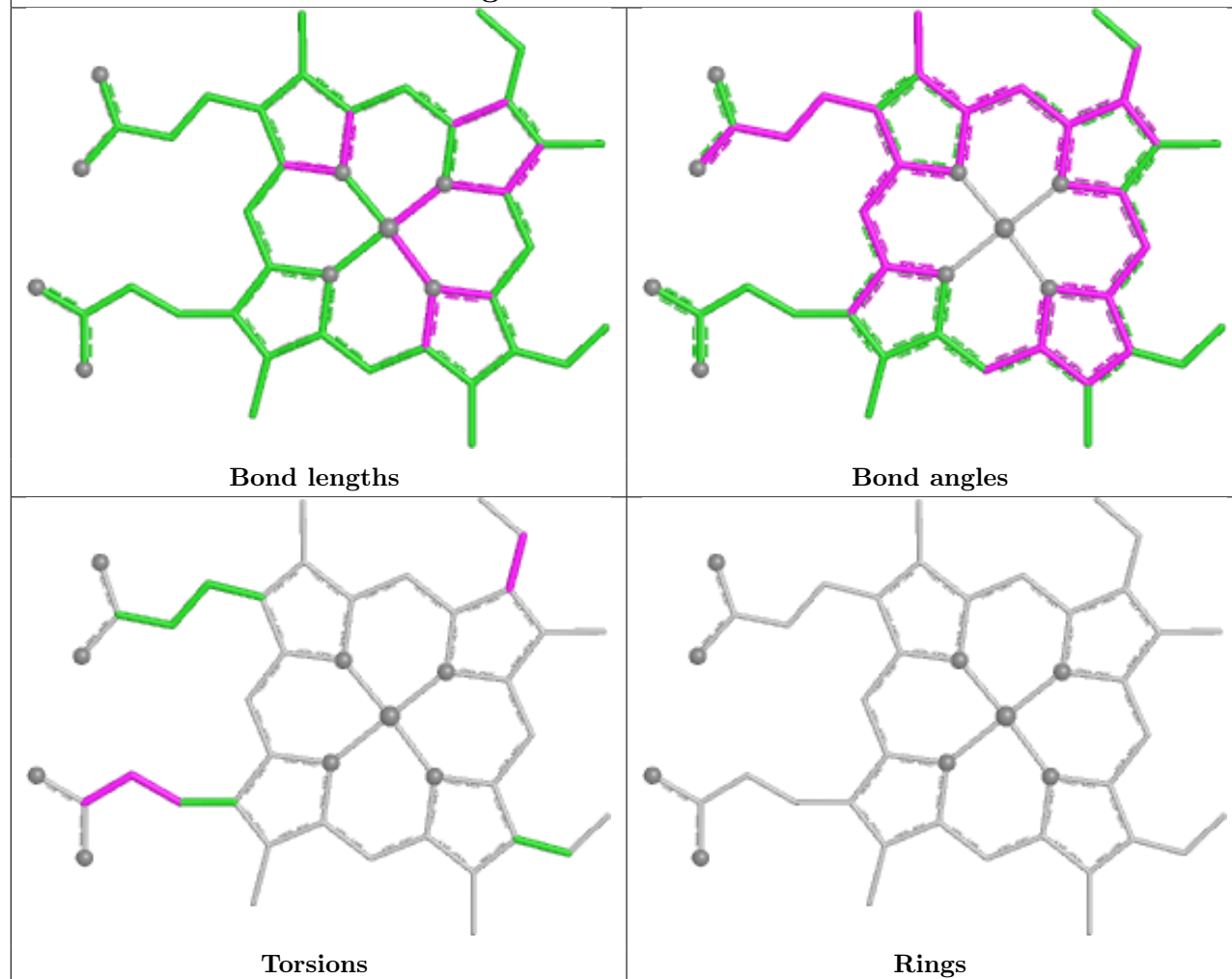
Ligand A1AER DDD 403

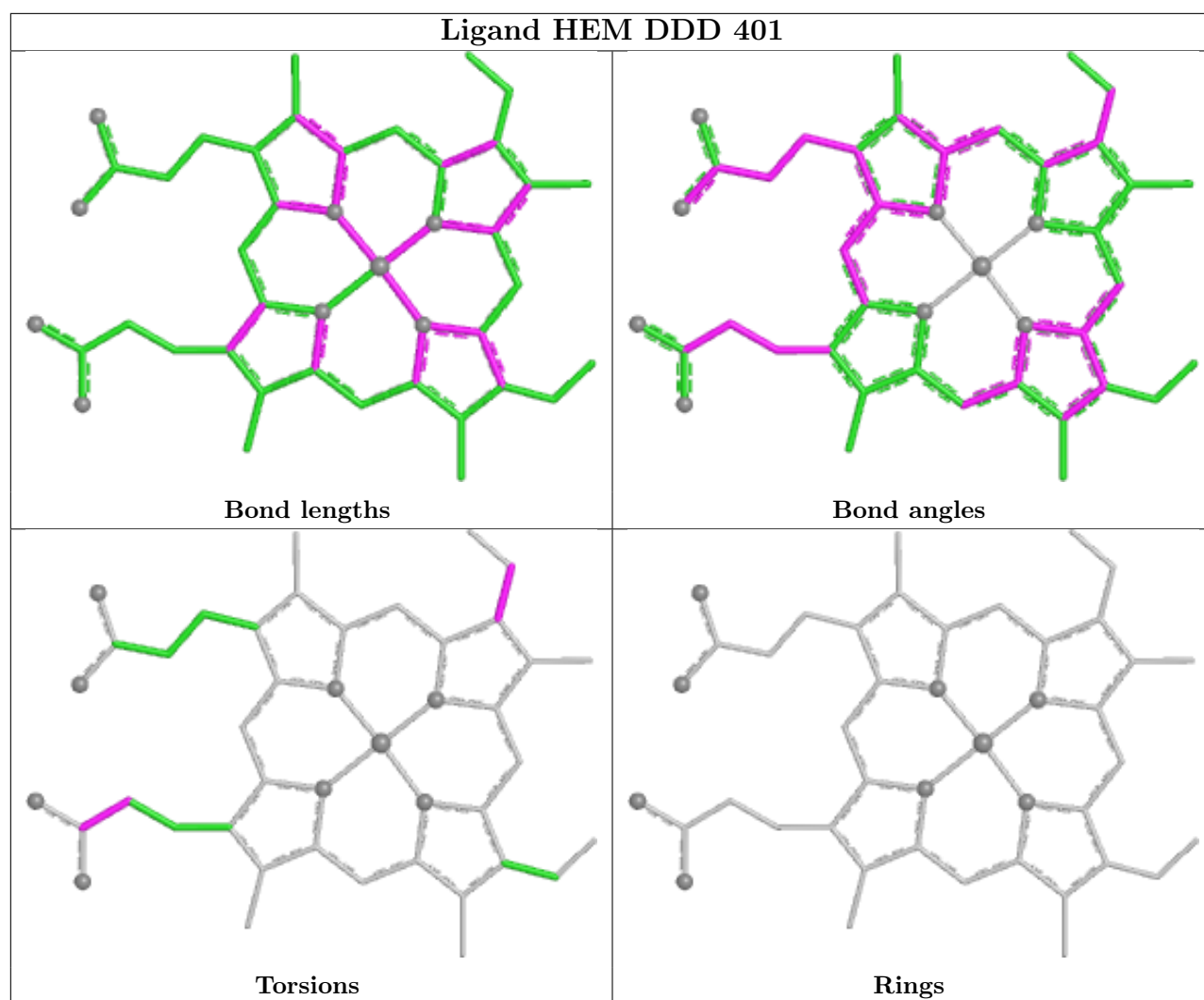


Ligand ZIQ CCC 402



Ligand HEM AAA 401





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	AAA	344/380 (90%)	0.07	11 (3%) 50 52	30, 53, 117, 141	0
1	BBB	344/380 (90%)	-0.05	16 (4%) 36 38	29, 46, 112, 136	0
1	CCC	326/380 (85%)	0.29	12 (3%) 45 48	31, 61, 118, 152	0
1	DDD	343/380 (90%)	-0.01	6 (1%) 69 70	31, 53, 104, 147	0
All	All	1357/1520 (89%)	0.08	45 (3%) 49 51	29, 53, 115, 152	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	385	ILE	4.8
1	AAA	175	TYR	4.8
1	AAA	385	ILE	4.6
1	BBB	340	ALA	4.6
1	DDD	338	SER	4.1
1	AAA	339	LYS	4.0
1	AAA	388	PHE	3.9
1	CCC	347	GLY	3.8
1	BBB	388	PHE	3.7
1	BBB	175	TYR	3.7
