



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 12:41 PM EDT

PDB ID : 9Q4X / pdb_00009q4x
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-((5-(2-(dimethylamino)ethyl)-2,3-difluorophenoxy)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2025-08-20
Resolution : 2.15 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

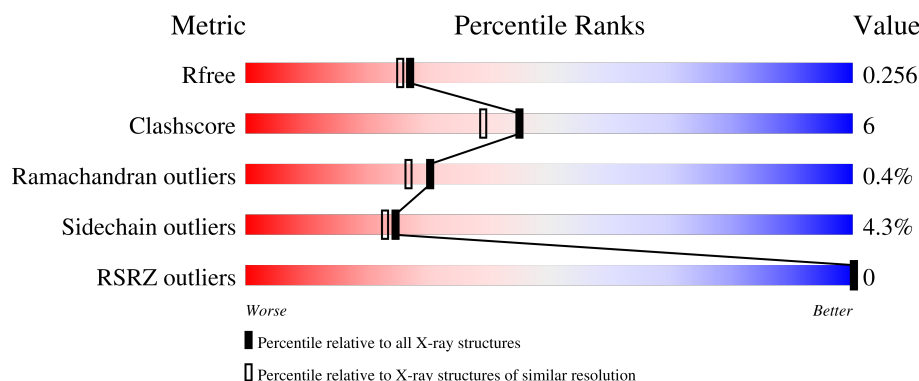
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.15 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	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	440	
1	B	440	
1	C	440	
1	D	440	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13841 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 Nitric oxide synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	1	0
			3191	2032	561	582	16			
1	B	402	Total	C	N	O	S	0	4	0
			3225	2054	566	589	16			
1	C	400	Total	C	N	O	S	0	1	0
			3200	2038	563	583	16			
1	D	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	conflict	UNP P29474
B	298	GLU	ASP	conflict	UNP P29474
C	298	GLU	ASP	conflict	UNP P29474
D	298	GLU	ASP	conflict	UNP P29474

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



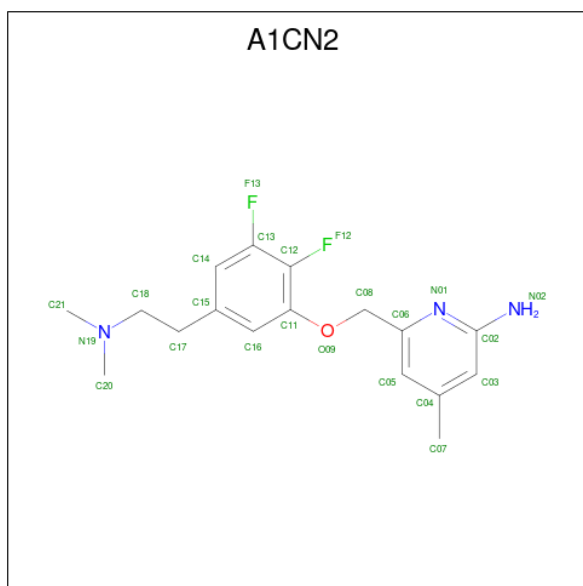
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-({5-[2-(dimethylamino)ethyl]-2,3-difluorophenoxy}methyl)-4-methylpyridin-2-amine (CCD ID: A1CN2) (formula: C₁₇H₂₁F₂N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			23	17	2	3	1		
4	B	1	Total	C	F	N	O	0	0
			23	17	2	3	1		
4	C	1	Total	C	F	N	O	0	0
			23	17	2	3	1		
4	D	1	Total	C	F	N	O	0	0
			23	17	2	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Gd 1 1	0	0
8	B	1	Total Gd 1 1	0	0
8	C	1	Total Gd 1 1	0	0
8	D	1	Total Gd 1 1	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Zn 1 1	0	0
9	C	1	Total Zn 1 1	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Ca 1 1	0	0
10	B	1	Total Ca 1 1	0	0


- Molecule 11 is water.

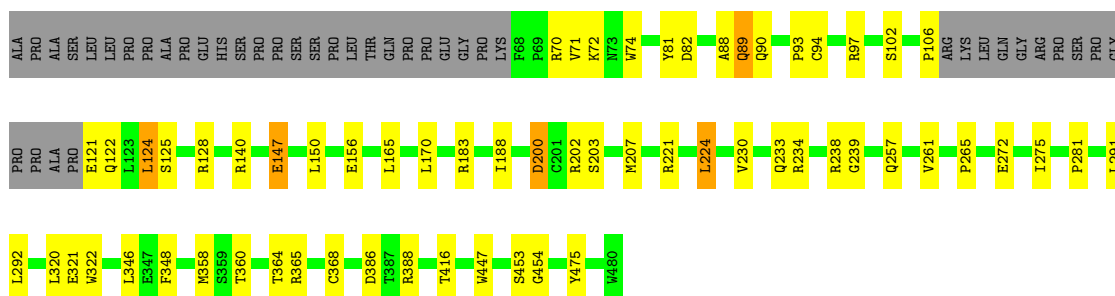
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	112	Total O 112 112	0	0
11	B	159	Total O 159 159	0	0
11	C	103	Total O 103 103	0	0
11	D	147	Total O 147 147	0	0

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.

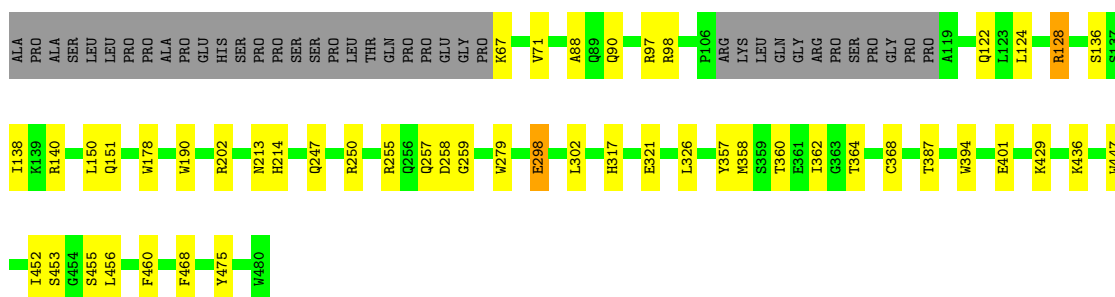
• Molecule 1: Nitric oxide synthase 3

Chain A: 



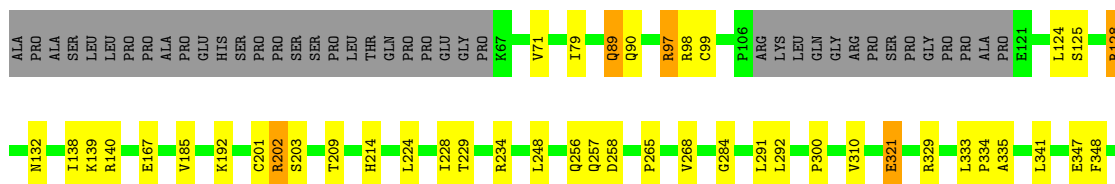
• Molecule 1: Nitric oxide synthase 3

Chain B: 



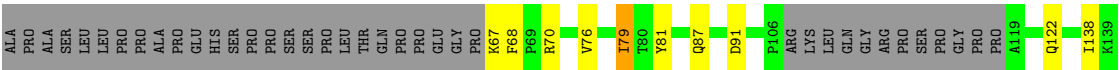
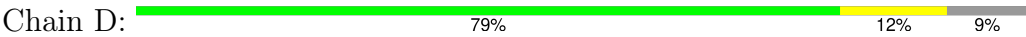
• Molecule 1: Nitric oxide synthase 3

Chain C: 





● Molecule 1: Nitric oxide synthase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.96Å 154.22Å 109.11Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	39.26 – 2.15 39.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.26-2.15) 94.4 (39.26-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.203 , 0.261 0.200 , 0.256	Depositor DCC
R_{free} test set	5066 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13841	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: GOL, CA, CL, GD, H4B, A1CN2, HEM, BTB, ZN

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	0.31	0/3285	0.52	0/4476
1	B	0.38	0/3329	0.55	0/4536
1	C	0.32	0/3294	0.49	0/4487
1	D	0.36	0/3307	0.56	0/4506
All	All	0.34	0/13215	0.53	0/18005

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	3191	0	3091	33	0
1	B	3225	0	3131	27	0
1	C	3200	0	3104	33	0
1	D	3212	0	3116	36	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	23	0	0	0	0
4	B	23	0	0	1	0
4	C	23	0	0	0	0
4	D	23	0	0	0	0
5	A	28	0	37	7	0
5	B	28	0	36	6	0
5	C	28	0	37	3	0
5	D	28	0	37	11	0
6	A	12	0	16	0	0
6	B	6	0	8	0	0
6	C	12	0	16	1	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	112	0	0	3	0
11	B	159	0	0	2	0
11	C	103	0	0	6	0
11	D	147	0	0	4	0
All	All	13841	0	12817	151	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 6.

