



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:10 am BST

PDB ID : 5UO9
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-[(3-Ethyl-5-((methylamino)methyl)phenoxy)methyl]quinolin-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

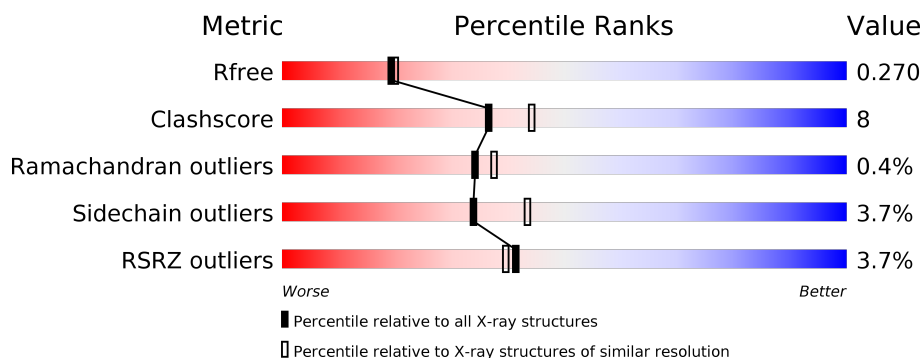
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 8%</div> </div> </div>
1	B	440	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 9%</div> </div> </div>
1	C	440	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	D	440	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13803 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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			

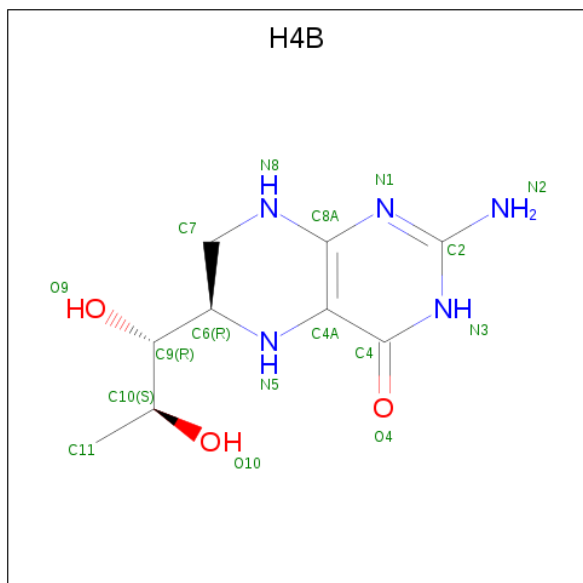
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Continued from previous page...

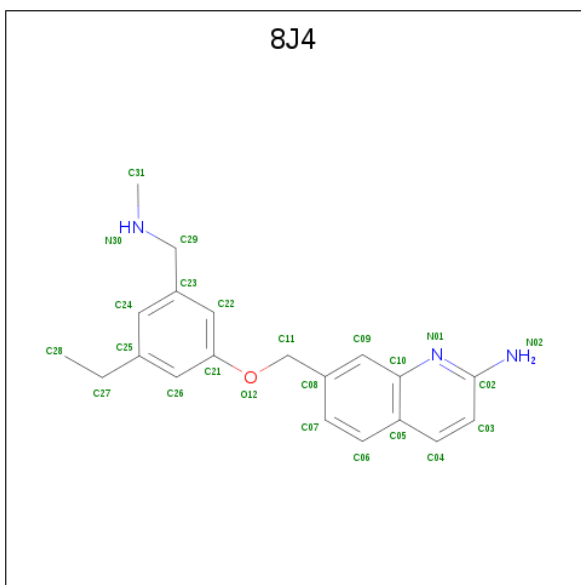
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



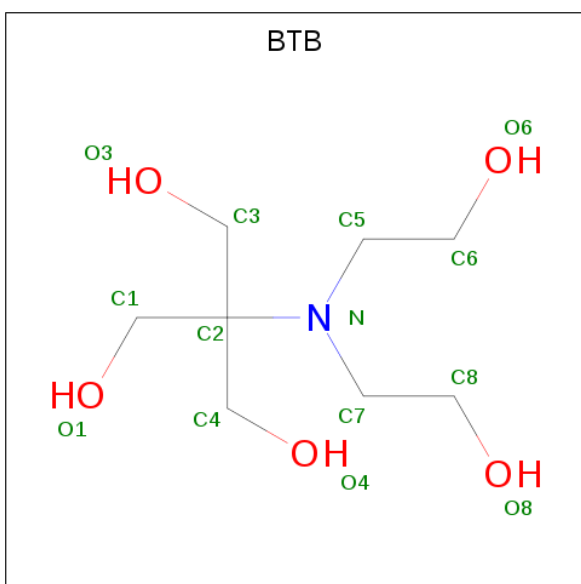
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-({3-ethyl-5-[(methylamino)methyl]phenoxy}methyl)quinolin-2-amine (three-letter code: 8J4) (formula: $C_{20}H_{23}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	3	1		
4	B	1	Total	C	N	O	0	0
			24	20	3	1		
4	C	1	Total	C	N	O	0	0
			24	20	3	1		
4	D	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



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	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	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	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		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		
8	D	2	Total	Cl	0	0
			2	2		
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Gd	0	0
			1	1		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

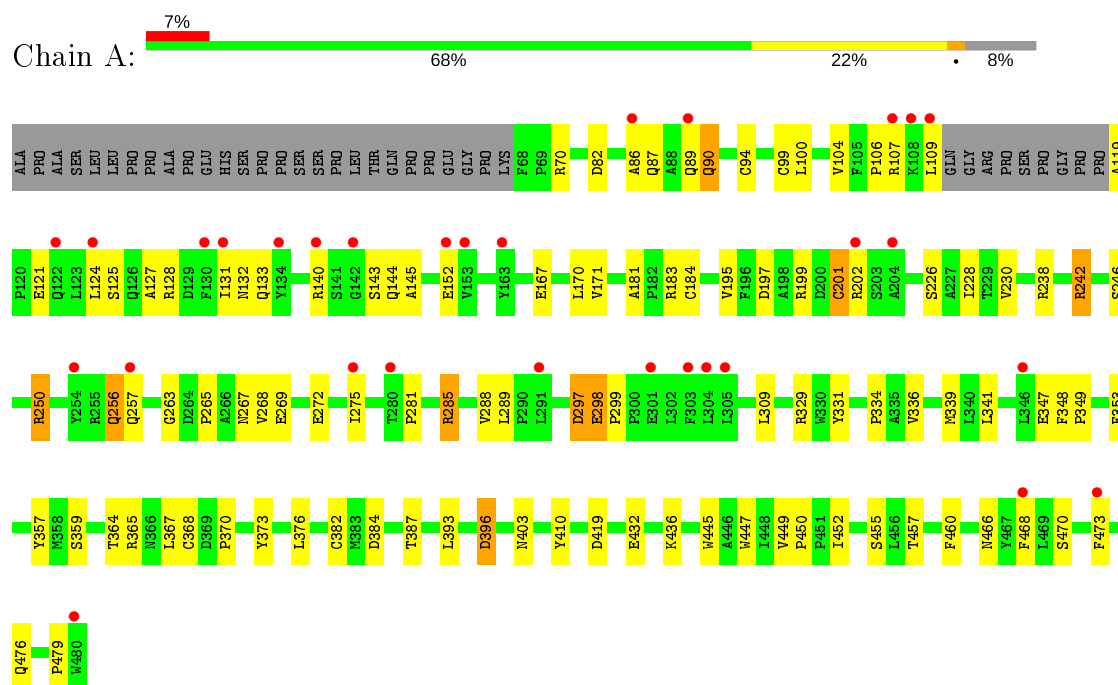
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	118	Total	O	0	0
			118	118		
12	C	76	Total	O	0	0
			76	76		
12	D	114	Total	O	0	0
			114	114		

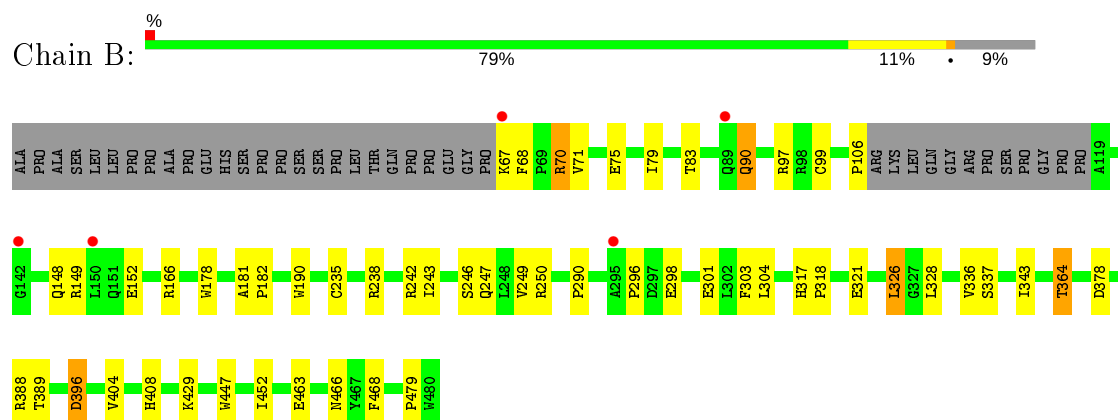
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.38 Å 152.09 Å 108.22 Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	38.87 – 2.19 38.86 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.0 (38.87-2.19) 92.3 (38.86-2.19)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.212 , 0.276 0.207 , 0.270	Depositor DCC
R_{free} test set	4651 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13803	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, MG, H4B, CL, CA, ZN, 8J4, GD, BTB, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3335	0.55	0/4543
1	B	0.43	0/3319	0.56	0/4523
1	C	0.38	0/3307	0.55	0/4507
1	D	0.44	0/3319	0.57	0/4523
All	All	0.40	0/13280	0.56	0/18096

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	3237	0	3146	59	0
1	B	3221	0	3126	35	0
1	C	3209	0	3109	53	0
1	D	3221	0	3126	41	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	1	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	1	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
5	A	28	0	38	5	0
5	B	84	0	111	12	0
5	C	14	0	19	4	0
5	D	42	0	54	10	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	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	2	0	0	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
11	D	1	0	0	0	0
12	A	78	0	0	11	0
12	B	118	0	0	6	0
12	C	76	0	0	6	0
12	D	114	0	0	4	0
All	All	13803	0	12925	207	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 8.