1	CCC	174	PRO	3.6
1	CCC	254	VAL	3.6
1	CCC	326	TYR	3.5
1	BBB	346	SER	3.4
1	AAA	179	HIS	3.2
1	AAA	389	LEU	3.2
1	DDD	243	ALA	3.1
1	DDD	383	PRO	3.1
1	CCC	179	HIS	3.0
1	CCC	40	LEU	2.9
1	BBB	385	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	CCC	391	HIS	2.8
1	AAA	338	SER	2.8
1	CCC	255	ALA	2.8
1	BBB	38	GLY	2.7
1	BBB	383	PRO	2.6
1	BBB	168	LEU	2.6
1	BBB	180	TYR	2.6
1	AAA	174	PRO	2.6
1	AAA	383	PRO	2.5
1	DDD	348	TYR	2.5
1	CCC	388	PHE	2.4
1	BBB	348	TYR	2.4
1	BBB	173	VAL	2.4
1	BBB	384	THR	2.4
1	CCC	193	LEU	2.4
1	BBB	386	HIS	2.4
1	AAA	384	THR	2.3
1	BBB	171	MET	2.2
1	AAA	149	PRO	2.1
1	DDD	386	HIS	2.1
1	CCC	39	GLY	2.1
1	DDD	40	LEU	2.0
1	BBB	333	HIS	2.0
1	BBB	174	PRO	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](#)