All (151) 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:C:292:LEU:HD22	1:C:300:PRO:HB2	1.62	0.81
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.66	0.74
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.71	0.73
1:D:70:ARG:HD2	1:D:79:ILE:HD13	1.69	0.72
5:D:504:BTB:O8	11:D:601:HOH:O	2.07	0.72
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.68	0.72
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.72	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.72	0.70
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.76	0.68
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.13	0.66
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.77	0.66
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.77	0.66
5:C:505:BTB:O4	5:C:505:BTB:O3	2.10	0.65
1:A:200:ASP:OD1	1:A:200:ASP:N	2.30	0.64
1:A:97:ARG:HG3	1:B:88:ALA:HB3	1.80	0.63
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.15	0.63
1:B:213[B]:ASN:ND2	11:B:601:HOH:O	2.32	0.63
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.13	0.63
1:B:128:ARG:HG3	1:B:150:LEU:HD22	1.81	0.62
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.30	0.61
1:C:321:GLU:H	1:C:321:GLU:CD	2.08	0.61
1:A:221:ARG:NH1	11:A:606:HOH:O	2.33	0.61
1:C:341:LEU:HB3	1:C:348:PHE:HB2	1.83	0.61
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.81	0.61
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.18	0.61
1:D:173:GLY:HA3	1:D:343:ILE:HD13	1.83	0.60
5:B:504:BTB:O8	5:B:504:BTB:H62	2.01	0.59
1:D:396:ASP:OD1	1:D:396:ASP:N	2.30	0.59
1:D:308:GLU:H	1:D:308:GLU:CD	2.11	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.83	0.59
1:A:102:SER:O	3:A:502:H4B:O10	2.21	0.58
1:D:298:GLU:OE2	5:D:505:BTB:O8	2.18	0.57
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.23	0.57
1:B:298:GLU:CD	5:B:505:BTB:H41	2.30	0.57
1:B:358:MET:HE3	1:B:360:THR:OG1	2.04	0.57
1:A:70:ARG:HG3	1:A:81:TYR:CE2	2.41	0.56
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.87	0.56
1:C:97:ARG:HG2	1:C:98:ARG:HG2	1.87	0.55
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.40	0.55
5:A:505:BTB:HO8	5:A:505:BTB:HO3	1.54	0.55
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.89	0.55
1:A:90:GLN:NE2	11:A:602:HOH:O	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:O	1:C:352:PRO:HD2	2.08	0.54
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.22	0.53
1:A:257:GLN:HG3	1:C:388:ARG:NH2	2.23	0.53
1:D:138:ILE:O	1:D:140:ARG:HG2	2.09	0.53
5:D:505:BTB:O6	5:D:505:BTB:O3	2.23	0.53
1:C:265:PRO:HA	1:C:268:VAL:HG23	1.91	0.53
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.90	0.53
1:A:89:GLN:NE2	1:A:90:GLN:OE1	2.42	0.53
1:C:201:CYS:O	1:C:202:ARG:NH1	2.41	0.53
1:C:185:VAL:HG23	1:C:448:ILE:HG23	1.90	0.52
1:A:386:ASP:OD2	1:A:388:ARG:HG2	2.09	0.52
1:A:364:THR:O	1:A:368:CYS:HB2	2.08	0.52
1:C:71:VAL:HG12	11:C:651:HOH:O	2.09	0.52
1:B:298:GLU:OE2	5:B:505:BTB:H41	2.10	0.52
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.44	0.51
1:C:455:SER:HA	1:C:460:PHE:CG	2.45	0.51
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.23	0.51
1:B:447:TRP:HA	3:B:502:H4B:N1	2.25	0.51
2:B:501:HEM:HBD1	4:B:503:A1CN2:F12	2.00	0.51
1:D:379:VAL:HG21	1:D:402:ILE:HD11	1.93	0.51
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.51	0.51
1:D:298:GLU:CD	5:D:505:BTB:H42	2.35	0.50
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.25	0.50
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.30	0.50
1:B:364:THR:O	1:B:368:CYS:HB2	2.11	0.50
5:D:504:BTB:O8	5:D:504:BTB:H62	2.12	0.50
1:C:434:GLU:OE1	11:C:603:HOH:O	2.20	0.50
1:C:447:TRP:NE1	11:C:601:HOH:O	2.07	0.49
1:D:91:ASP:OD1	11:D:602:HOH:O	2.20	0.49
1:D:320:LEU:HD13	1:D:322:TRP:CZ2	2.47	0.49
5:B:505:BTB:H72	5:B:505:BTB:H12	1.35	0.49
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.94	0.49
1:C:378:ASP:OD1	11:C:602:HOH:O	2.19	0.49
1:D:358:MET:HE3	1:D:360:THR:OG1	2.13	0.49
5:A:504:BTB:O3	5:A:504:BTB:O4	2.27	0.48
1:D:234:ARG:NH1	1:D:347:GLU:OE1	2.42	0.48
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.49	0.48
1:C:284:GLY:N	11:C:608:HOH:O	2.46	0.48
1:A:165:LEU:HG	1:A:346:LEU:HD12	1.96	0.48
1:B:138:ILE:O	1:B:140:ARG:HG2	2.14	0.48
5:D:504:BTB:H32	5:D:504:BTB:H51	1.59	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:504:BTB:H72	5:A:504:BTB:H12	1.55	0.47
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.55	0.47
1:D:67:LYS:HG3	1:D:68:PHE:H	1.80	0.47
1:B:90:GLN:HB3	1:B:468:PHE:CD2	2.51	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.46
1:A:238:ARG:HD3	1:A:239:GLY:O	2.16	0.46
1:B:387:THR:HA	1:B:394:TRP:CD1	2.51	0.46
5:A:505:BTB:H72	5:A:505:BTB:O4	2.13	0.45
1:A:320:LEU:HD13	1:A:322:TRP:CZ2	2.52	0.45
1:B:357:TYR:CD2	1:B:362:ILE:HD11	2.51	0.45
1:A:70:ARG:HG3	1:A:81:TYR:CZ	2.52	0.45
5:C:504:BTB:H51	5:C:504:BTB:H32	1.54	0.45
1:D:357:TYR:CG	1:D:362:ILE:HD11	2.52	0.45
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.98	0.45
5:C:505:BTB:H11	5:C:505:BTB:H51	1.52	0.45
1:D:255:ARG:HG3	1:D:256:GLN:O	2.17	0.45
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.52	0.44
1:C:89:GLN:HG3	1:C:90:GLN:N	2.31	0.44
5:D:505:BTB:H11	5:D:505:BTB:H51	1.49	0.44
5:A:505:BTB:H51	5:A:505:BTB:H11	1.44	0.44
1:D:70:ARG:HB2	1:D:81:TYR:CE2	2.53	0.44
5:D:504:BTB:H72	5:D:504:BTB:H11	1.65	0.44
1:A:72:LYS:HD3	1:A:74:TRP:CZ2	2.53	0.43
1:C:128:ARG:O	1:C:132:ASN:ND2	2.51	0.43
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.88	0.43
1:A:88:ALA:O	1:B:97:ARG:NH2	2.51	0.43
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.82	0.43
1:C:248:LEU:HD12	1:C:335:ALA:HB1	2.00	0.43
1:C:192:LYS:HE2	11:C:627:HOH:O	2.19	0.43
1:D:321:GLU:CD	5:D:504:BTB:O4	2.61	0.43
1:A:453:SER:HA	1:B:452:ILE:HG22	2.00	0.43
1:C:167:GLU:OE1	6:C:506:GOL:O3	2.33	0.43
1:A:89:GLN:HG3	1:A:90:GLN:N	2.34	0.42
1:D:238:ARG:HD3	11:D:630:HOH:O	2.19	0.42
1:D:364:THR:O	1:D:368:CYS:HB2	2.19	0.42
5:A:504:BTB:H51	5:A:504:BTB:H32	1.62	0.42
1:C:138:ILE:O	1:C:140:ARG:HG2	2.19	0.42
1:A:93:PRO:HG3	1:A:106:PRO:HB3	2.00	0.42
5:D:505:BTB:H42	5:D:505:BTB:H72	1.77	0.42
1:C:397:LYS:NZ	11:D:605:HOH:O	2.53	0.42
5:A:505:BTB:O3	5:A:505:BTB:O8	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ALA:O	1:D:224:LEU:HA	2.20	0.42
1:A:124:LEU:O	1:A:128:ARG:HG3	2.19	0.42
1:C:333:LEU:HD12	1:C:334:PRO:HD2	2.02	0.42
1:D:339:MET:HE3	1:D:475:TYR:CD1	2.55	0.42
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.02	0.42
1:C:453:SER:HA	1:D:452:ILE:HG22	2.01	0.42
1:A:82:ASP:OD2	11:A:601:HOH:O	2.20	0.42
1:D:242:ARG:HD2	1:D:242:ARG:HA	1.88	0.42
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.91	0.41
1:A:147:GLU:HA	1:A:150:LEU:HD12	2.02	0.41
1:C:214:HIS:CD2	1:C:214:HIS:C	2.98	0.41
1:C:99:CYS:HB3	1:D:466:ASN:HB3	2.01	0.41
1:D:214:HIS:CD2	1:D:214:HIS:C	2.98	0.41
1:D:257:GLN:C	1:D:259:GLY:H	2.29	0.41
1:A:224:LEU:HB2	1:A:416:THR:HB	2.02	0.41
1:A:358:MET:HE3	1:A:360:THR:OG1	2.21	0.41
1:C:258:ASP:OD1	1:C:258:ASP:N	2.54	0.41
1:B:455:SER:HA	1:B:460:PHE:CG	2.56	0.41
1:A:261:VAL:HG11	1:A:265:PRO:HA	2.02	0.41
1:B:214:HIS:CD2	1:B:214:HIS:C	2.98	0.41
1:A:94:CYS:HB2	11:B:709:HOH:O	2.21	0.40
5:B:505:BTB:H32	5:B:505:BTB:H51	1.47	0.40
1:C:386:ASP:OD2	1:C:388:ARG:HG3	2.20	0.40
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.57	0.40
1:B:247:GLN:CB	1:B:250:ARG:HD3	2.42	0.40
1:B:257:GLN:C	1:B:259:GLY:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/440 (90%)	379 (96%)	16 (4%)	1 (0%)	37	34
1	B	402/440 (91%)	388 (96%)	13 (3%)	1 (0%)	44	44
1	C	397/440 (90%)	384 (97%)	10 (2%)	3 (1%)	16	11
1	D	399/440 (91%)	382 (96%)	16 (4%)	1 (0%)	37	34
All	All	1594/1760 (91%)	1533 (96%)	55 (4%)	6 (0%)	30	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	GLY
1	D	144	GLN
1	B	255	ARG
1	C	454	GLY
1	C	203	SER
1	C	89	GLN

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	340/373 (91%)	321 (94%)	19 (6%)	17	14
1	B	345/373 (92%)	332 (96%)	13 (4%)	28	27
1	C	341/373 (91%)	322 (94%)	19 (6%)	17	14
1	D	342/373 (92%)	333 (97%)	9 (3%)	41	43
All	All	1368/1492 (92%)	1308 (96%)	60 (4%)	25	22

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

Mol	Chain	Res	Type
1	A	71	VAL
1	A	89	GLN
1	A	121	GLU
1	A	122	GLN
1	A	124	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	SER
1	A	140	ARG
1	A	147	GLU
1	A	156	GLU
1	A	188	ILE
1	A	200	ASP
1	A	202	ARG
1	A	203	SER
1	A	207	MET
1	A	224	LEU
1	A	234	ARG
1	A	272	GLU
1	A	291	LEU
1	A	321	GLU
1	B	67	LYS
1	B	71	VAL
1	B	98	ARG
1	B	122	GLN
1	B	128	ARG
1	B	136	SER
1	B	151	GLN
1	B	202	ARG
1	B	258	ASP
1	B	298	GLU
1	B	326	LEU
1	B	429	LYS
1	B	436	LYS
1	C	79	ILE
1	C	97	ARG
1	C	124	LEU
1	C	125	SER
1	C	128	ARG
1	C	139	LYS
1	C	202	ARG
1	C	209	THR
1	C	224	LEU
1	C	228	ILE
1	C	256	GLN
1	C	257	GLN
1	C	291	LEU
1	C	310	VAL
1	C	321	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	329	ARG
1	C	388	ARG
1	C	417	ILE
1	C	474	ARG
1	D	76	VAL
1	D	79	ILE
1	D	87	GLN
1	D	122	GLN
1	D	168[A]	SER
1	D	168[B]	SER
1	D	326	LEU
1	D	342	GLU
1	D	396	ASP

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	194	GLN
1	B	466	ASN
1	C	220	ASN