All (207) 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:347:GLU:OE2	12:C:601:HOH:O	2.03	0.76
1:A:144:GLN:O	12:A:601:HOH:O	2.03	0.75
1:C:235:CYS:H	1:C:238:ARG:HD3	1.51	0.75
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.70	0.72
1:A:201:CYS:SG	12:A:639:HOH:O	2.47	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.70	0.71
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.74	0.70
5:A:505:BTB:O1	5:A:505:BTB:O4	2.04	0.69
1:C:378:ASP:OD1	12:C:602:HOH:O	2.09	0.69
1:B:408:HIS:ND1	12:B:604:HOH:O	2.26	0.69
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.75	0.69
1:B:70:ARG:HE	1:B:79:ILE:HD13	1.58	0.68
1:B:149:ARG:NH1	1:B:152:GLU:OE1	2.26	0.68
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.13	0.67
1:B:326:LEU:HD12	5:B:510:BTB:H72	1.77	0.67
1:A:201:CYS:O	1:A:202:ARG:NH1	2.24	0.67
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.75	0.67
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.77	0.67
1:A:432:GLU:HG2	1:A:436:LYS:HE3	1.78	0.66
1:A:70:ARG:NH1	12:A:609:HOH:O	2.27	0.66
1:A:125:SER:HA	1:A:128:ARG:HE	1.60	0.66
1:D:209:THR:O	1:D:213:ASN:ND2	2.28	0.66
1:A:331:TYR:O	1:A:410:TYR:OH	2.14	0.65
1:A:89:GLN:O	12:A:602:HOH:O	2.15	0.65
1:C:262:ARG:NH1	1:C:283:ASN:O	2.31	0.64
1:A:167:GLU:OE2	7:A:507:GOL:O1	2.15	0.63
1:A:256:GLN:O	12:A:603:HOH:O	2.15	0.63
1:A:87:GLN:O	1:A:89:GLN:NE2	2.31	0.63
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.80	0.63
1:D:101:GLY:N	12:D:604:HOH:O	2.30	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.82	0.62
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.17	0.62
5:B:510:BTB:O3	1:C:384:ASP:OD2	2.18	0.62
5:B:511:BTB:HO3	5:B:511:BTB:HO1	1.37	0.62
1:D:336:VAL:HG21	4:D:503:8J4:C07	2.31	0.60
1:A:476:GLN:OE1	12:A:604:HOH:O	2.16	0.59
1:A:119:ALA:N	12:A:611:HOH:O	2.34	0.58
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.85	0.57
1:C:336:VAL:HG21	4:C:503:8J4:C07	2.35	0.57
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.20	0.56
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.33	0.55
1:A:86:ALA:O	1:B:97:ARG:NH2	2.39	0.55
1:C:200:ASP:OD1	1:C:200:ASP:N	2.37	0.55
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:NH1	1:D:152:GLU:OE1	2.39	0.55
1:C:128:ARG:O	1:C:132:ASN:ND2	2.40	0.55
1:C:143:SER:O	1:C:145:ALA:N	2.40	0.55
1:C:170:LEU:HD11	1:C:230:VAL:HG21	1.88	0.55
1:D:124:LEU:HD21	1:D:154:GLU:HG2	1.87	0.55
1:A:339:MET:HE2	1:A:473:PHE:HB3	1.89	0.55
1:D:447:TRP:HA	3:D:502:H4B:N1	2.22	0.54
1:D:67:LYS:O	12:D:601:HOH:O	2.18	0.54
1:C:379:VAL:HG21	1:C:402:ILE:HD11	1.89	0.54
2:B:501:HEM:HHB	2:B:501:HEM:HBB2	1.90	0.54
1:C:149:ARG:NE	1:C:169:GLU:OE2	2.38	0.53
5:A:504:BTB:O8	5:A:504:BTB:H42	2.09	0.53
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.53
1:A:171:VAL:HA	1:A:195:VAL:HG21	1.91	0.53
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.44	0.53
1:C:451:PRO:HB2	1:D:455:SER:OG	2.09	0.52
5:D:504:BTB:O4	5:D:504:BTB:O3	2.28	0.52
1:C:78:SER:OG	12:C:603:HOH:O	2.19	0.52
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.45	0.52
1:A:263:GLY:HA2	1:A:285:ARG:HA	1.92	0.52
1:A:455:SER:HA	1:A:460:PHE:CG	2.45	0.52
1:A:450:PRO:HG3	1:A:457:THR:HG21	1.90	0.52
5:A:505:BTB:O4	12:A:605:HOH:O	2.19	0.52
1:A:143:SER:OG	1:A:144:GLN:N	2.44	0.51
5:D:504:BTB:O8	8:D:510:CL:CL	2.64	0.51
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.91	0.51
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.93	0.51
1:C:166:ARG:N	1:C:169:GLU:OE1	2.44	0.51
1:D:100:LEU:N	12:D:604:HOH:O	2.43	0.51
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.51
1:A:387:THR:O	5:A:505:BTB:H61	2.10	0.50
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.50
1:C:450:PRO:HG3	1:C:457:THR:HG21	1.93	0.50
1:C:156:GLU:OE2	1:C:164:GLN:N	2.43	0.50
1:A:367:LEU:HA	1:A:373:TYR:HB2	1.94	0.50
1:B:378:ASP:OD1	5:B:507:BTB:H71	2.12	0.50
1:B:106:PRO:HB3	12:B:668:HOH:O	2.11	0.49
1:C:453:SER:HA	1:D:452:ILE:HG22	1.94	0.49
1:A:341:LEU:HB3	1:A:348:PHE:HB2	1.95	0.49
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.94	0.49
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.94	0.48
1:D:271:THR:O	1:D:275:ILE:HG12	2.12	0.48
5:C:504:BTB:O8	5:C:504:BTB:O6	2.20	0.48
1:B:336:VAL:HG21	4:B:503:8J4:C07	2.44	0.48
1:C:240:ASP:OD1	1:C:349:PRO:HG2	2.14	0.48
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.47	0.48
1:C:229:THR:O	1:C:352:PRO:HD2	2.14	0.48
1:A:250:ARG:NH1	1:A:267:ASN:OD1	2.46	0.48
1:B:68:PHE:CD2	1:B:83:THR:HG22	2.49	0.47
1:C:367:LEU:HA	1:C:373:TYR:HB2	1.95	0.47
1:D:138:ILE:HD12	1:D:140:ARG:HD3	1.95	0.47
1:A:347:GLU:O	1:A:349:PRO:HD3	2.15	0.47
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.44	0.47
1:B:243:ILE:HG21	1:B:337:SER:HB2	1.97	0.47
1:C:119:ALA:N	12:C:611:HOH:O	2.47	0.47
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.97	0.47
5:B:511:BTB:H71	5:B:511:BTB:H32	1.50	0.47
1:C:316[B]:GLU:OE1	12:C:605:HOH:O	2.20	0.47
1:C:428:MET:HG3	1:C:458:PRO:HB2	1.95	0.47
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.50	0.47
1:B:90:GLN:HB2	1:B:468:PHE:CD1	2.50	0.46
5:D:505:BTB:H71	5:D:505:BTB:H42	1.51	0.46