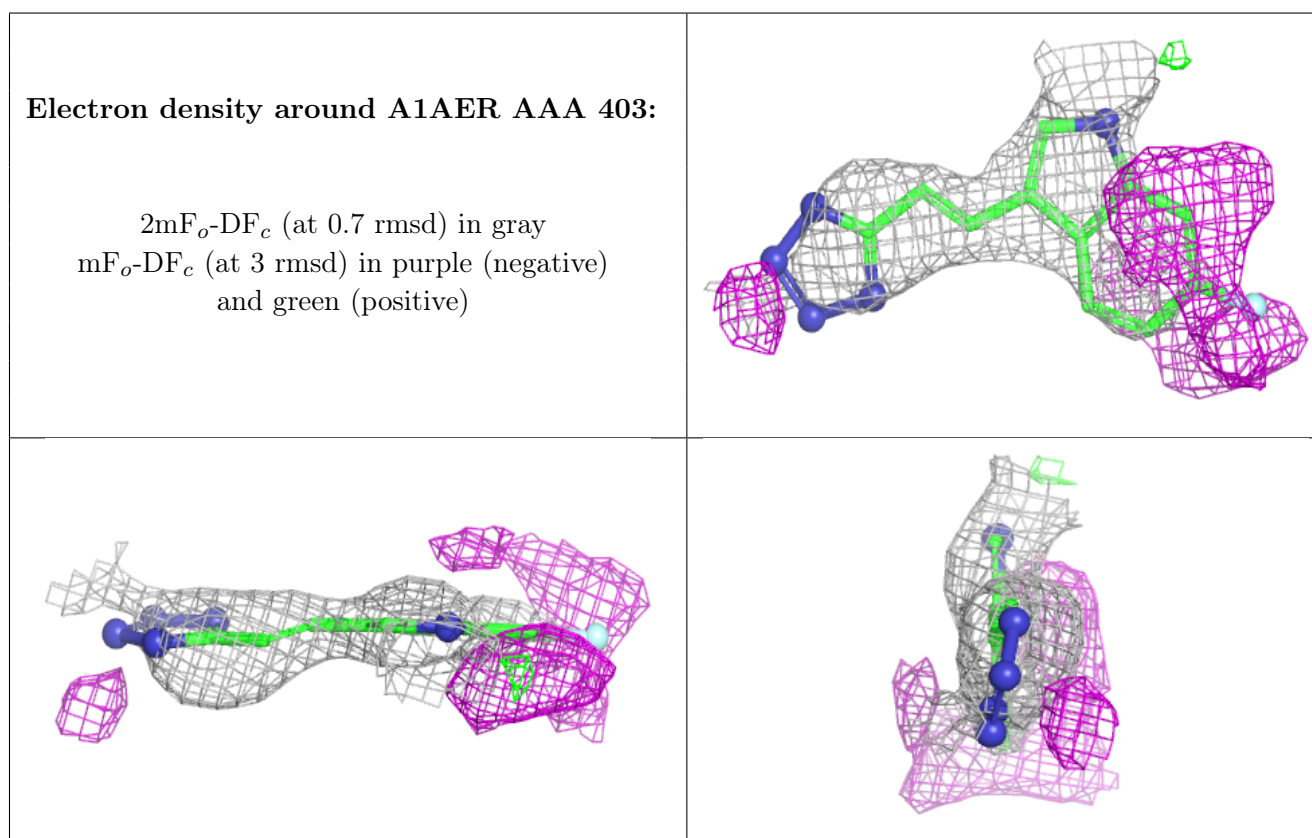
There are no oligosaccharides in this entry.

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.