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 38 ligands modelled in this entry, 12 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	501	1	42,50,50	1.46	6 (14%)	46,82,82	1.98	12 (26%)
4	A1CN2	D	503	-	24,24,24	0.46	0	31,33,33	1.22	2 (6%)
4	A1CN2	B	503	-	24,24,24	0.56	0	31,33,33	1.24	2 (6%)
3	H4B	A	502	-	16,18,18	1.07	1 (6%)	14,26,26	2.49	4 (28%)
6	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.44	0
4	A1CN2	C	503	-	24,24,24	0.41	0	31,33,33	1.36	2 (6%)
5	BTB	C	504	8	13,13,13	0.39	0	7,16,16	0.90	0
5	BTB	D	504	8	13,13,13	0.55	0	7,16,16	0.57	0
2	HEM	B	501	1	42,50,50	1.61	7 (16%)	46,82,82	1.81	9 (19%)
5	BTB	C	505	-	13,13,13	0.51	0	7,16,16	0.92	1 (14%)
6	GOL	C	506	-	5,5,5	0.32	0	5,5,5	0.46	0
6	GOL	D	506	-	5,5,5	0.33	0	5,5,5	0.22	0
6	GOL	C	507	-	5,5,5	0.36	0	5,5,5	0.30	0
6	GOL	B	506	-	5,5,5	0.43	0	5,5,5	0.18	0
5	BTB	A	505	-	13,13,13	0.76	0	7,16,16	1.09	1 (14%)
5	BTB	B	504	8	13,13,13	0.63	0	7,16,16	1.02	1 (14%)
3	H4B	C	502	-	16,18,18	0.97	0	14,26,26	2.58	6 (42%)
5	BTB	B	505	-	13,13,13	0.46	0	7,16,16	0.77	0
4	A1CN2	A	503	-	24,24,24	0.44	0	31,33,33	1.45	3 (9%)
3	H4B	D	502	-	16,18,18	0.93	0	14,26,26	2.66	8 (57%)
2	HEM	A	501	1	42,50,50	1.52	6 (14%)	46,82,82	1.71	11 (23%)
5	BTB	D	505	-	13,13,13	0.46	0	7,16,16	1.29	0
6	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.29	0
3	H4B	B	502	-	16,18,18	0.89	0	14,26,26	2.32	6 (42%)
2	HEM	C	501	1	42,50,50	1.56	6 (14%)	46,82,82	1.79	9 (19%)
5	BTB	A	504	8	13,13,13	0.56	0	7,16,16	0.88	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
2	HEM	D	501	1	-	6/12/54/54	-
4	A1CN2	D	503	-	-	3/10/10/10	0/2/2/2
4	A1CN2	B	503	-	-	1/10/10/10	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
6	GOL	A	507	-	-	1/4/4/4	-
4	A1CN2	C	503	-	-	0/10/10/10	0/2/2/2
5	BTB	C	504	8	-	7/21/21/21	-
5	BTB	D	504	8	-	8/21/21/21	-
2	HEM	B	501	1	-	6/12/54/54	-
5	BTB	C	505	-	-	10/21/21/21	-
6	GOL	C	506	-	-	4/4/4/4	-
6	GOL	D	506	-	-	2/4/4/4	-
6	GOL	C	507	-	-	4/4/4/4	-
6	GOL	B	506	-	-	2/4/4/4	-
5	BTB	A	505	-	-	13/21/21/21	-
5	BTB	B	504	8	-	3/21/21/21	-
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
5	BTB	B	505	-	-	12/21/21/21	-
4	A1CN2	A	503	-	-	0/10/10/10	0/2/2/2
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
2	HEM	A	501	1	-	6/12/54/54	-
5	BTB	D	505	-	-	13/21/21/21	-
6	GOL	A	506	-	-	4/4/4/4	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	6/12/54/54	-
5	BTB	A	504	8	-	5/21/21/21	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-4.16	1.34	1.40
2	B	501	HEM	FE-NB	3.86	2.19	1.98
2	C	501	HEM	C3C-C2C	-3.84	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	C	501	HEM	FE-NB	3.51	2.17	1.98
2	D	501	HEM	C3C-C4C	3.45	1.46	1.41
2	B	501	HEM	C3C-CAC	3.39	1.55	1.47
2	C	501	HEM	C3C-CAC	3.34	1.55	1.47
2	B	501	HEM	C3C-C4C	3.31	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-CAC	3.19	1.54	1.47
2	C	501	HEM	CAB-C3B	3.18	1.55	1.47
2	C	501	HEM	C3C-C4C	3.09	1.45	1.41
2	B	501	HEM	CAB-C3B	3.01	1.55	1.47
2	A	501	HEM	C3C-C4C	2.99	1.45	1.41
2	A	501	HEM	CAB-C3B	2.97	1.55	1.47
2	A	501	HEM	FE-NB	2.84	2.13	1.98
2	D	501	HEM	C3C-CAC	2.77	1.53	1.47
2	D	501	HEM	CAB-C3B	2.75	1.54	1.47
3	A	502	H4B	C7-C6	2.63	1.54	1.52
2	B	501	HEM	C2C-C1C	2.54	1.48	1.42
2	B	501	HEM	C3C-C2C	-2.50	1.37	1.40
2	B	501	HEM	CMD-C2D	2.33	1.55	1.50
2	A	501	HEM	CMB-C2B	2.28	1.55	1.50
2	C	501	HEM	CMB-C2B	2.26	1.55	1.50
2	D	501	HEM	CMB-C2B	2.20	1.55	1.50
2	D	501	HEM	CHA-C4D	2.01	1.39	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CBA-CAA-C2A	-6.65	101.36	112.54
2	D	501	HEM	CBA-CAA-C2A	-6.00	102.45	112.54
2	C	501	HEM	CBA-CAA-C2A	-5.90	102.62	112.54
4	A	503	A1CN2	C02-N01-C06	5.80	122.41	118.07
3	A	502	H4B	C8A-C4A-C4	5.69	119.68	114.50
3	C	502	H4B	C8A-C4A-C4	5.56	119.56	114.50
4	C	503	A1CN2	C02-N01-C06	5.38	122.09	118.07
3	D	502	H4B	C8A-C4A-C4	4.96	119.01	114.50
3	B	502	H4B	C8A-C4A-C4	4.80	118.87	114.50
2	A	501	HEM	C4B-CHC-C1C	4.58	128.60	122.56
4	B	503	A1CN2	C02-N01-C06	4.54	121.47	118.07
3	D	502	H4B	C11-C10-C9	-4.29	106.86	112.11
2	C	501	HEM	C4B-CHC-C1C	4.17	128.06	122.56
4	D	503	A1CN2	C02-N01-C06	3.85	120.95	118.07
3	C	502	H4B	C2-N3-C4	3.84	121.30	115.96
2	A	501	HEM	CBA-CAA-C2A	-3.77	106.21	112.54
2	B	501	HEM	C4B-CHC-C1C	3.71	127.45	122.56
3	B	502	H4B	N1-C2-N3	-3.69	119.82	125.48
3	D	502	H4B	N1-C2-N3	-3.64	119.90	125.48
3	C	502	H4B	N1-C2-N3	-3.61	119.95	125.48
2	D	501	HEM	C3B-C4B-NB	-3.59	106.89	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C2-N3-C4	3.57	120.93	115.96
2	D	501	HEM	C4C-CHD-C1D	3.39	127.04	122.56
3	A	502	H4B	N1-C2-N3	-3.37	120.32	125.48
3	B	502	H4B	C2-N3-C4	3.36	120.64	115.96
3	C	502	H4B	C11-C10-C9	-3.31	108.06	112.11
2	D	501	HEM	C4D-ND-C1D	3.21	109.00	105.21
3	D	502	H4B	C2-N3-C4	3.19	120.39	115.96
2	D	501	HEM	C4B-CHC-C1C	3.11	126.67	122.56
2	B	501	HEM	CHC-C4B-C3B	3.07	129.27	124.57
2	B	501	HEM	C1B-NB-C4B	3.04	108.81	105.21
2	D	501	HEM	C1B-NB-C4B	2.98	108.73	105.21
3	B	502	H4B	C2-N1-C8A	2.96	121.62	114.59
2	B	501	HEM	CMC-C2C-C3C	2.93	130.55	124.68
2	A	501	HEM	C4D-ND-C1D	2.90	108.65	105.21
2	B	501	HEM	C4C-CHD-C1D	2.88	126.36	122.56
2	C	501	HEM	C3B-C2B-C1B	2.88	108.57	106.41
2	A	501	HEM	C3D-C4D-ND	-2.86	107.03	110.17
3	D	502	H4B	C2-N1-C8A	2.86	121.39	114.59
2	D	501	HEM	C2D-C1D-ND	-2.86	106.59	109.90
2	B	501	HEM	C3B-C2B-C1B	2.77	108.49	106.41
2	D	501	HEM	C3B-C2B-C1B	2.75	108.47	106.41
2	D	501	HEM	C3D-C4D-ND	-2.69	107.22	110.17
4	D	503	A1CN2	O09-C11-C12	2.60	119.84	115.92
2	A	501	HEM	C1B-NB-C4B	2.60	108.29	105.21
3	B	502	H4B	C4-C4A-N5	2.59	122.27	118.57
2	D	501	HEM	CMC-C2C-C3C	2.58	129.84	124.68
3	D	502	H4B	N2-C2-N3	2.57	121.08	117.22
2	A	501	HEM	C3B-C4B-NB	-2.52	107.66	109.47
3	A	502	H4B	C2-N1-C8A	2.51	120.56	114.59
2	C	501	HEM	CMA-C3A-C4A	-2.49	124.81	128.46
2	B	501	HEM	C3B-C4B-NB	-2.46	107.70	109.47
5	B	504	BTB	O3-C3-C2	2.45	117.17	111.40
3	C	502	H4B	C2-N1-C8A	2.44	120.39	114.59
2	C	501	HEM	C4D-ND-C1D	2.42	108.08	105.21
2	A	501	HEM	C3B-C2B-C1B	2.40	108.21	106.41
3	D	502	H4B	C4-C4A-N5	2.35	121.93	118.57
2	A	501	HEM	CHD-C1D-ND	2.29	126.90	124.44
4	A	503	A1CN2	N02-C02-N01	2.29	120.27	116.59
2	A	501	HEM	CMC-C2C-C3C	2.28	129.24	124.68
3	B	502	H4B	N2-C2-N3	2.27	120.62	117.22
2	A	501	HEM	CMA-C3A-C4A	-2.21	125.21	128.46
2	C	501	HEM	C1B-NB-C4B	2.21	107.82	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1CN2	C05-C06-N01	-2.13	120.30	122.73
2	B	501	HEM	C2B-C1B-NB	-2.13	107.40	109.84
3	D	502	H4B	O10-C10-C9	2.12	113.28	109.77
2	A	501	HEM	C2D-C1D-ND	-2.10	107.48	109.90
5	A	505	BTB	O1-C1-C2	-2.10	106.47	111.40
2	C	501	HEM	C3D-C4D-ND	-2.09	107.88	110.17
2	D	501	HEM	CAD-CBD-CGD	-2.09	108.12	113.67
3	C	502	H4B	O10-C10-C9	2.09	113.23	109.77
4	C	503	A1CN2	C05-C06-N01	-2.08	120.35	122.73
4	B	503	A1CN2	C07-C04-C05	-2.08	118.10	120.92
2	C	501	HEM	C3B-C4B-NB	-2.07	107.98	109.47
2	C	501	HEM	C2D-C1D-ND	-2.04	107.55	109.90
2	D	501	HEM	C3C-C4C-NC	-2.03	107.11	110.94
5	C	505	BTB	O3-C3-C2	-2.00	106.70	111.40