1:B:447:TRP:HA	3:B:502:H4B:N1	2.30	0.46
1:C:238:ARG:HE	1:C:240:ASP:CG	2.18	0.46
1:C:160:THR:HG23	1:C:162:THR:HG22	1.98	0.46
5:C:504:BTB:H52	5:C:504:BTB:H42	1.59	0.46
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.81	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.46
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.97	0.46
1:D:171:VAL:HG12	1:D:175:LYS:HE3	1.98	0.46
5:B:505:BTB:H72	12:B:602:HOH:O	2.16	0.45
1:C:203:SER:OG	1:C:204:ALA:N	2.47	0.45
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.98	0.45
1:C:248:LEU:HD12	1:C:335:ALA:HB1	1.99	0.45
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.97	0.45
5:B:506:BTB:H32	5:B:506:BTB:H52	1.51	0.45
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.72	0.45
1:C:85:SER:HB3	1:C:467:TYR:CE2	2.52	0.45
1:C:298:GLU:OE1	5:C:504:BTB:N	2.50	0.45
1:D:298:GLU:OE1	5:D:505:BTB:N	2.50	0.45
5:D:505:BTB:H11	5:D:505:BTB:H51	1.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:505:BTB:H61	5:D:505:BTB:H72	1.46	0.45
1:C:91:ASP:OD1	12:C:604:HOH:O	2.20	0.44
5:B:507:BTB:O8	12:B:602:HOH:O	2.21	0.44
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.57	0.44
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.98	0.44
1:A:275:ILE:HG12	1:A:281:PRO:HG3	1.98	0.44
5:D:504:BTB:H42	5:D:504:BTB:H71	1.53	0.44
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.99	0.44
1:A:396:ASP:N	1:A:396:ASP:OD1	2.49	0.44
1:A:336:VAL:HG21	4:A:503:8J4:C07	2.47	0.44
1:B:247:GLN:HB2	1:B:250:ARG:HG2	2.00	0.44
1:D:200:ASP:O	1:D:202:ARG:HG2	2.17	0.44
1:A:144:GLN:CG	1:A:145:ALA:H	2.30	0.43
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.00	0.43
1:C:451:PRO:HB2	1:D:455:SER:HG	1.82	0.43
1:A:70:ARG:NH2	12:A:614:HOH:O	2.43	0.43
1:B:106:PRO:O	12:B:603:HOH:O	2.21	0.43
1:A:334:PRO:HB3	1:A:357:TYR:CZ	2.53	0.43
1:A:127:ALA:O	1:A:131:ILE:HG12	2.19	0.43
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.31	0.43
1:A:90:GLN:HB2	1:A:468:PHE:CD1	2.53	0.43
1:B:149:ARG:HD3	1:B:166:ARG:CZ	2.48	0.43
1:B:321:GLU:OE1	5:B:504:BTB:H62	2.18	0.43
1:B:388:ARG:HB2	1:B:388:ARG:HE	1.44	0.43
1:B:71:VAL:HG13	1:B:463:GLU:HB2	2.00	0.43
1:A:94:CYS:SG	1:A:100:LEU:N	2.70	0.43
5:B:505:BTB:H52	5:B:505:BTB:H32	1.50	0.43
5:D:506:BTB:H11	5:D:506:BTB:H71	1.76	0.43
1:A:269:GLU:O	1:A:272:GLU:HB3	2.19	0.43
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.54	0.43
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.53	0.43
1:B:67:LYS:N	12:B:622:HOH:O	2.52	0.43
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.43
1:A:242:ARG:NE	1:A:479:PRO:HD3	2.33	0.42
5:B:507:BTB:H52	5:B:507:BTB:H11	1.50	0.42
1:C:396:ASP:OD2	1:D:453:SER:OG	2.18	0.42
1:A:246:SER:OG	1:A:250:ARG:HD2	2.19	0.42
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.54	0.42
1:D:199:ARG:O	1:D:232:PRO:HG3	2.19	0.42
1:C:397:LYS:HG3	1:D:400:VAL:HG11	2.02	0.42
1:C:358:MET:HB3	1:C:358:MET:HE2	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:O	1:B:250:ARG:HG2	2.18	0.42
1:D:204:ALA:O	1:D:207:MET:HB2	2.20	0.42
1:D:478:ASP:HA	1:D:479:PRO:HD3	1.81	0.42
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.55	0.42
1:A:228:ILE:HG13	1:A:353:PHE:HB3	2.00	0.42
1:A:359:SER:OG	1:A:419:ASP:HA	2.20	0.42
1:C:369:ASP:HB2	1:C:372:ARG:HG2	2.02	0.42
1:A:298:GLU:OE2	12:A:606:HOH:O	2.22	0.41
1:A:382:CYS:HA	5:A:504:BTB:H11	2.02	0.41
1:C:224:LEU:HD12	1:C:356:TRP:HB3	2.02	0.41
1:D:72:LYS:H	1:D:463:GLU:HB2	1.86	0.41
5:D:506:BTB:H32	5:D:506:BTB:H52	1.59	0.41
1:B:301:GLU:HB3	1:B:303:PHE:HE1	1.85	0.41
1:B:396:ASP:N	1:B:396:ASP:OD1	2.47	0.41
1:D:213:ASN:N	1:D:213:ASN:HD22	2.19	0.41
5:C:504:BTB:H71	5:C:504:BTB:H32	1.77	0.41
1:D:249:VAL:HA	12:D:611:HOH:O	2.21	0.41
1:D:301:GLU:HB3	1:D:303:PHE:HE1	1.86	0.41
1:A:128:ARG:O	1:A:132:ASN:ND2	2.53	0.41
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.03	0.41
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.33	0.41
5:B:510:BTB:H32	1:C:382:CYS:HA	2.01	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.41
1:A:370:PRO:HB2	1:B:75:GLU:HG3	2.03	0.41
1:D:235[B]:CYS:HA	1:D:236:PRO:HD3	1.93	0.41
1:A:384:ASP:HB3	12:A:656:HOH:O	2.21	0.41
1:D:435:GLN:O	1:D:439:GLY:HA2	2.21	0.41
1:A:393:LEU:HD12	1:B:404:VAL:HG23	2.03	0.40
1:A:104:VAL:O	1:A:106:PRO:HD3	2.21	0.40
1:A:288:VAL:HG12	1:A:289:LEU:O	2.21	0.40
1:C:238:ARG:NH2	1:C:240:ASP:OD2	2.50	0.40
1:D:387:THR:HA	1:D:394:TRP:CD1	2.56	0.40
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.40
1:A:466:ASN:HB3	1:B:99:CYS:HB3	2.03	0.40
1:B:429:LYS:HA	1:B:429:LYS:HD2	1.89	0.40
1:C:207:MET:HE2	1:C:293:LEU:HB3	2.03	0.40
1:D:162:THR:OG1	1:D:163:TYR:N	2.54	0.40
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.04	0.40
1:B:364:THR:HG21	1:B:452:ILE:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/440 (91%)	369 (92%)	29 (7%)	4 (1%)	15	14
1	B	401/440 (91%)	387 (96%)	14 (4%)	0	100	100
1	C	399/440 (91%)	380 (95%)	16 (4%)	3 (1%)	19	19
1	D	401/440 (91%)	388 (97%)	13 (3%)	0	100	100
All	All	1603/1760 (91%)	1524 (95%)	72 (4%)	7 (0%)	34	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	A	90	GLN
1	C	89	GLN
1	C	143	SER
1	A	297	ASP
1	A	107	ARG
1	A	181	ALA