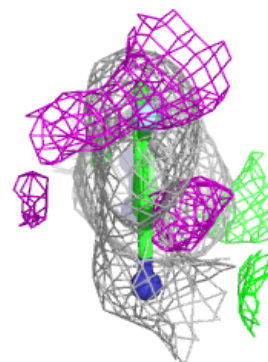
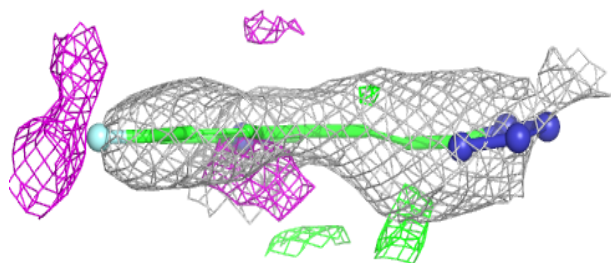
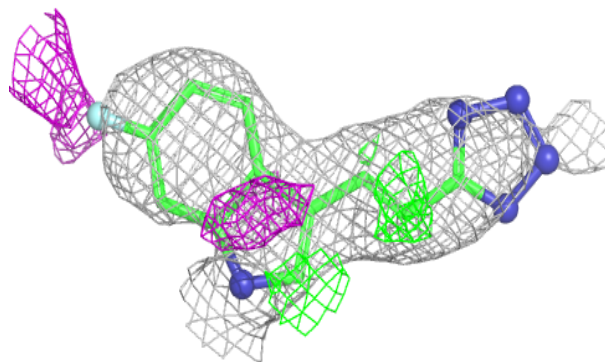
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1AER	AAA	403	17/17	0.86	0.19	94,103,122,123	0
4	A1AER	BBB	403	17/17	0.86	0.18	79,90,123,124	0
4	A1AER	DDD	403	17/17	0.91	0.15	80,90,100,117	0
3	ZIQ	CCC	402	16/16	0.95	0.07	45,51,62,68	0
3	ZIQ	DDD	402	16/16	0.96	0.06	42,47,54,57	0
3	ZIQ	BBB	402	16/16	0.97	0.05	33,36,38,41	0
2	HEM	CCC	401	43/43	0.97	0.07	47,61,71,85	0
2	HEM	BBB	401	43/43	0.98	0.05	37,45,61,63	0
2	HEM	AAA	401	43/43	0.98	0.06	40,51,64,74	0
3	ZIQ	AAA	402	16/16	0.98	0.04	32,37,53,64	0
2	HEM	DDD	401	43/43	0.99	0.06	36,44,66,81	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.

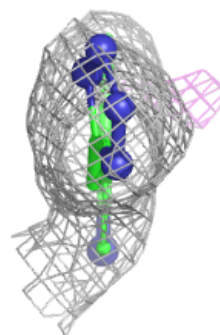
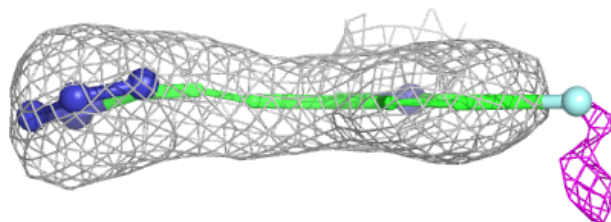
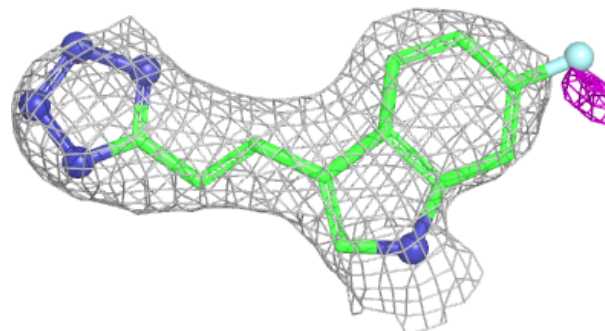


Electron density around A1AER BBB 403:

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

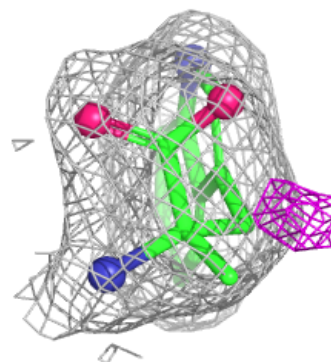
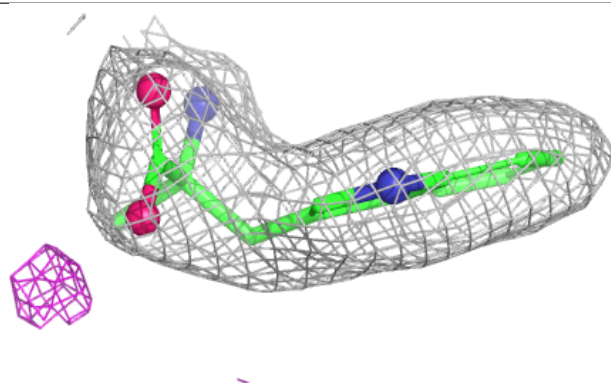
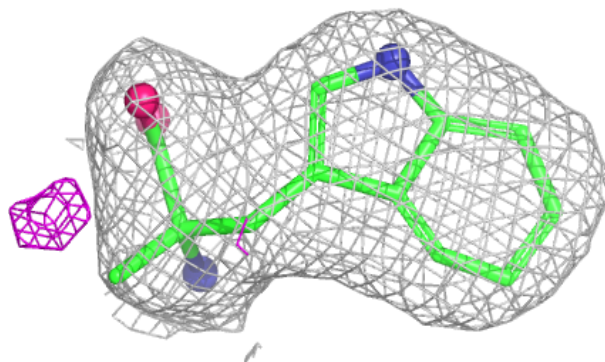
**Electron density around A1AER DDD 403:**