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	N-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	O1-C1-C2-C3
5	B	505	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-N
5	B	505	BTB	N-C2-C4-O4
5	B	505	BTB	C1-C2-N-C7
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C1-C2-C3-O3
5	C	504	BTB	N-C2-C3-O3
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C7
6	A	506	GOL	O1-C1-C2-C3
6	A	506	GOL	C1-C2-C3-O3
6	C	506	GOL	O1-C1-C2-C3
6	C	506	GOL	C1-C2-C3-O3
6	D	506	GOL	O1-C1-C2-C3
2	B	501	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	C3D-CAD-CBD-CGD
5	D	504	BTB	N-C5-C6-O6
5	A	504	BTB	N-C7-C8-O8
5	D	505	BTB	N-C5-C6-O6
5	C	505	BTB	N-C7-C8-O8
6	C	506	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
5	C	504	BTB	N-C7-C8-O8
6	A	507	GOL	O1-C1-C2-C3
6	B	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
4	B	503	A1CN2	C15-C17-C18-N19
6	A	506	GOL	O2-C2-C3-O3
6	C	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O1-C1-C2-O2
2	D	501	HEM	C4B-C3B-CAB-CBB
6	A	506	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	506	GOL	O1-C1-C2-O2
5	D	505	BTB	N-C7-C8-O8
5	B	505	BTB	N-C7-C8-O8
5	B	505	BTB	C1-C2-C4-O4
6	B	506	GOL	O1-C1-C2-O2
6	C	507	GOL	O2-C2-C3-O3
2	A	501	HEM	C3D-CAD-CBD-CGD
6	C	507	GOL	C1-C2-C3-O3
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C7
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C7
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C4-C2-N-C5
3	C	502	H4B	C7-C6-C9-C10
2	C	501	HEM	C3D-CAD-CBD-CGD
5	B	504	BTB	N-C5-C6-O6
4	D	503	A1CN2	C17-C18-N19-C20
2	C	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O2D
5	C	505	BTB	C1-C2-C4-O4
2	C	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
5	A	504	BTB	N-C5-C6-O6
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	502	H4B	C7-C6-C9-O9
2	A	501	HEM	CAD-CBD-CGD-O2D
4	D	503	A1CN2	C16-C15-C17-C18
3	B	502	H4B	N5-C6-C9-O9
3	C	502	H4B	N5-C6-C9-O9
2	A	501	HEM	CAD-CBD-CGD-O1D
3	D	502	H4B	C7-C6-C9-O9
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C4-C2-N-C5
5	B	505	BTB	C4-C2-N-C5
5	C	505	BTB	O1-C1-C2-N
5	D	504	BTB	C4-C2-N-C5
5	D	505	BTB	N-C2-C4-O4
4	D	503	A1CN2	C14-C15-C17-C18
5	D	504	BTB	N-C7-C8-O8

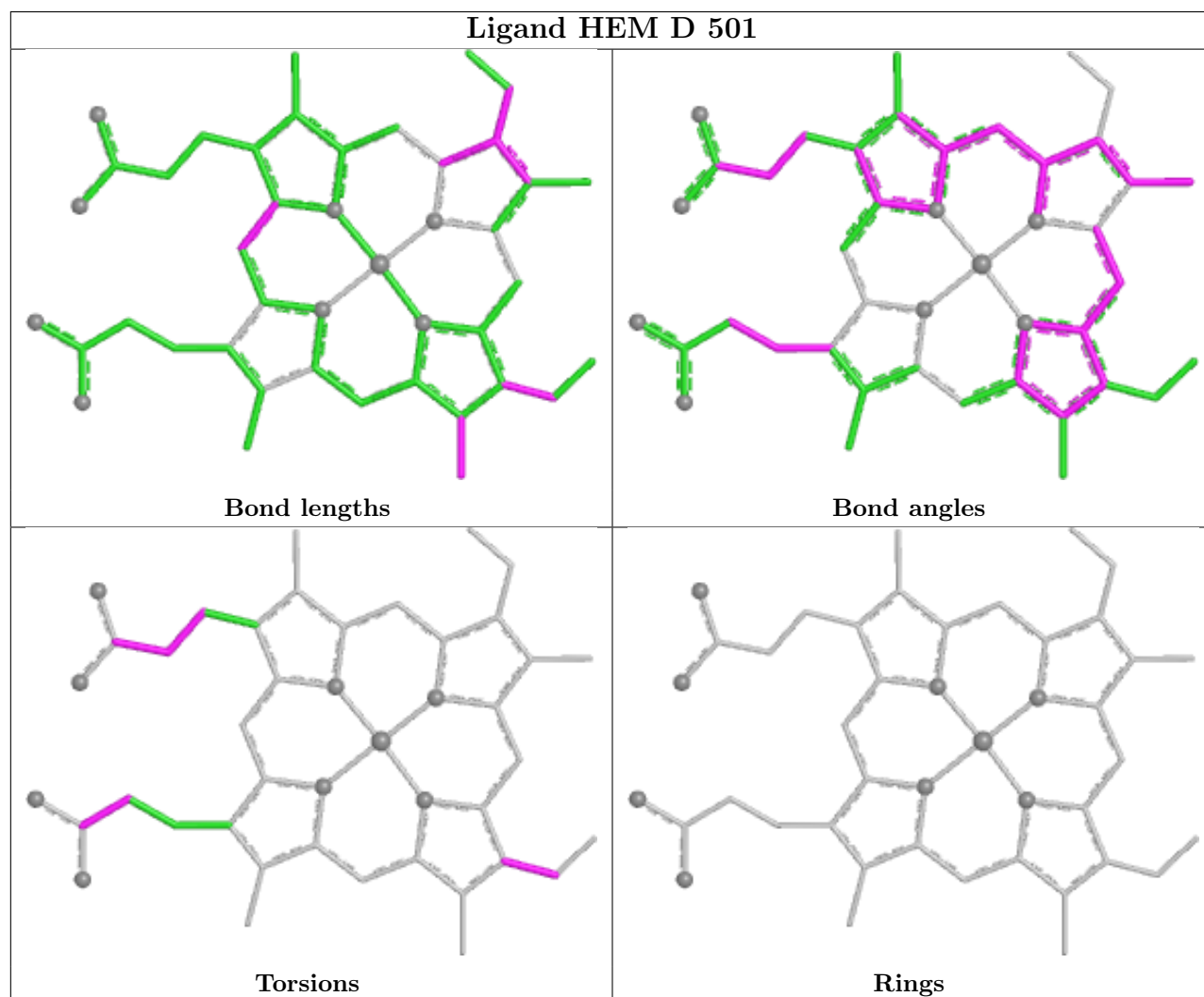
There are no ring outliers.

17 monomers are involved in 44 short contacts:

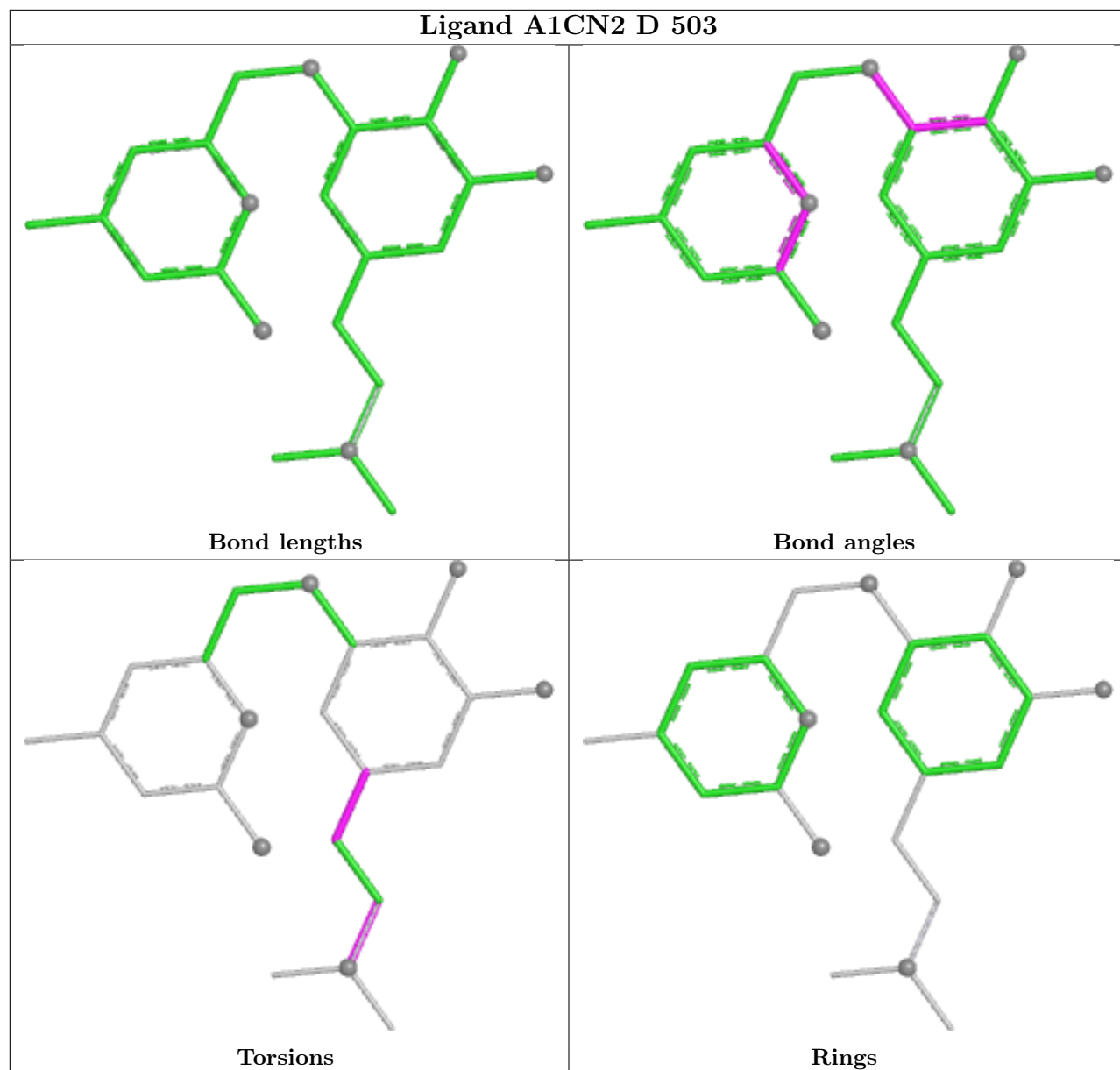
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	3	0
4	B	503	A1CN2	1	0
3	A	502	H4B	2	0
5	C	504	BTB	1	0
5	D	504	BTB	6	0
2	B	501	HEM	4	0
5	C	505	BTB	2	0
6	C	506	GOL	1	0
5	A	505	BTB	4	0
5	B	504	BTB	2	0
3	C	502	H4B	1	0
5	B	505	BTB	4	0
2	A	501	HEM	2	0
5	D	505	BTB	5	0
3	B	502	H4B	1	0
2	C	501	HEM	3	0
5	A	504	BTB	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