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	345/373 (92%)	323 (94%)	22 (6%)	17	20
1	B	344/373 (92%)	332 (96%)	12 (4%)	36	46
1	C	342/373 (92%)	330 (96%)	12 (4%)	36	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	344/373 (92%)	339 (98%)	5 (2%)	65	78
All	All	1375/1492 (92%)	1324 (96%)	51 (4%)	34	43

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	109	LEU
1	A	121	GLU
1	A	124	LEU
1	A	133	GLN
1	A	140	ARG
1	A	152	GLU
1	A	201	CYS
1	A	226	SER
1	A	238	ARG
1	A	242	ARG
1	A	250	ARG
1	A	256	GLN
1	A	257	GLN
1	A	285	ARG
1	A	297	ASP
1	A	298	GLU
1	A	309	LEU
1	A	329	ARG
1	A	396	ASP
1	A	403	ASN
1	A	470	SER
1	B	70	ARG
1	B	90	GLN
1	B	148	GLN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	246	SER
1	B	298	GLU
1	B	326	LEU
1	B	343	ILE
1	B	364	THR
1	B	389	THR
1	B	396	ASP
1	C	71	VAL
1	C	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	137	SER
1	C	154	GLU
1	C	160	THR
1	C	216	LYS
1	C	221	ARG
1	C	234	ARG
1	C	240	ASP
1	C	257	GLN
1	C	309	LEU
1	C	321	GLU
1	D	71	VAL
1	D	97	ARG
1	D	98	ARG
1	D	136	SER
1	D	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	213	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 13 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
5	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.55	0
2	HEM	B	501	1	27,50,50	2.10	5 (18%)	17,82,82	2.23	4 (23%)
5	BTB	B	510	9	13,13,13	0.44	0	7,16,16	0.56	0
7	GOL	A	507	-	5,5,5	0.45	0	5,5,5	0.31	0
3	H4B	C	502	-	16,18,18	0.88	0	11,26,26	2.66	6 (54%)
4	8J4	A	503	-	26,26,26	0.88	0	33,35,35	0.92	0
5	BTB	A	504	9	13,13,13	0.38	0	7,16,16	0.40	0
3	H4B	D	502	-	16,18,18	0.91	0	11,26,26	2.86	5 (45%)
3	H4B	B	502	-	16,18,18	0.89	0	11,26,26	2.75	6 (54%)
2	HEM	A	501	1	27,50,50	2.06	5 (18%)	17,82,82	1.49	3 (17%)
5	BTB	B	505	-	13,13,13	0.34	0	7,16,16	0.43	0
5	BTB	B	507	-	13,13,13	0.37	0	7,16,16	0.68	0
5	BTB	B	504	9	13,13,13	0.40	0	7,16,16	0.38	0
3	H4B	A	502	-	16,18,18	0.88	0	11,26,26	2.68	6 (54%)
2	HEM	C	501	1	27,50,50	2.19	6 (22%)	17,82,82	1.51	4 (23%)
7	GOL	C	506	-	5,5,5	0.42	0	5,5,5	0.49	0
4	8J4	C	503	-	26,26,26	0.92	0	33,35,35	1.10	3 (9%)
4	8J4	B	503	-	26,26,26	0.94	0	33,35,35	1.10	2 (6%)
5	BTB	D	505	-	13,13,13	0.42	0	7,16,16	0.75	0
5	BTB	B	506	-	13,13,13	0.69	0	7,16,16	0.73	0
5	BTB	D	506	-	13,13,13	0.43	0	7,16,16	0.76	0
4	8J4	D	503	-	26,26,26	0.81	0	33,35,35	1.01	1 (3%)
2	HEM	D	501	1	27,50,50	2.08	5 (18%)	17,82,82	2.19	5 (29%)
5	BTB	B	511	-	13,13,13	0.62	0	7,16,16	0.95	0
5	BTB	C	504	-	13,13,13	0.34	0	7,16,16	0.36	0
5	BTB	D	504	9	13,13,13	0.45	0	7,16,16	0.40	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
5	BTB	A	505	-	-	5/21/21/21	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	0/6/54/54	-
5	BTB	B	510	9	-	5/21/21/21	-
7	GOL	A	507	-	-	3/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	8J4	A	503	-	-	2/9/19/19	0/3/3/3
5	BTB	A	504	9	-	7/21/21/21	-
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
2	HEM	A	501	1	-	3/6/54/54	-
5	BTB	B	505	-	-	8/21/21/21	-
5	BTB	B	507	-	-	4/21/21/21	-
5	BTB	B	504	9	-	3/21/21/21	-
3	H4B	A	502	-	-	1/8/17/17	0/2/2/2
2	HEM	C	501	1	-	5/6/54/54	-
7	GOL	C	506	-	-	4/4/4/4	-
4	8J4	C	503	-	-	2/9/19/19	0/3/3/3
4	8J4	B	503	-	-	0/9/19/19	0/3/3/3
5	BTB	D	505	-	-	9/21/21/21	-
5	BTB	B	506	-	-	4/21/21/21	-
5	BTB	D	506	-	-	5/21/21/21	-
4	8J4	D	503	-	-	2/9/19/19	0/3/3/3
2	HEM	D	501	1	-	0/6/54/54	-
5	BTB	B	511	-	-	6/21/21/21	-
5	BTB	C	504	-	-	0/21/21/21	-
5	BTB	D	504	9	-	8/21/21/21	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	5.50	1.54	1.37
2	B	501	HEM	C3D-C2D	5.08	1.52	1.37
2	D	501	HEM	C3D-C2D	5.06	1.52	1.37
2	A	501	HEM	C3D-C2D	4.94	1.52	1.37
2	B	501	HEM	C3B-C2B	-4.79	1.33	1.40
2	C	501	HEM	C3B-C2B	-4.70	1.33	1.40
2	D	501	HEM	C3B-C2B	-4.36	1.34	1.40
2	B	501	HEM	C3B-CAB	4.12	1.56	1.47
2	A	501	HEM	C3B-C2B	-4.10	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-CAC	3.78	1.55	1.47
2	C	501	HEM	C3B-CAB	3.75	1.55	1.47
2	D	501	HEM	C3C-CAC	3.75	1.55	1.47
2	C	501	HEM	C3C-CAC	3.75	1.55	1.47
2	D	501	HEM	C3B-CAB	3.67	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.64	1.35	1.40
2	A	501	HEM	C3B-CAB	3.61	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.60	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.55	1.35	1.40
2	B	501	HEM	C3C-CAC	3.53	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.48	1.35	1.40
2	C	501	HEM	CAA-C2A	2.18	1.55	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-6.44	100.61	112.48
3	D	502	H4B	C4-C4A-C8A	6.09	119.97	114.57
2	B	501	HEM	CBA-CAA-C2A	-5.35	102.61	112.49
3	C	502	H4B	C4-C4A-C8A	5.26	119.24	114.57
3	A	502	H4B	C4-C4A-C8A	5.24	119.22	114.57
2	B	501	HEM	CBD-CAD-C3D	-5.00	103.27	112.48
3	B	502	H4B	C4-C4A-C8A	4.91	118.93	114.57
3	B	502	H4B	N3-C2-N1	-3.70	119.61	125.42
2	A	501	HEM	CBD-CAD-C3D	-3.67	105.71	112.48
3	B	502	H4B	C4-C4A-N5	3.65	122.18	119.12
3	C	502	H4B	N3-C2-N1	-3.30	120.24	125.42
2	B	501	HEM	CAD-CBD-CGD	-3.25	107.22	112.67
3	B	502	H4B	C4-N3-C2	3.24	121.07	115.93
3	A	502	H4B	C4-C4A-N5	3.23	121.83	119.12
3	A	502	H4B	N3-C2-N1	-3.22	120.37	125.42
3	D	502	H4B	N3-C2-N1	-3.17	120.44	125.42
3	A	502	H4B	C4-N3-C2	3.16	120.95	115.93
2	D	501	HEM	C1D-C2D-C3D	-3.13	104.82	107.00
2	D	501	HEM	CBA-CAA-C2A	-3.13	106.72	112.49
4	C	503	8J4	C23-C29-N30	-3.13	104.94	112.67
3	D	502	H4B	C4-N3-C2	3.12	120.88	115.93
3	B	502	H4B	C2-N1-C8A	3.11	121.51	114.54
3	C	502	H4B	C4-C4A-N5	3.07	121.70	119.12
3	D	502	H4B	C4-C4A-N5	2.98	121.62	119.12
3	C	502	H4B	C4-N3-C2	2.94	120.60	115.93
3	C	502	H4B	C2-N1-C8A	2.92	121.08	114.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C2-N1-C8A	2.85	120.93	114.54
3	A	502	H4B	C2-N1-C8A	2.80	120.81	114.54
2	D	501	HEM	C4A-C3A-C2A	2.78	108.93	107.00
2	C	501	HEM	C4A-C3A-C2A	2.78	108.93	107.00
4	B	503	8J4	O12-C11-C08	2.66	117.15	109.16
3	C	502	H4B	N2-C2-N3	2.62	121.33	117.25
4	B	503	8J4	C03-C02-N01	-2.49	119.08	122.08
3	A	502	H4B	N2-C2-N3	2.47	121.09	117.25
2	C	501	HEM	C1D-C2D-C3D	-2.30	105.39	107.00
2	C	501	HEM	CMC-C2C-C3C	2.25	128.89	124.68
4	C	503	8J4	O12-C11-C08	2.23	115.85	109.16
2	C	501	HEM	CBD-CAD-C3D	-2.22	108.38	112.48
2	B	501	HEM	CMC-C2C-C3C	2.22	128.83	124.68
2	D	501	HEM	CMC-C2C-C3C	2.22	128.83	124.68
2	A	501	HEM	C4A-C3A-C2A	2.17	108.50	107.00
2	A	501	HEM	CMC-C2C-C3C	2.16	128.72	124.68
4	C	503	8J4	C29-C23-C24	-2.04	116.23	120.64
3	B	502	H4B	N2-C2-N1	2.02	120.40	117.25
4	D	503	8J4	C03-C02-N01	-2.01	119.66	122.08

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	510	BTB	O1-C1-C2-C3
5	B	510	BTB	O1-C1-C2-C4
5	B	510	BTB	O1-C1-C2-N
7	A	507	GOL	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
5	B	505	BTB	O1-C1-C2-C3
5	B	505	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	505	BTB	N-C5-C6-O6
5	B	507	BTB	C3-C2-C4-O4
5	B	507	BTB	N-C2-C4-O4
5	B	504	BTB	O1-C1-C2-C4
2	C	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C3D-CAD-CBD-CGD
7	C	506	GOL	O1-C1-C2-C3
7	C	506	GOL	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	C6-C5-N-C7
5	B	506	BTB	O1-C1-C2-C3
5	D	506	BTB	C1-C2-C4-O4
5	D	506	BTB	C3-C2-C4-O4
5	D	506	BTB	N-C2-C4-O4
5	B	511	BTB	C3-C2-N-C5
5	B	511	BTB	C3-C2-N-C7
5	B	511	BTB	C4-C2-N-C5
5	B	511	BTB	C6-C5-N-C7
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
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	B	505	BTB	N-C7-C8-O8
5	B	506	BTB	N-C5-C6-O6
5	D	504	BTB	N-C5-C6-O6
4	C	503	8J4	C26-C21-O12-C11
4	C	503	8J4	C22-C21-O12-C11
5	B	510	BTB	N-C5-C6-O6
5	D	505	BTB	N-C5-C6-O6
3	B	502	H4B	C7-C6-C9-O9
5	B	507	BTB	N-C7-C8-O8
7	A	507	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
5	A	504	BTB	C6-C5-N-C7
4	D	503	8J4	C26-C21-O12-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	503	8J4	C22-C21-O12-C11
7	C	506	GOL	O2-C2-C3-O3
5	D	504	BTB	N-C7-C8-O8
3	B	502	H4B	C7-C6-C9-C10
5	D	506	BTB	N-C5-C6-O6
5	B	507	BTB	C1-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	B	506	BTB	O1-C1-C2-C4
2	A	501	HEM	C3A-C2A-CAA-CBA
5	B	504	BTB	O1-C1-C2-N
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C2D-C3D-CAD-CBD
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-N-C5
5	B	506	BTB	O1-C1-C2-N
5	B	511	BTB	C1-C2-N-C5
5	B	511	BTB	C1-C2-N-C7
4	A	503	8J4	C26-C21-O12-C11
5	A	505	BTB	N-C5-C6-O6
4	A	503	8J4	C22-C21-O12-C11
5	D	506	BTB	N-C7-C8-O8
3	D	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	A	502	H4B	N5-C6-C9-O9
5	A	505	BTB	O1-C1-C2-C4
5	B	510	BTB	C4-C2-C3-O3
5	B	504	BTB	O1-C1-C2-C3
7	A	507	GOL	O2-C2-C3-O3

There are no ring outliers.