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

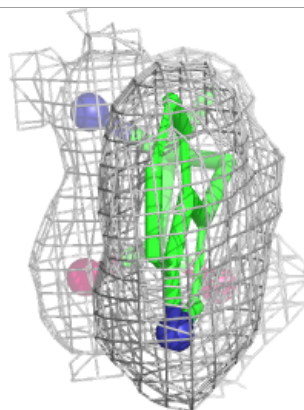
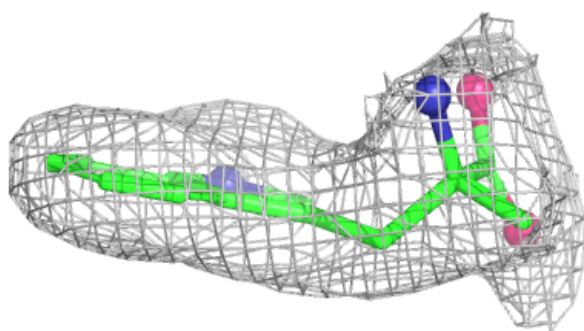
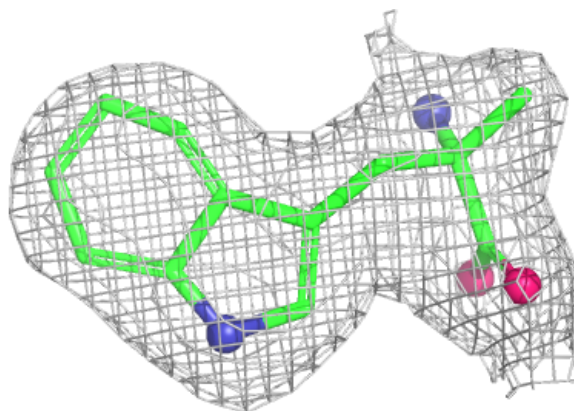


Electron density around ZIQ CCC 402:

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

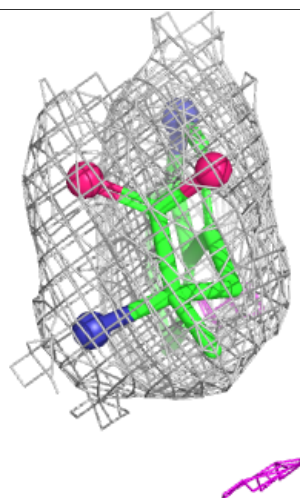
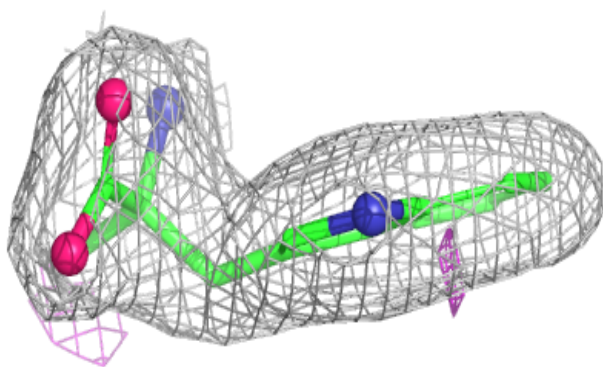
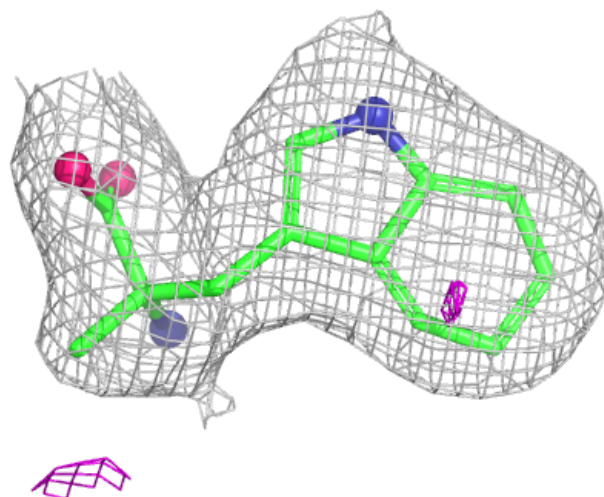
**Electron density around ZIQ DDD 402:**