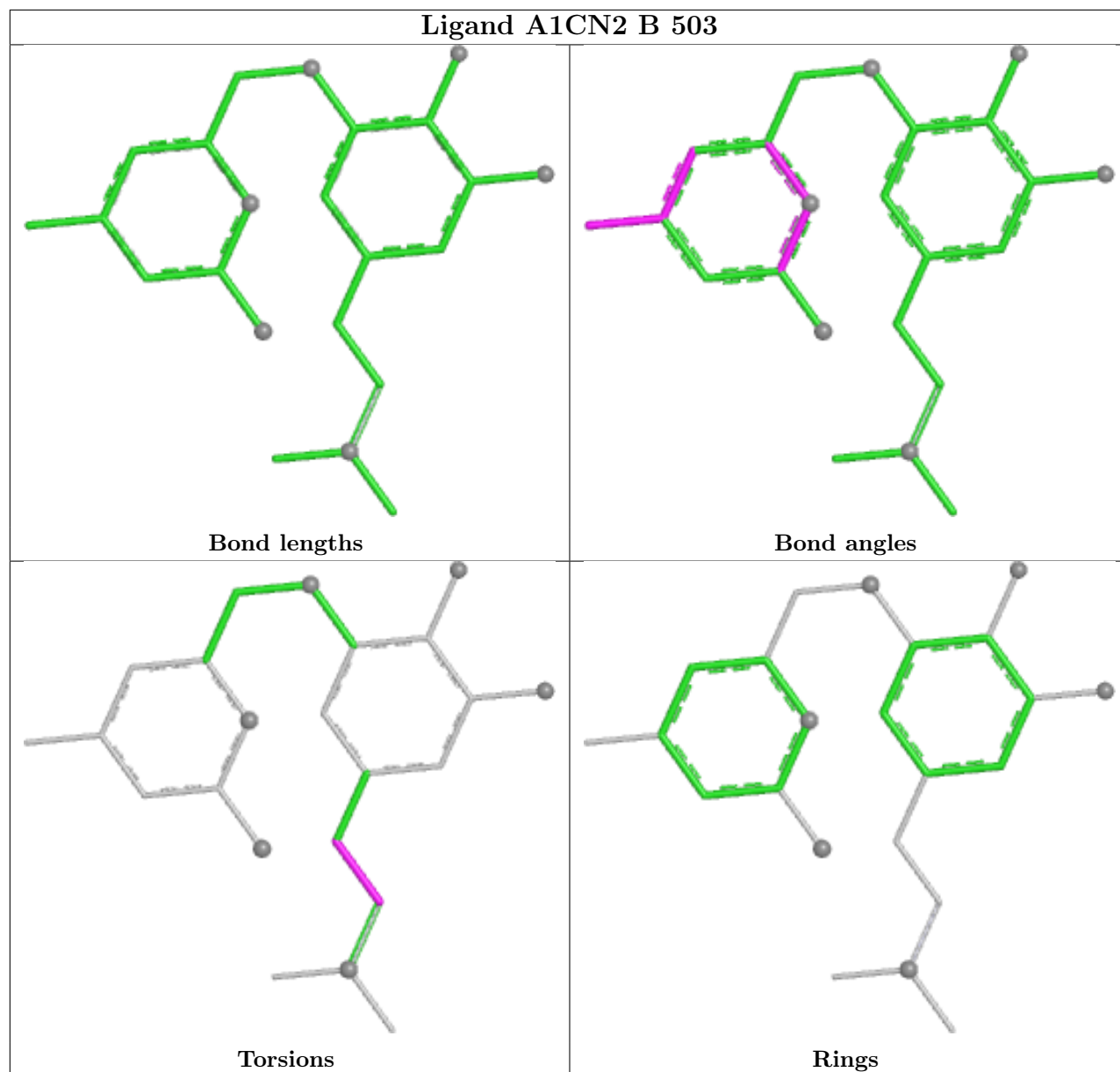
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