25 monomers are involved in 51 short contacts:

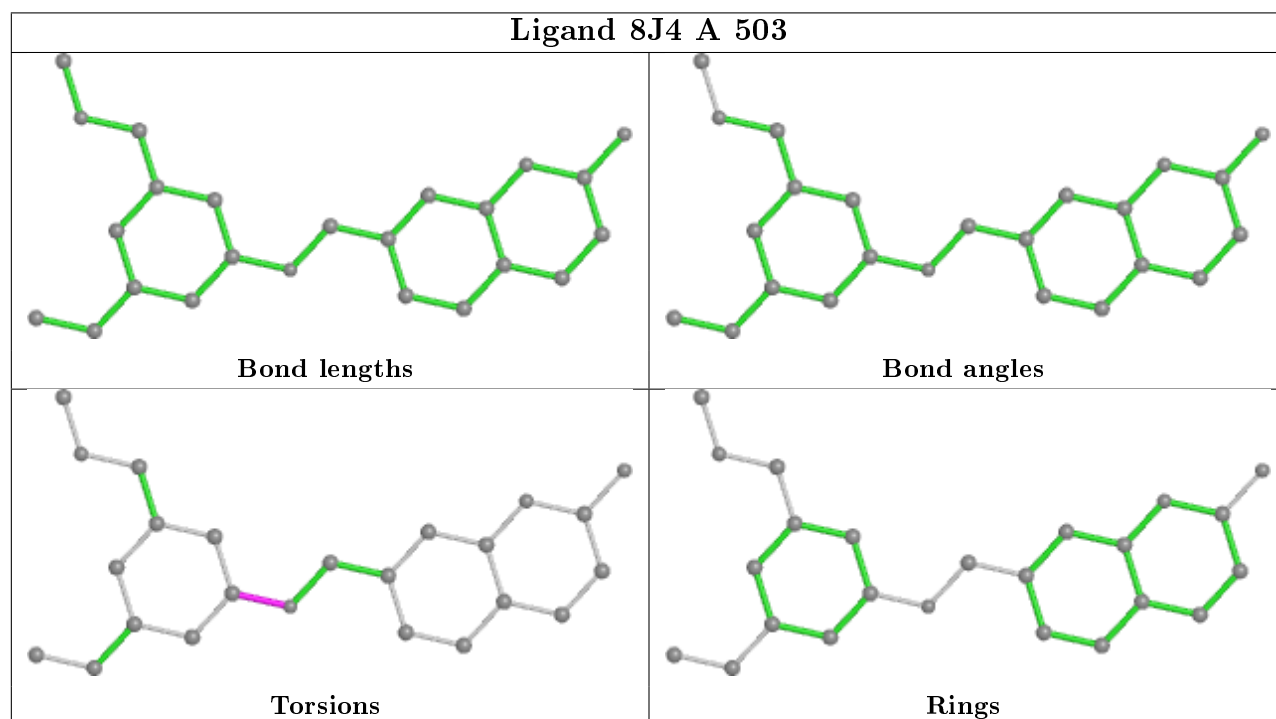
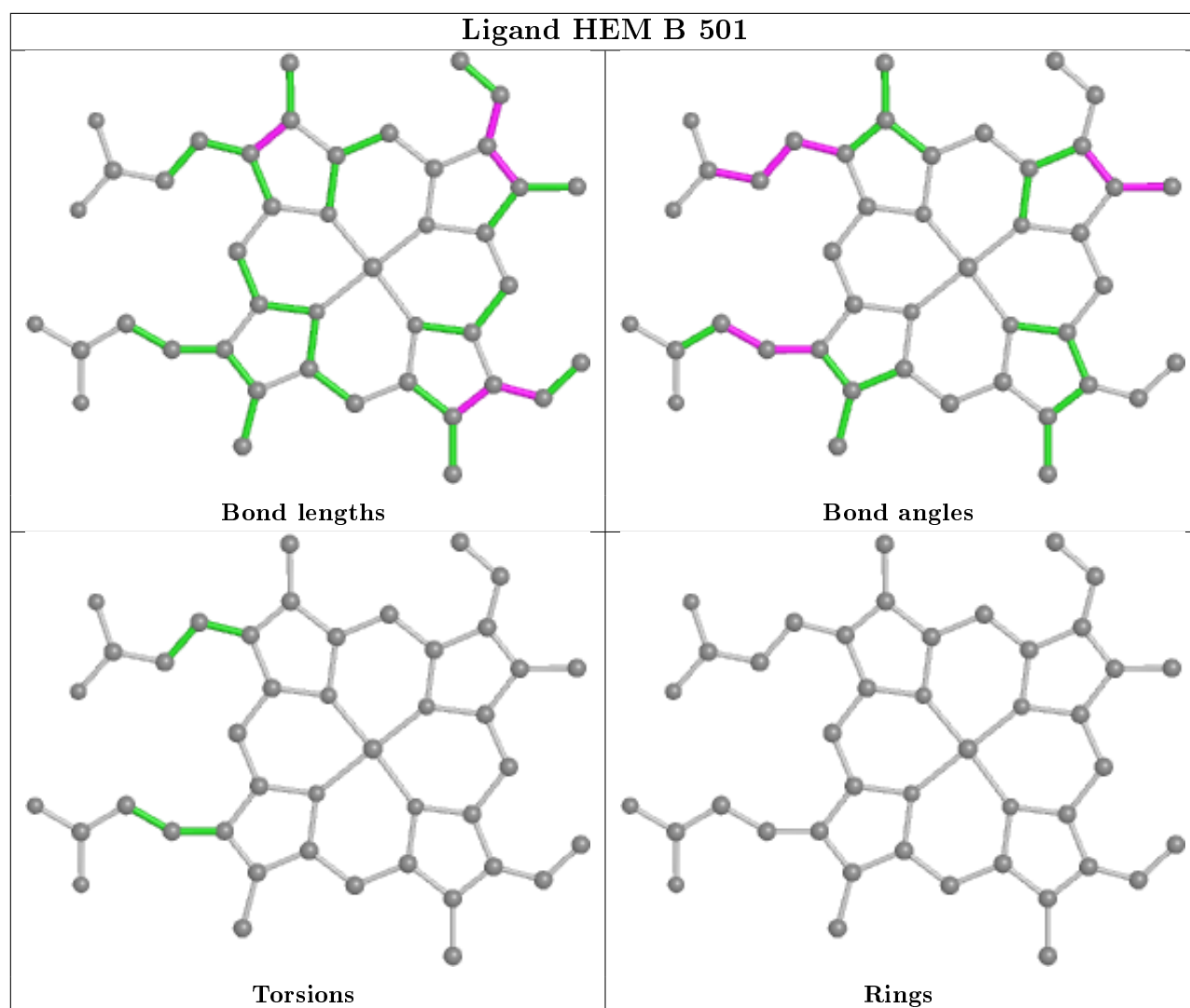
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	BTB	3	0
2	B	501	HEM	2	0
5	B	510	BTB	3	0
7	A	507	GOL	1	0
3	C	502	H4B	1	0
4	A	503	8J4	1	0
5	A	504	BTB	2	0