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



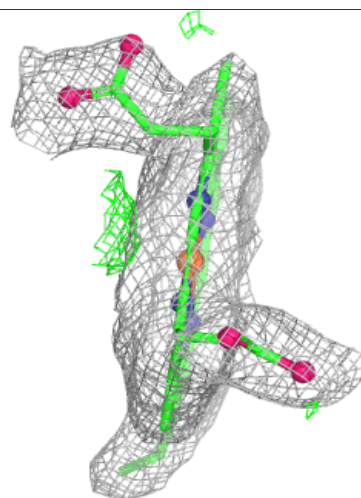
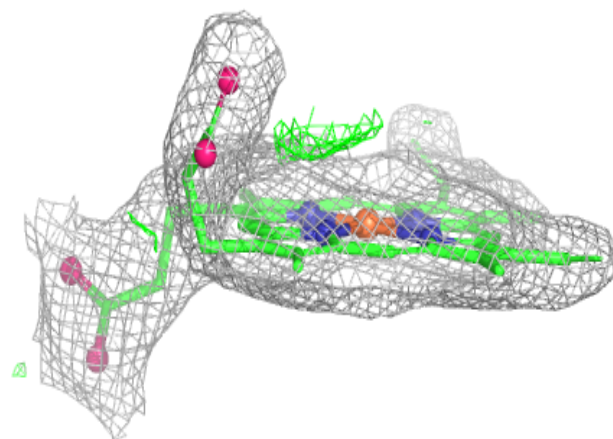
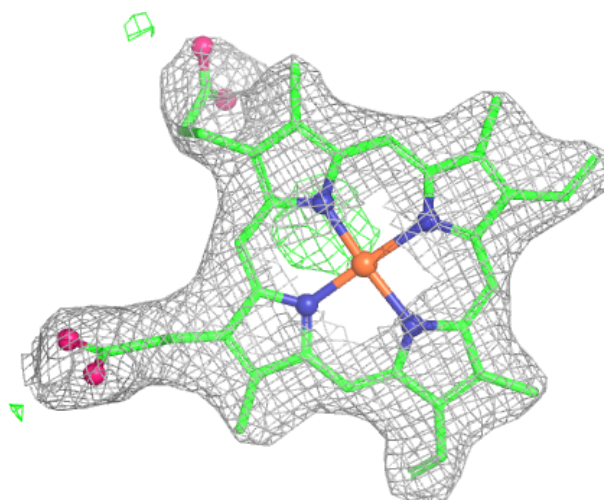
Electron density around ZIQ BBB 402:

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



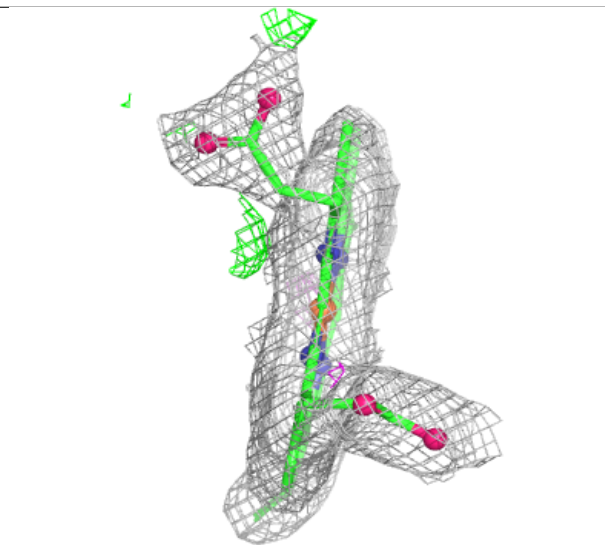
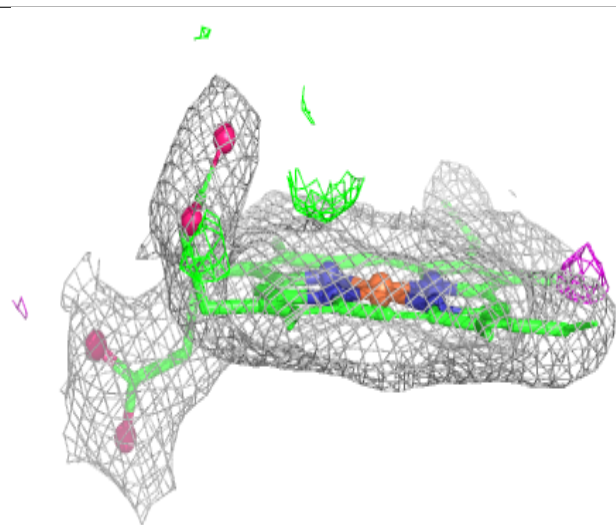
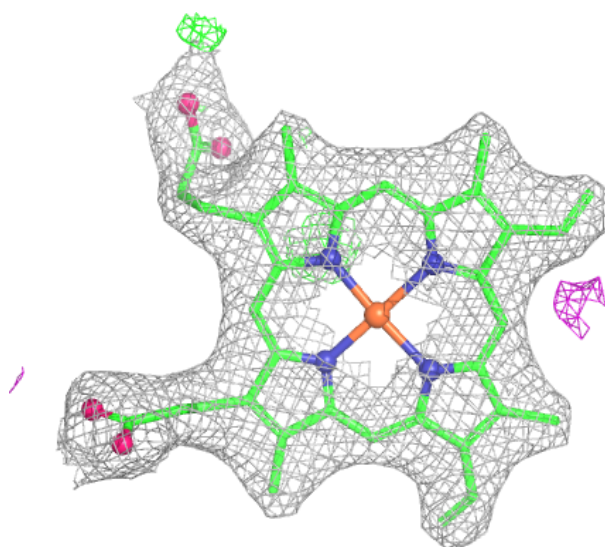
Electron density around HEM CCC 401:

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



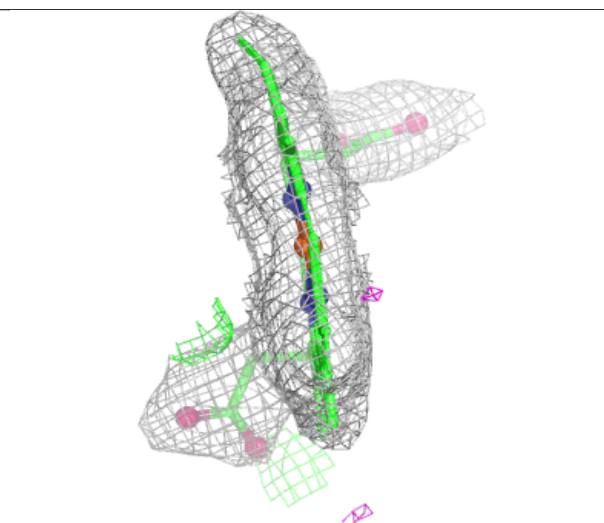
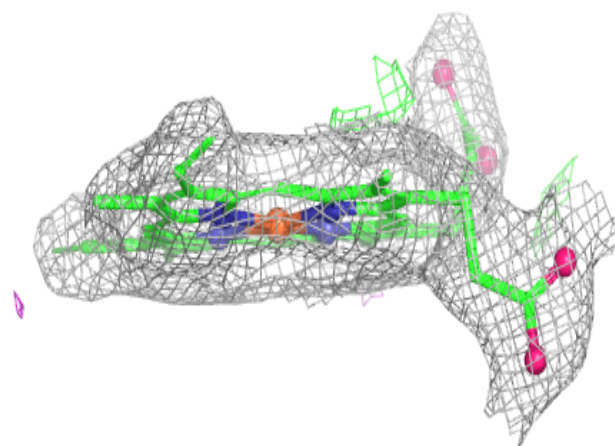
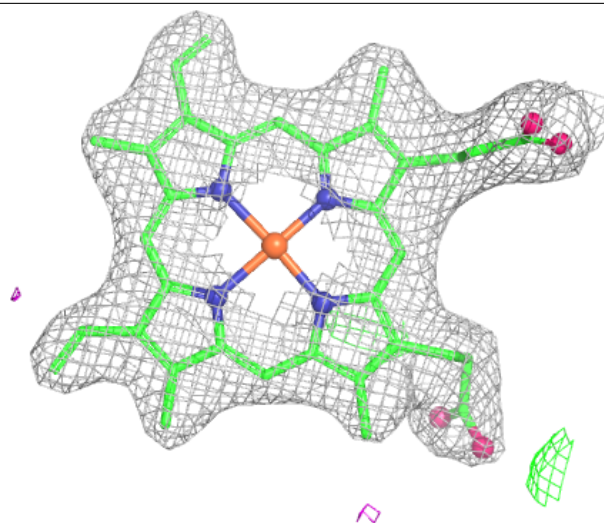
Electron density around HEM BBB 401:

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



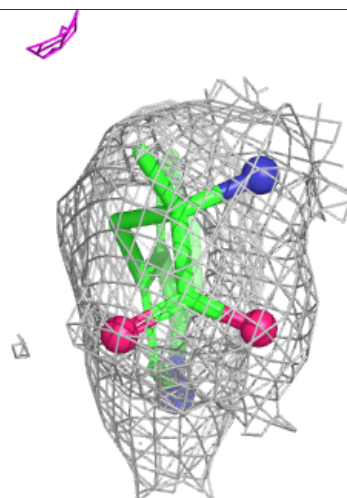
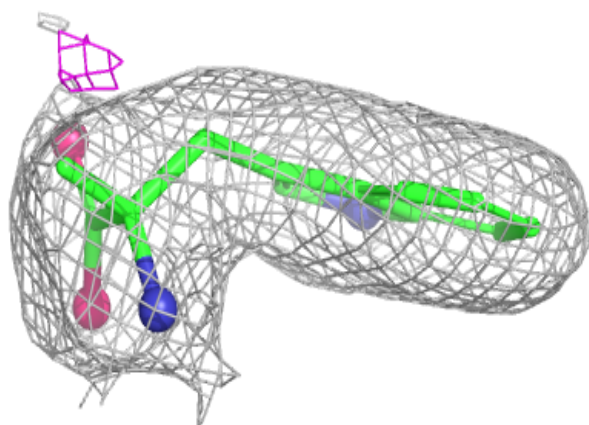
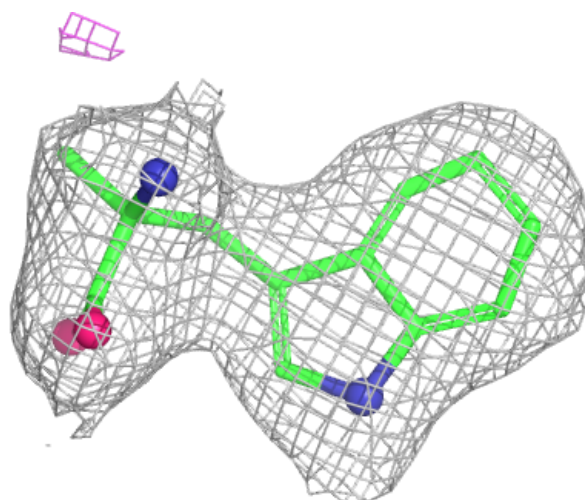
Electron density around HEM AAA 401:

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



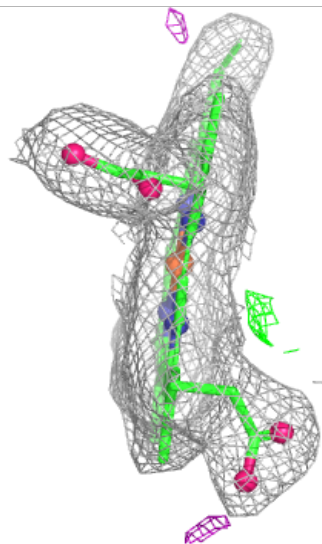
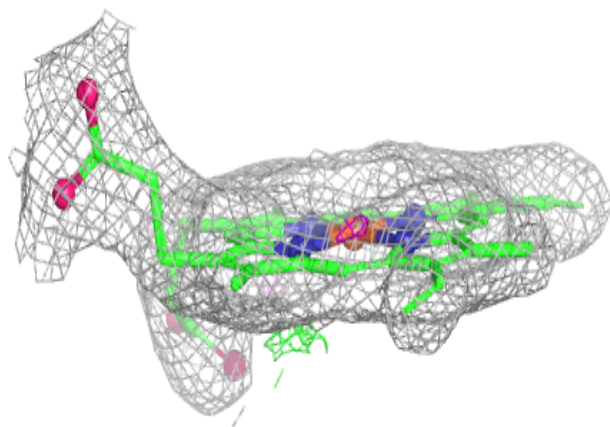
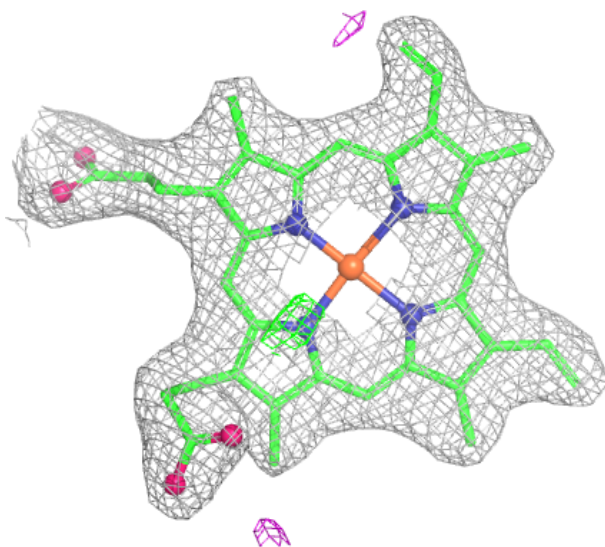
Electron density around ZIQ AAA 402:

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



Electron density around HEM DDD 401:

$2mF_o-DF_c$ (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.