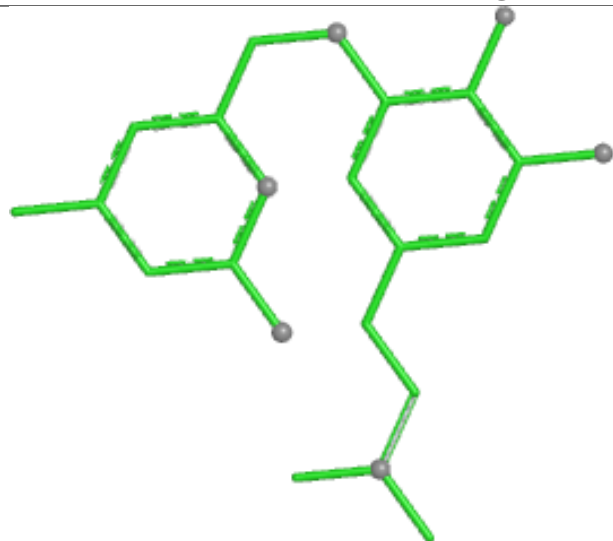
Ligand A1CN2 D 503



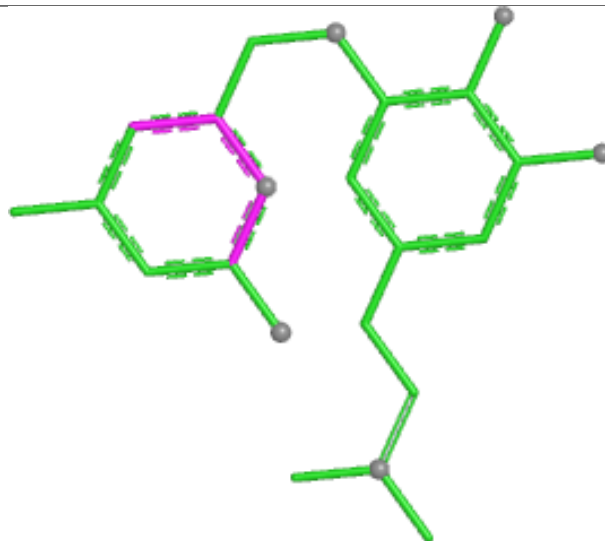
Ligand A1CN2 B 503



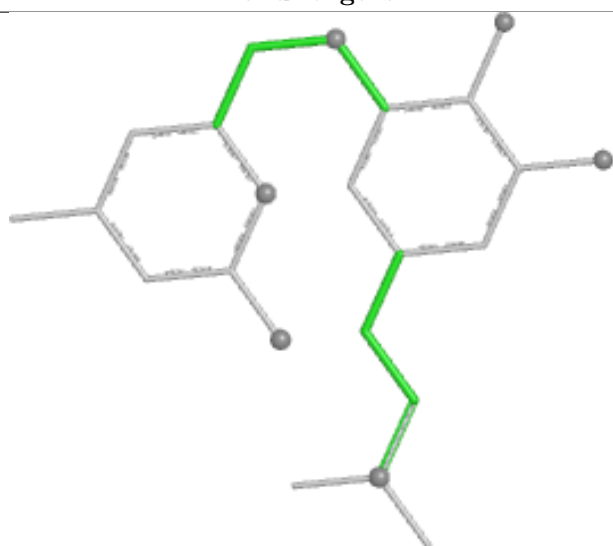
Ligand A1CN2 C 503



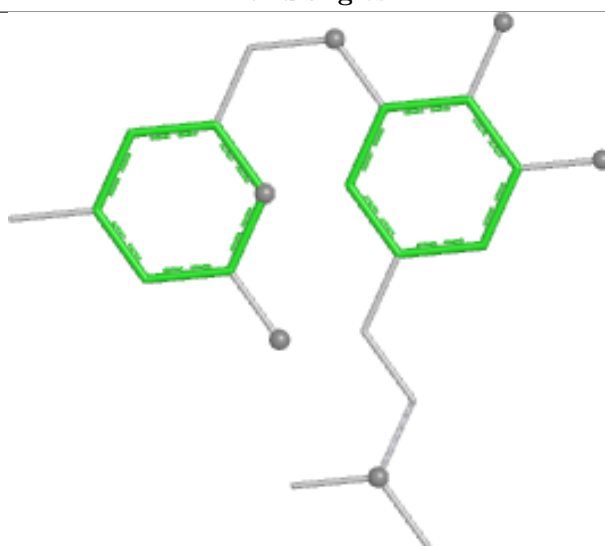
Bond lengths



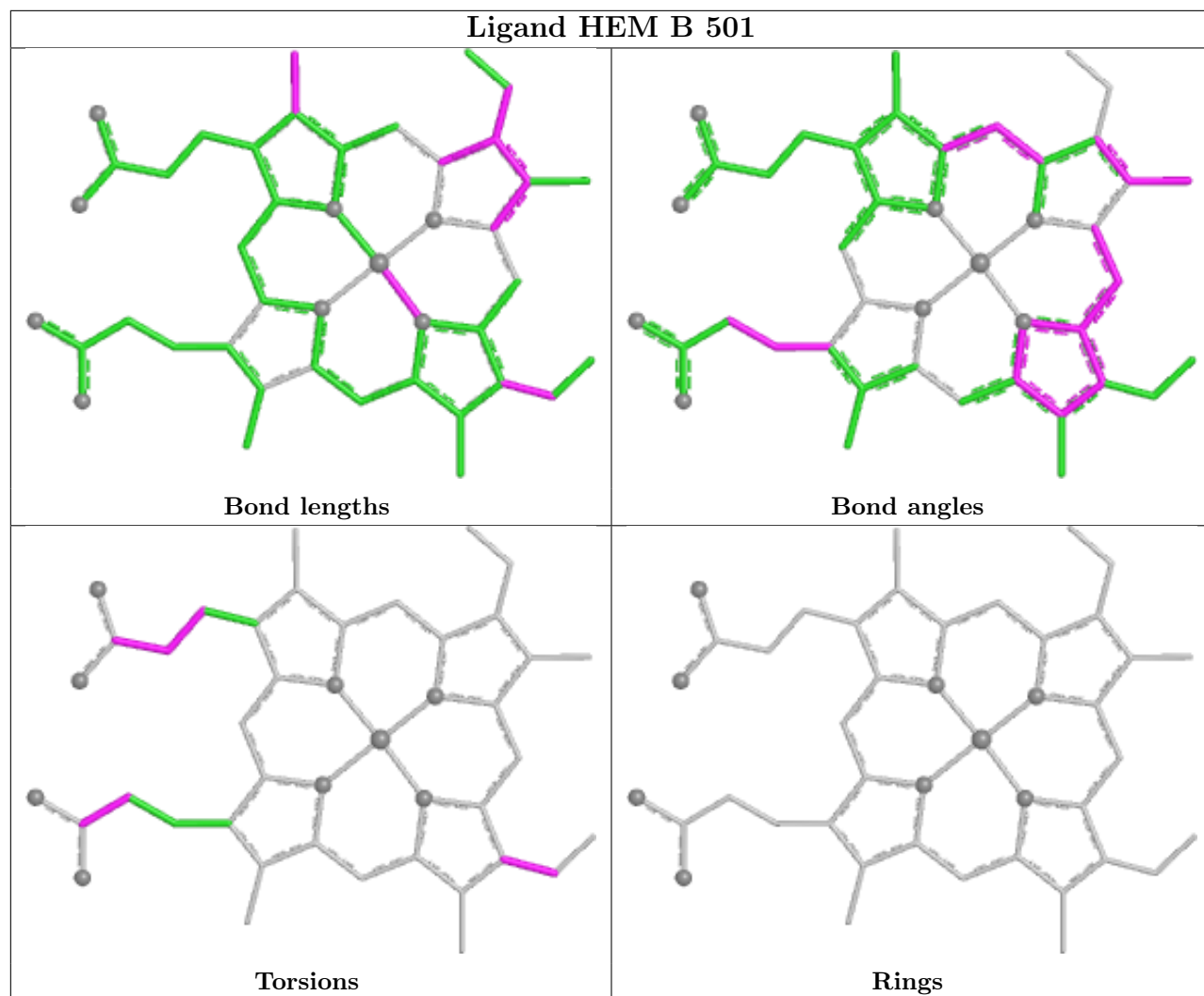
Bond angles



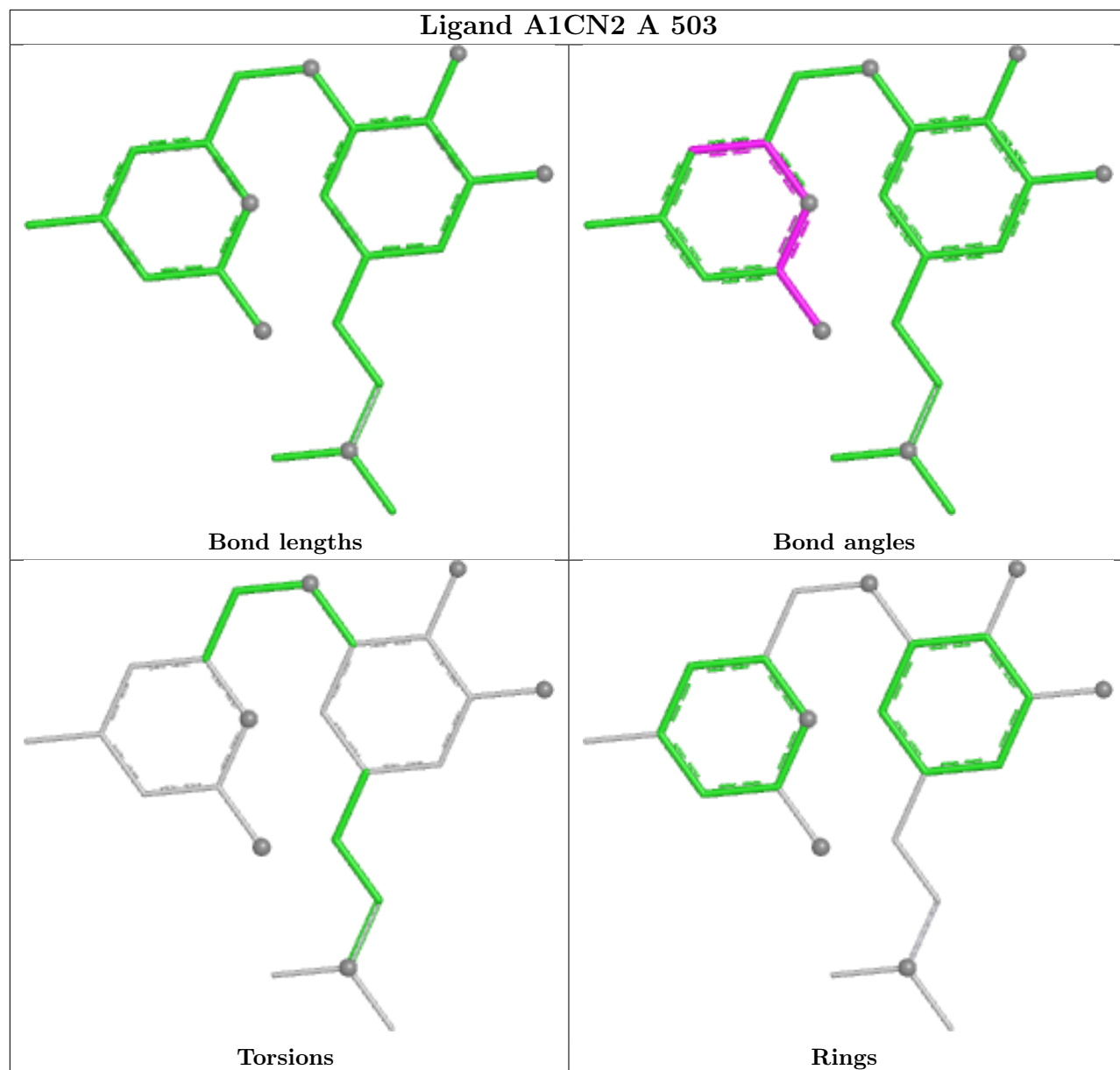
Torsions

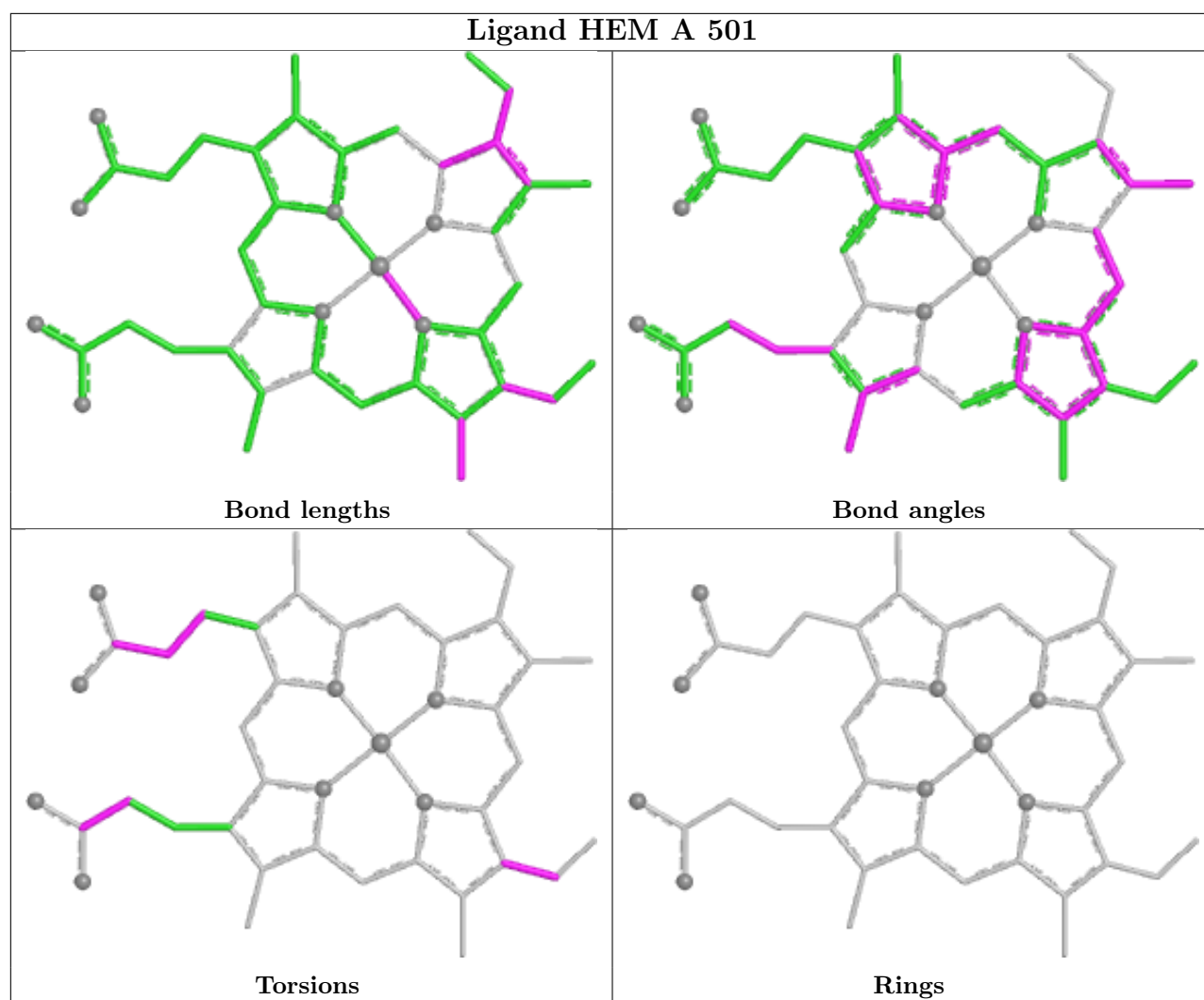


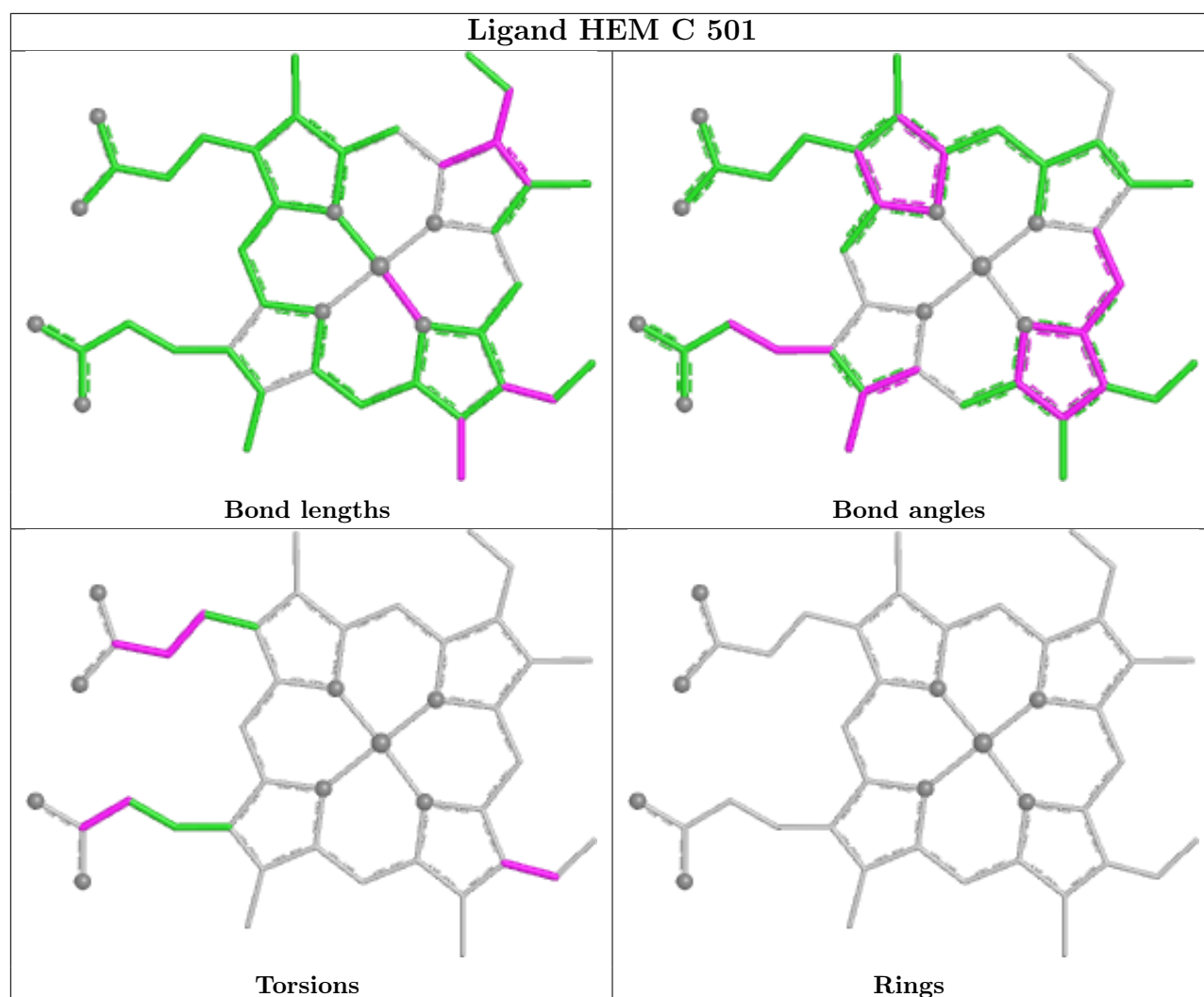
Rings



Ligand A1CN2 A 503







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/440 (90%)	-1.40	0 100 100	30, 53, 96, 127	1 (0%)
1	B	402/440 (91%)	-1.57	0 100 100	23, 40, 74, 131	4 (0%)
1	C	400/440 (90%)	-1.30	0 100 100	26, 56, 102, 128	1 (0%)
1	D	402/440 (91%)	-1.51	0 100 100	25, 42, 79, 136	1 (0%)
All	All	1603/1760 (91%)	-1.44	0 100 100	23, 48, 94, 136	7 (0%)

There are no RSRZ outliers to report.

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
6	GOL	A	507	6/6	0.96	0.04	86,88,90,92	0
5	BTB	B	505	14/14	0.98	0.04	68,84,92,94	0
4	A1CN2	C	503	23/23	0.98	0.06	44,75,88,93	0
6	GOL	C	507	6/6	0.98	0.03	68,75,81,84	0

Continued on next page...

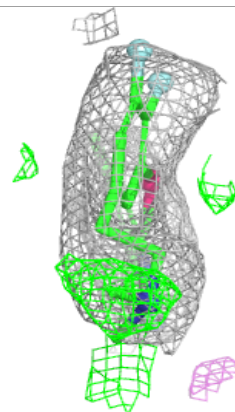
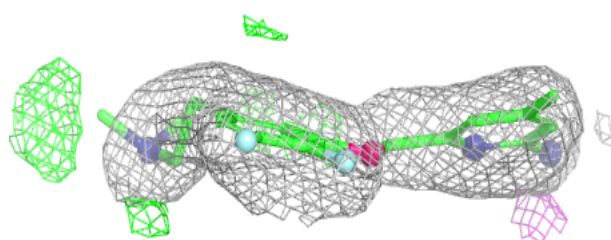
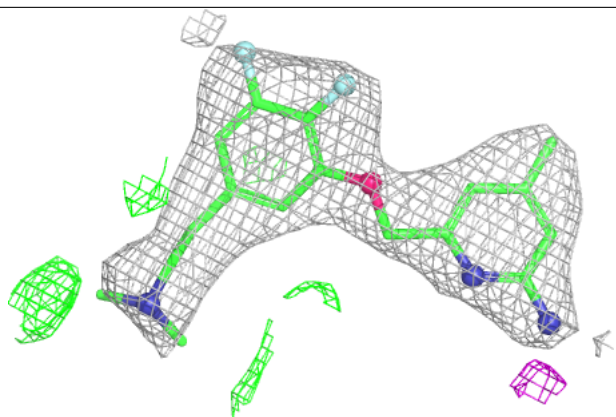
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	A1CN2	B	503	23/23	0.99	0.06	25,63,80,81	0
3	H4B	A	502	17/17	0.99	0.03	40,55,67,70	0
4	A1CN2	D	503	23/23	0.99	0.05	27,74,93,96	0
5	BTB	A	504	14/14	0.99	0.03	48,74,91,93	0
5	BTB	A	505	14/14	0.99	0.03	40,70,79,83	0
5	BTB	B	504	14/14	0.99	0.03	43,73,86,90	0