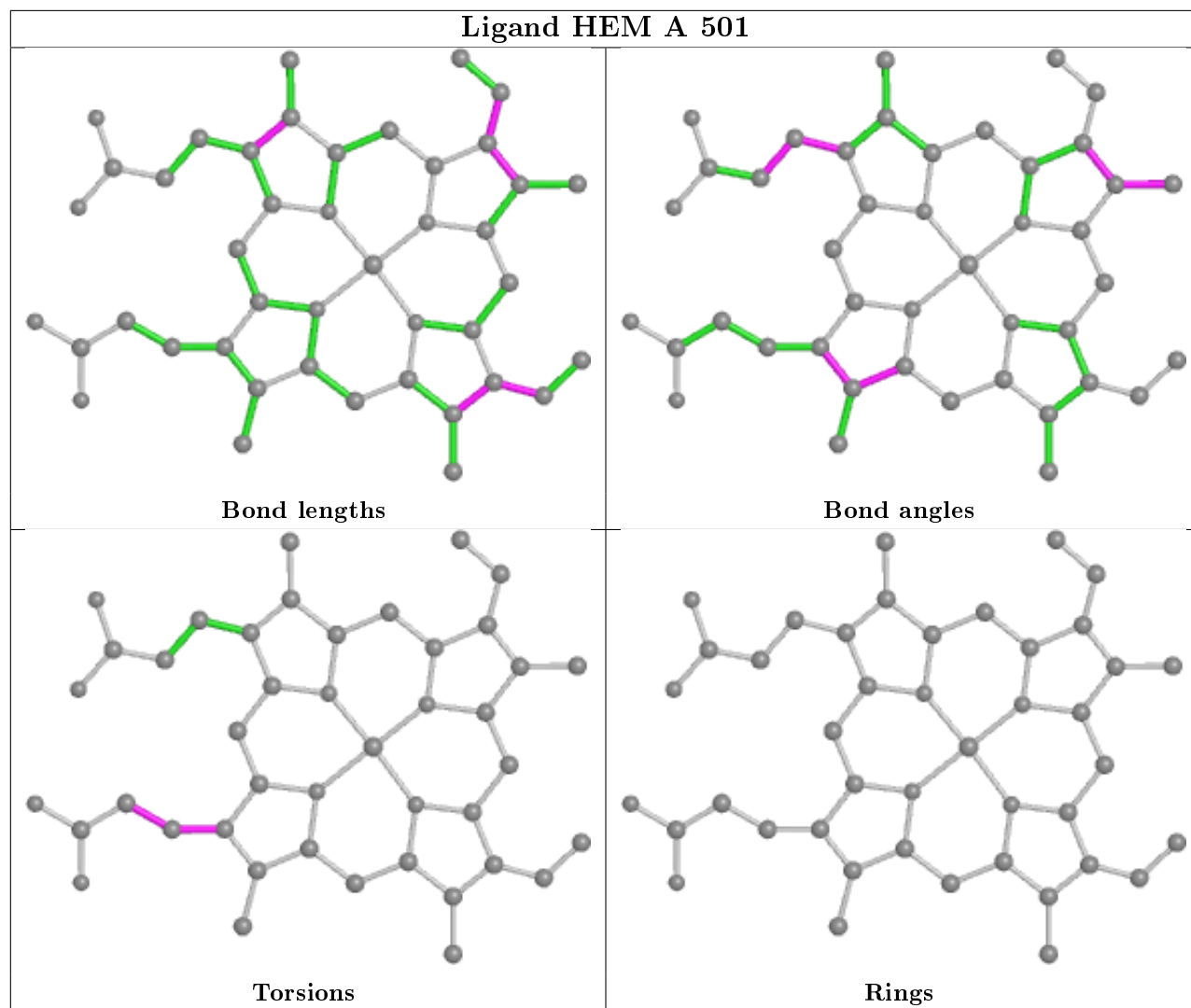
Continued on next page...

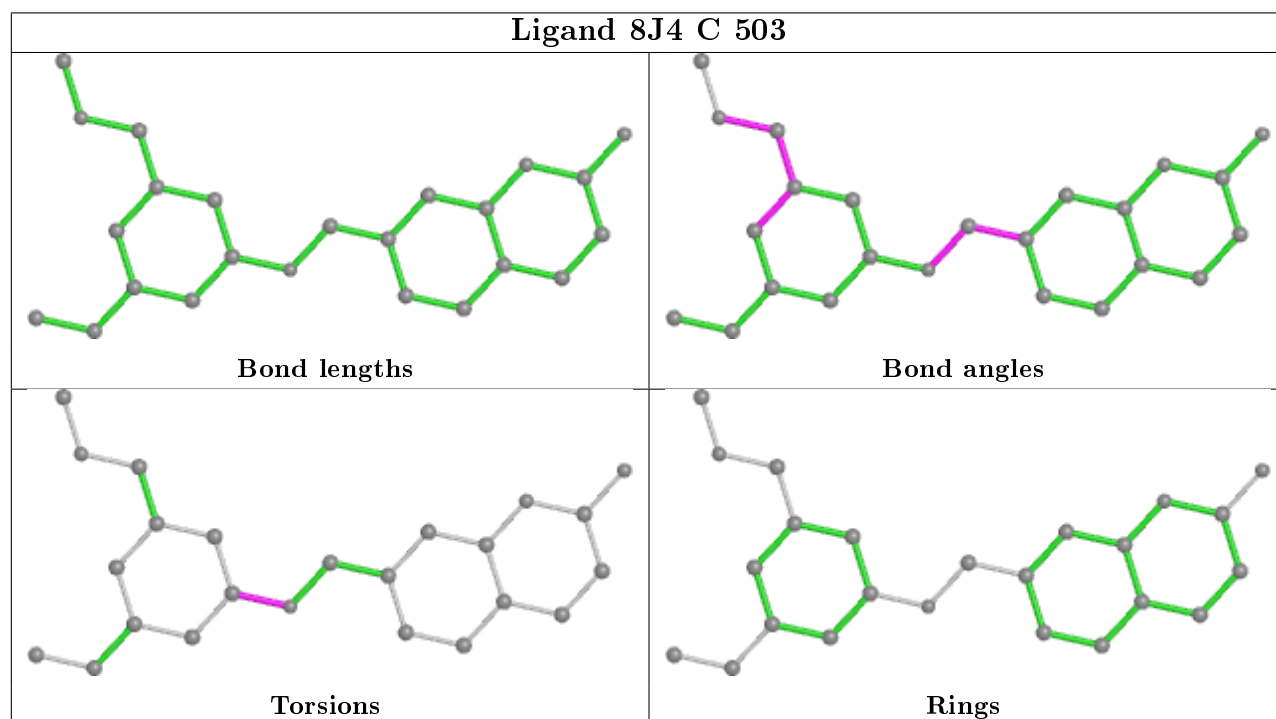
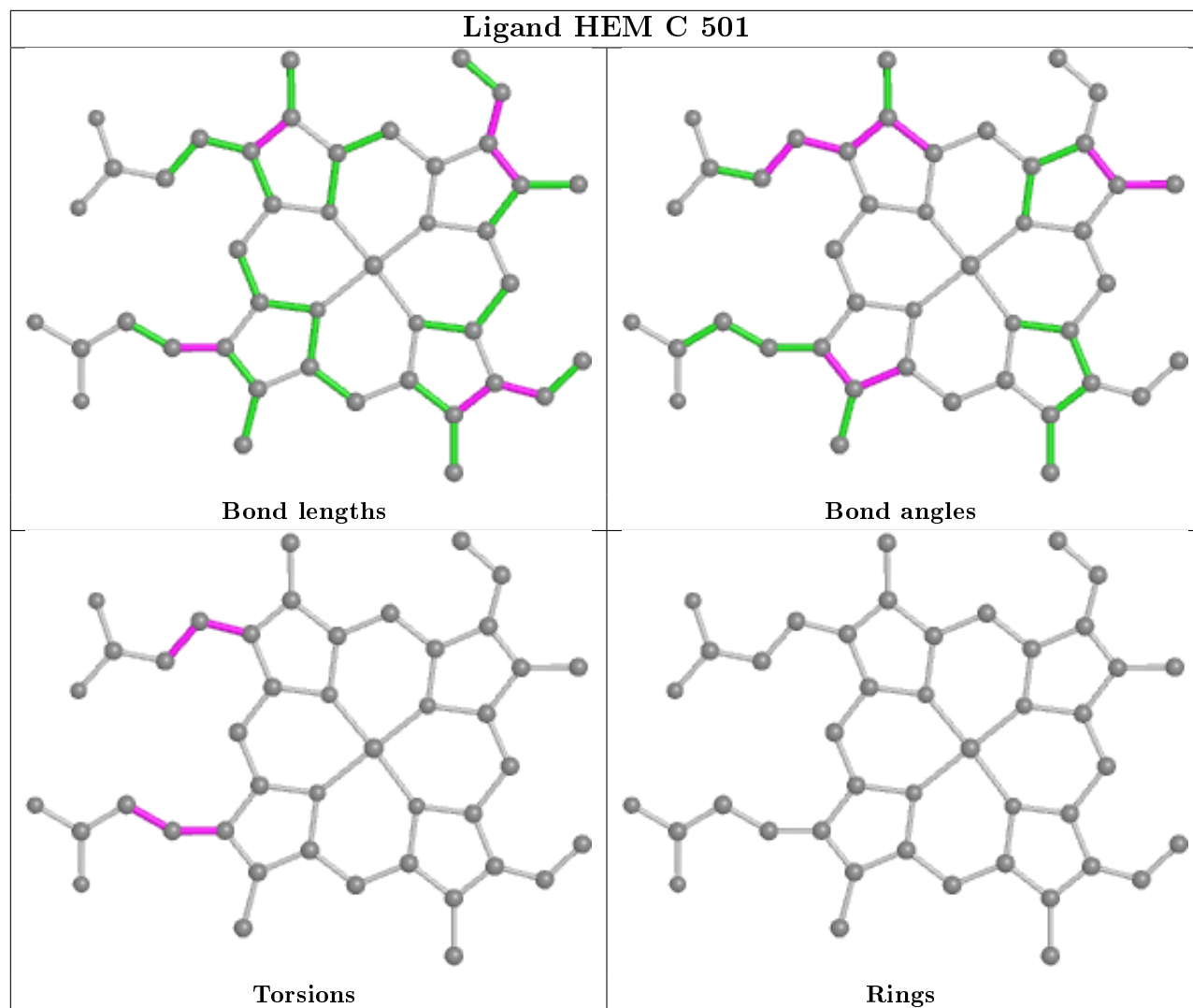
Continued from previous page...

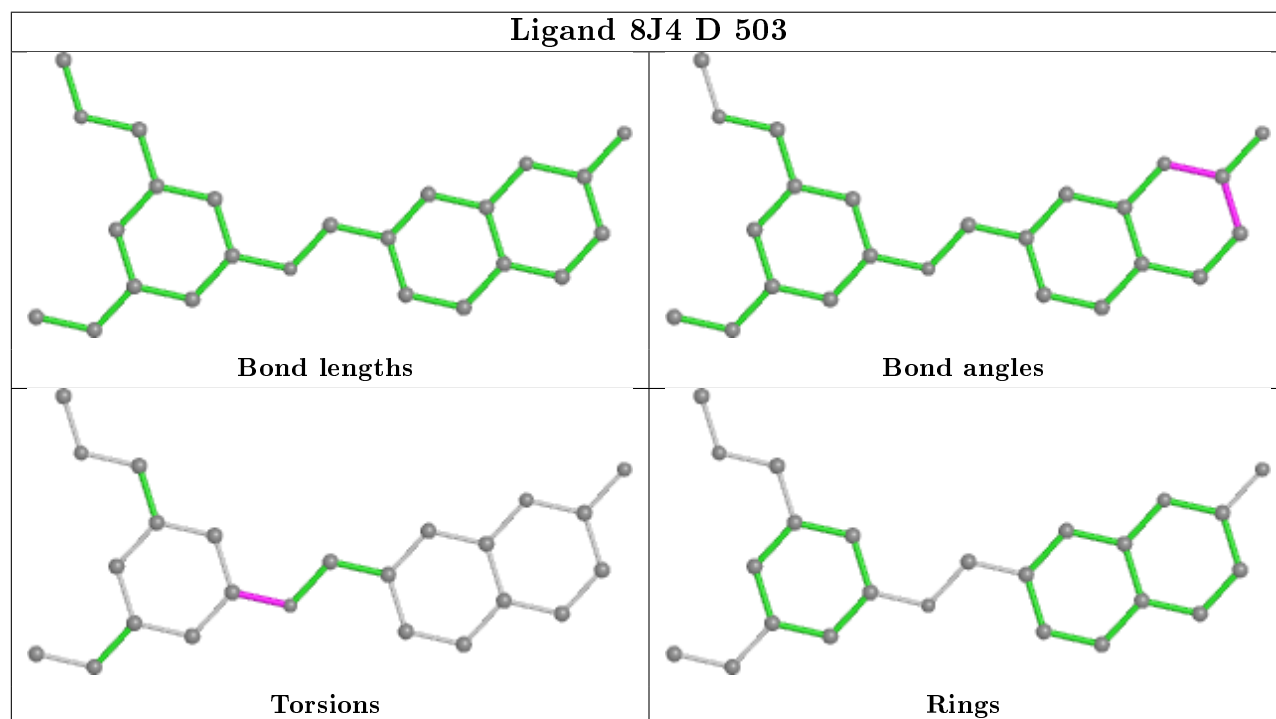
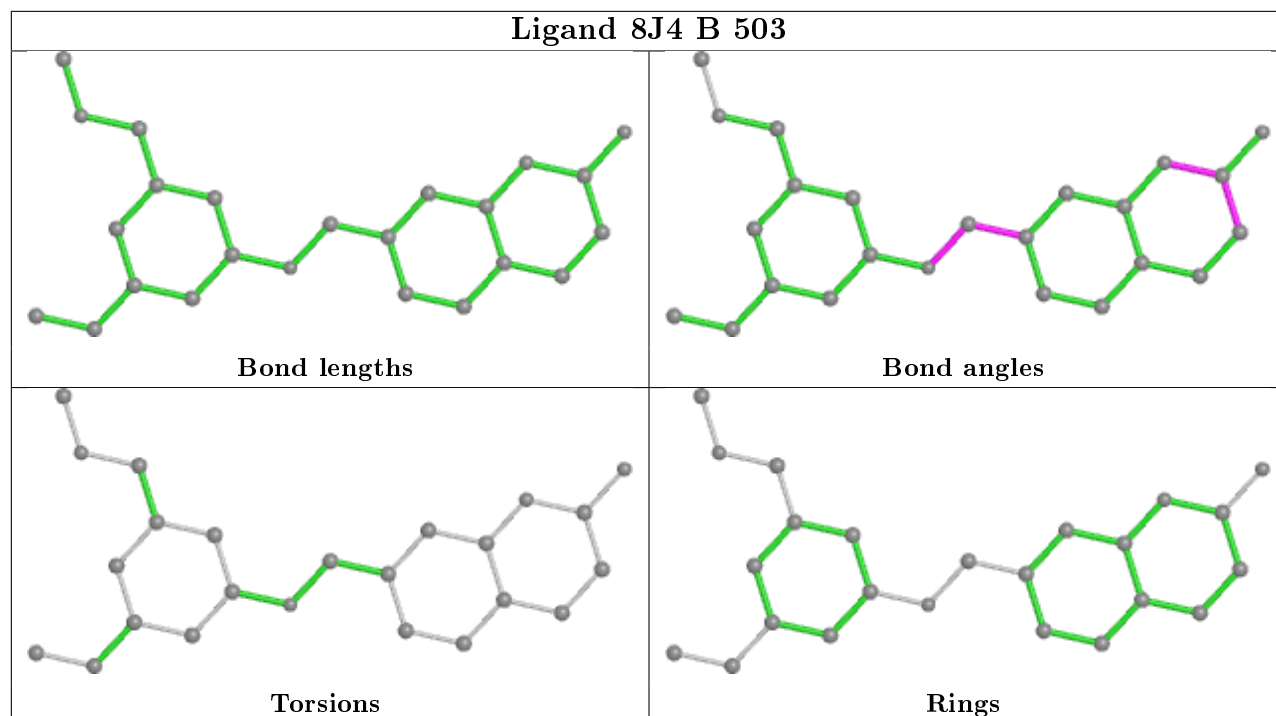
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	H4B	1	0
3	B	502	H4B	1	0
2	A	501	HEM	4	0
5	B	505	BTB	2	0
5	B	507	BTB	3	0
5	B	504	BTB	1	0
3	A	502	H4B	1	0
2	C	501	HEM	2	0
4	C	503	8J4	1	0
4	B	503	8J4	1	0
5	D	505	BTB	4	0
5	B	506	BTB	1	0
5	D	506	BTB	2	0
4	D	503	8J4	1	0
2	D	501	HEM	3	0
5	B	511	BTB	2	0
5	C	504	BTB	4	0
5	D	504	BTB	4	0