3	H4B	B	502	17/17	0.99	0.03	30,48,59,63	0
5	BTB	C	504	14/14	0.99	0.04	67,88,96,102	0
5	BTB	C	505	14/14	0.99	0.04	60,79,86,89	0
5	BTB	D	505	14/14	0.99	0.03	41,77,91,92	0
6	GOL	A	506	6/6	0.99	0.03	48,57,58,60	0
3	H4B	C	502	17/17	0.99	0.04	48,60,74,78	0
6	GOL	B	506	6/6	0.99	0.05	62,88,90,95	0
6	GOL	C	506	6/6	0.99	0.04	43,86,87,88	0
4	A1CN2	A	503	23/23	0.99	0.05	44,70,87,89	0
6	GOL	D	506	6/6	0.99	0.03	59,62,65,76	0
2	HEM	A	501	43/43	1.00	0.03	35,49,60,79	0
2	HEM	B	501	43/43	1.00	0.02	17,29,58,65	0
2	HEM	C	501	43/43	1.00	0.03	35,51,66,72	0
3	H4B	D	502	17/17	1.00	0.02	35,57,64,70	0
5	BTB	D	504	14/14	1.00	0.03	28,58,75,82	0
2	HEM	D	501	43/43	1.00	0.02	18,29,55,89	0
7	CL	A	508	1/1	1.00	0.02	49,49,49,49	0
7	CL	B	507	1/1	1.00	0.02	41,41,41,41	0
7	CL	C	508	1/1	1.00	0.02	50,50,50,50	0
7	CL	D	507	1/1	1.00	0.01	37,37,37,37	0
8	GD	A	509	1/1	1.00	0.01	111,111,111,111	0
8	GD	B	508	1/1	1.00	0.01	52,52,52,52	0
8	GD	C	509	1/1	1.00	0.01	147,147,147,147	0
8	GD	D	508	1/1	1.00	0.01	49,49,49,49	0
9	ZN	A	510	1/1	1.00	0.01	36,36,36,36	0
9	ZN	C	510	1/1	1.00	0.01	41,41,41,41	0
10	CA	A	511	1/1	1.00	0.02	54,54,54,54	0
10	CA	B	509	1/1	1.00	0.02	44,44,44,44	0

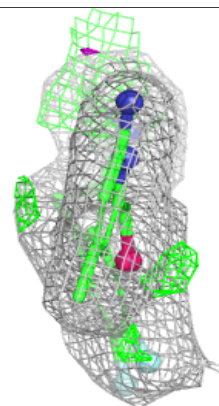
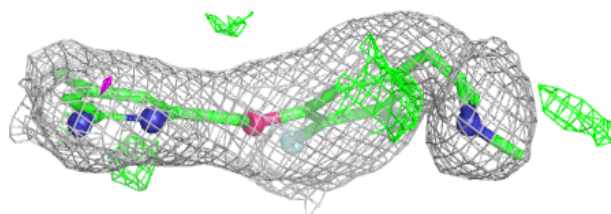
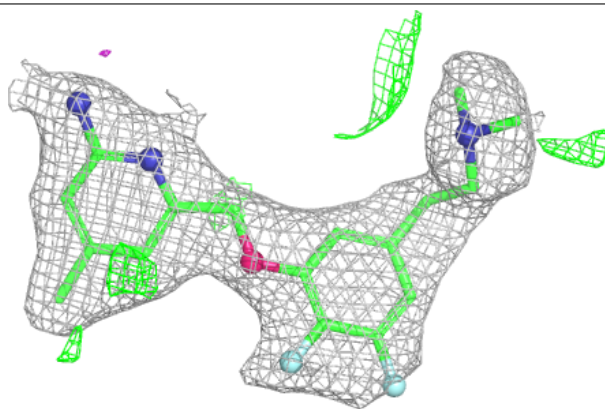
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CN2 C 503:

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

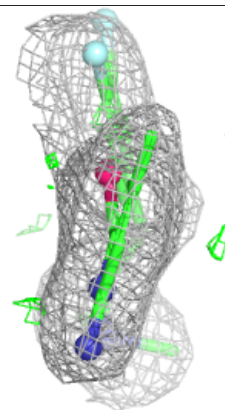
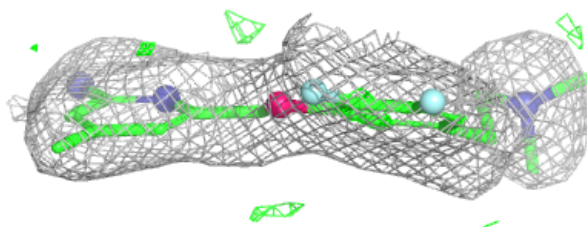
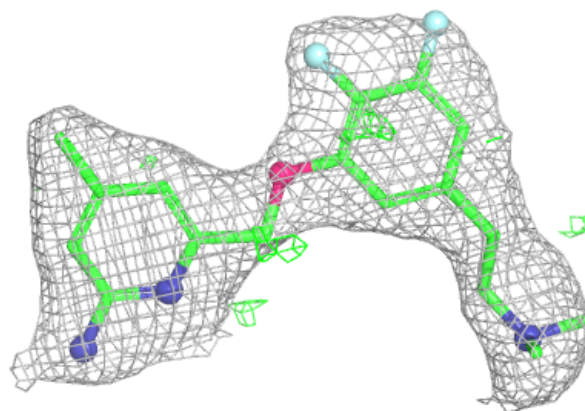
**Electron density around A1CN2 B 503:**

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



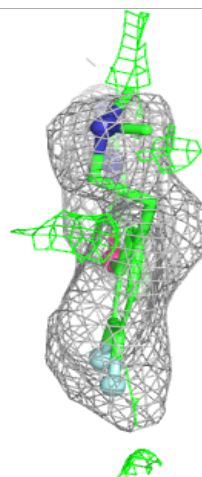
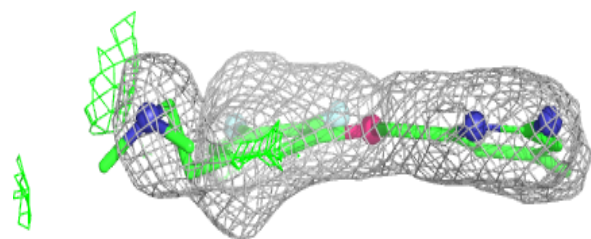
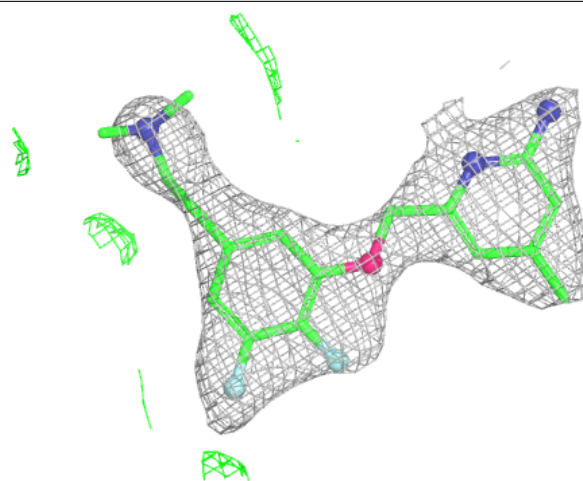
Electron density around A1CN2 D 503:

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



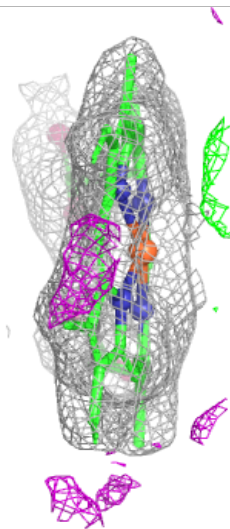
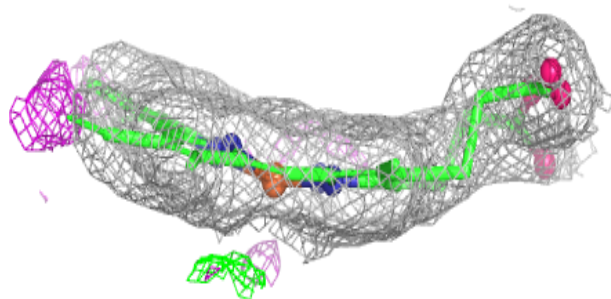
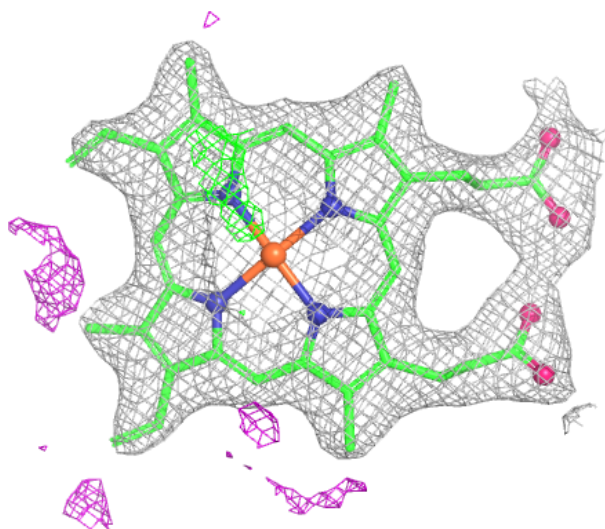
Electron density around A1CN2 A 503:

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



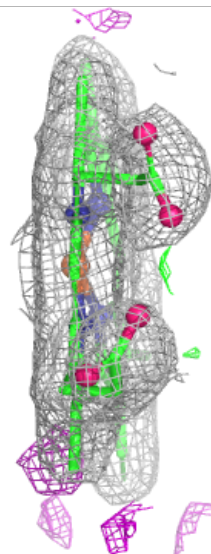
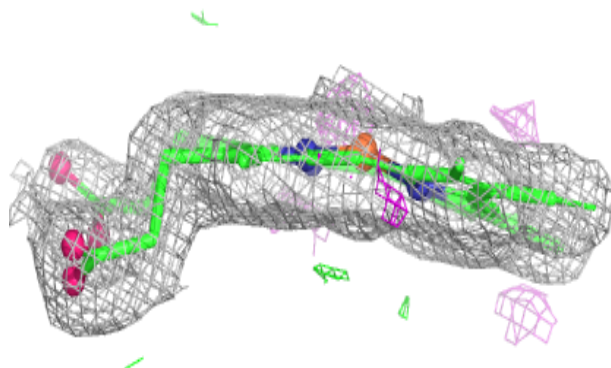
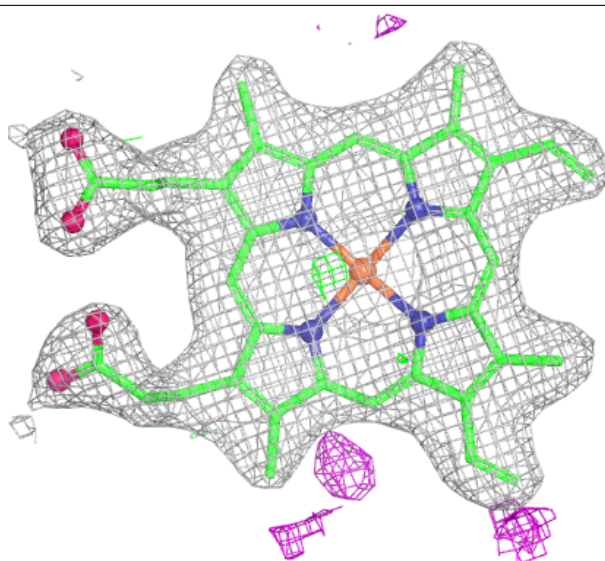
Electron density around HEM A 501:

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



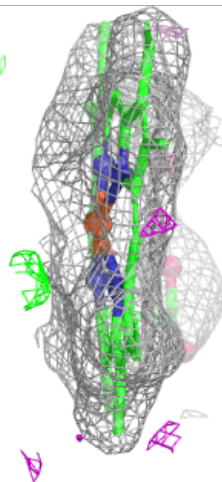
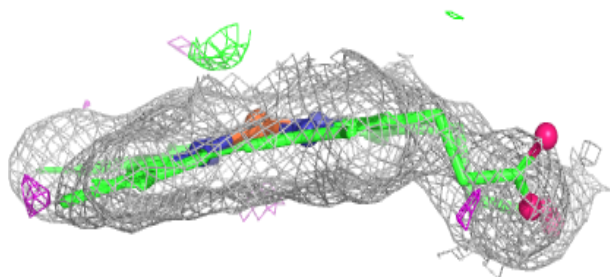
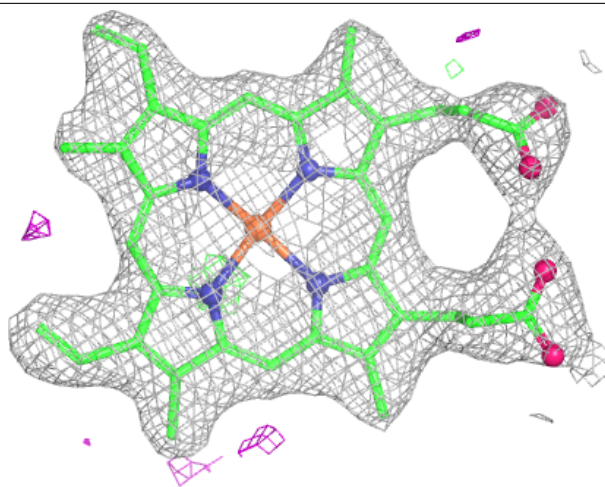
Electron density around HEM B 501:

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



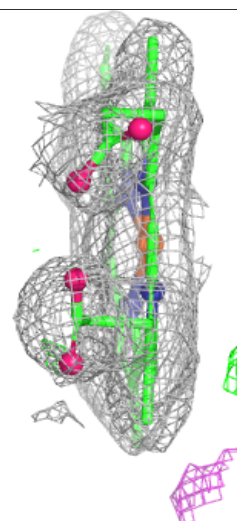
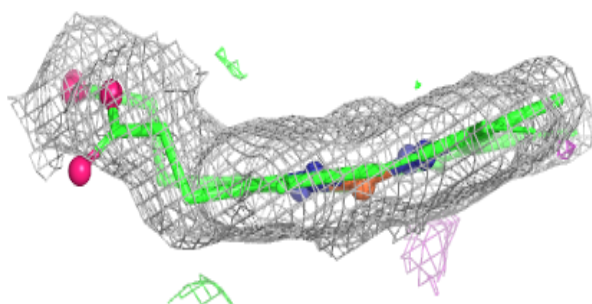
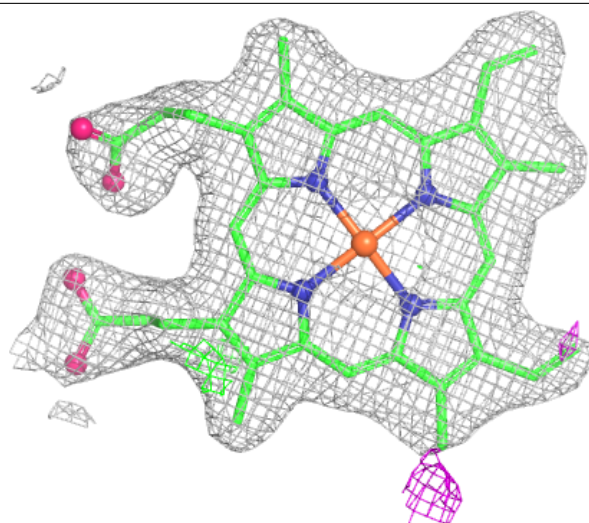
Electron density around HEM C 501:

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



Electron density around HEM D 501:

$2mF_o-DF_c$ (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.