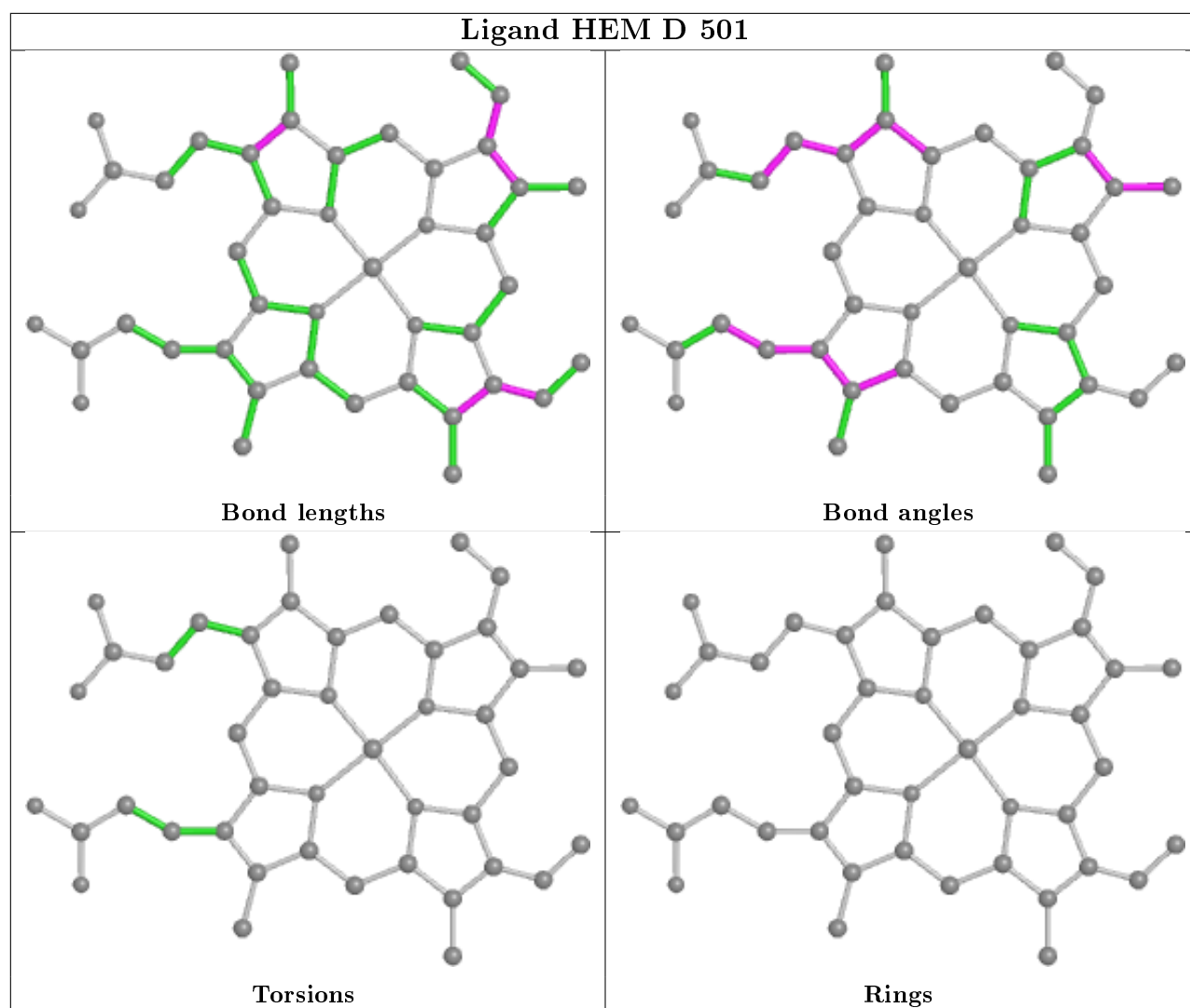
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	0.53	30 (7%) 14 13	31, 60, 107, 126	0
1	B	402/440 (91%)	0.10	5 (1%) 79 77	29, 44, 77, 108	0
1	C	401/440 (91%)	0.28	19 (4%) 31 30	32, 55, 95, 118	0
1	D	402/440 (91%)	0.04	6 (1%) 73 72	28, 43, 71, 117	0
All	All	1609/1760 (91%)	0.24	60 (3%) 41 39	28, 50, 93, 126	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	TRP	6.9
1	A	107	ARG	6.1
1	A	109	LEU	6.1
1	A	142	GLY	5.2
1	D	67	LYS	4.9
1	C	301	GLU	4.0
1	D	89	GLN	3.9
1	A	301	GLU	3.9
1	A	346	LEU	3.9
1	B	89	GLN	3.6
1	A	89	GLN	3.6
1	C	292	LEU	3.4
1	C	480	TRP	3.4
1	A	163	TYR	3.2
1	C	305	LEU	3.1
1	A	153	VAL	3.1
1	A	152	GLU	2.9
1	A	202	ARG	2.9
1	A	140	ARG	2.9
1	A	254	TYR	2.9
1	A	257	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	304	LEU	2.8
1	A	305	LEU	2.7
1	A	134	TYR	2.7
1	B	150	LEU	2.7
1	C	148	GLN	2.7
1	C	238	ARG	2.7
1	A	468	PHE	2.6
1	A	86	ALA	2.5
1	C	280	THR	2.5
1	C	140	ARG	2.4
1	A	204	ALA	2.4
1	A	124	LEU	2.4
1	A	275	ILE	2.4
1	D	90	GLN	2.4
1	A	108	LYS	2.4
1	A	291	LEU	2.3
1	A	303	PHE	2.3
1	C	294	GLN	2.3
1	C	303	PHE	2.3
1	A	280	THR	2.3
1	A	473	PHE	2.3
1	B	67	LYS	2.3
1	D	141[A]	SER	2.3
1	C	293	LEU	2.3
1	C	468	PHE	2.3
1	A	122	GLN	2.3
1	C	174	ALA	2.2
1	C	144	GLN	2.1
1	C	122	GLN	2.1
1	A	304	LEU	2.1
1	B	142	GLY	2.1
1	D	468	PHE	2.1
1	A	131	ILE	2.1
1	C	131	ILE	2.1
1	D	255	ARG	2.1
1	C	134	TYR	2.1
1	A	130	PHE	2.0
1	B	295	ALA	2.0
1	C	259	GLY	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 carbohydrates 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.

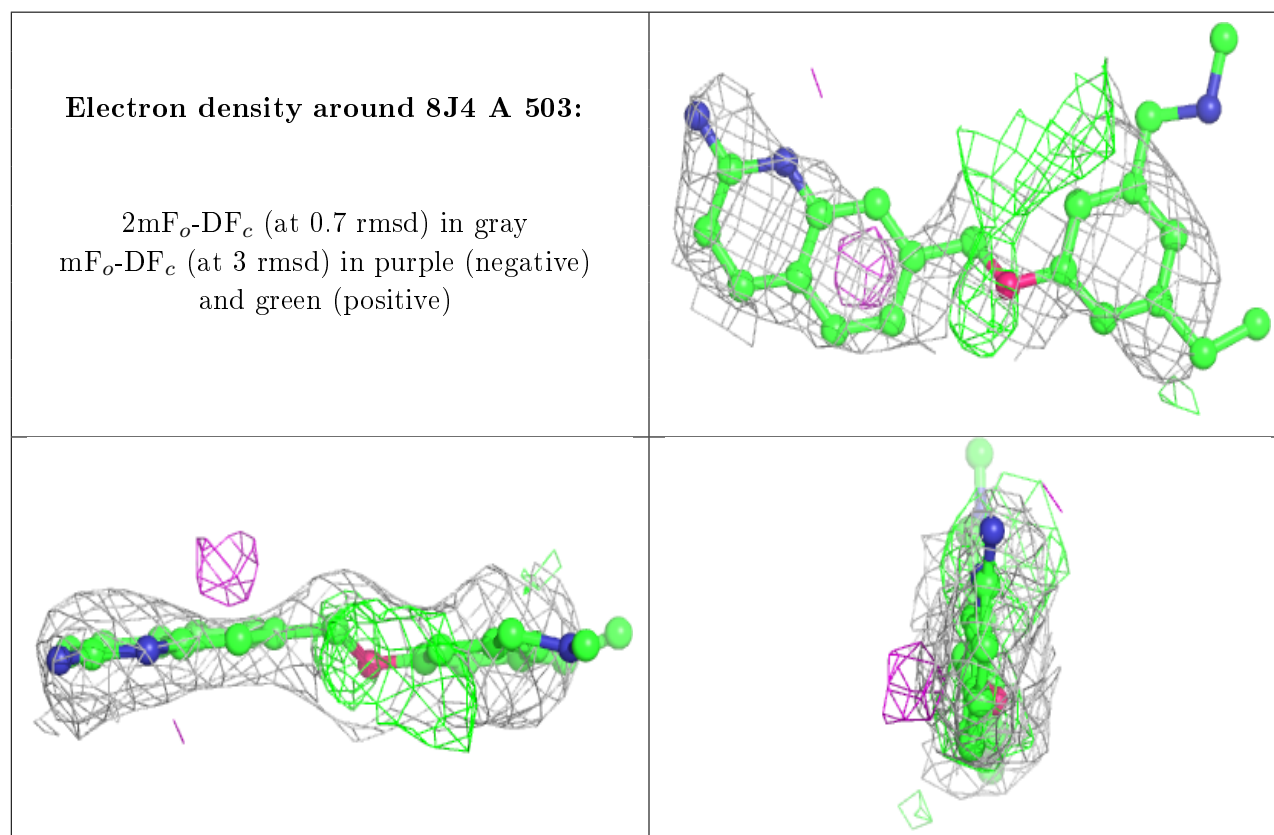
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BTB	B	507	14/14	0.66	0.17	77,82,89,90	0
9	GD	A	509	1/1	0.68	0.10	129,129,129,129	1
4	8J4	A	503	24/24	0.72	0.29	79,97,117,122	0
5	BTB	B	506	14/14	0.72	0.25	74,83,88,90	0
4	8J4	C	503	24/24	0.73	0.23	67,76,92,96	0
5	BTB	D	504	14/14	0.76	0.21	46,65,77,81	0
5	BTB	B	505	14/14	0.77	0.16	82,95,103,105	0
5	BTB	C	504	14/14	0.79	0.16	75,87,92,94	0
5	BTB	B	504	14/14	0.82	0.15	35,55,72,73	0
5	BTB	D	506	14/14	0.83	0.17	95,101,106,106	0
5	BTB	B	511	14/14	0.83	0.23	59,63,87,90	0
4	8J4	B	503	24/24	0.84	0.26	50,66,103,106	0
3	H4B	C	502	17/17	0.86	0.20	55,66,78,80	0
7	GOL	C	506	6/6	0.86	0.21	57,65,71,71	0
5	BTB	A	505	14/14	0.86	0.16	72,84,90,90	0
4	8J4	D	503	24/24	0.87	0.23	48,61,96,108	0
9	GD	C	508	1/1	0.88	0.11	111,111,111,111	1
3	H4B	A	502	17/17	0.89	0.14	48,60,66,69	0
5	BTB	B	510	14/14	0.89	0.18	39,68,83,83	0
3	H4B	D	502	17/17	0.90	0.13	27,46,52,52	0
5	BTB	A	504	14/14	0.92	0.19	75,85,93,96	0
3	H4B	B	502	17/17	0.92	0.11	34,46,54,61	0
5	BTB	D	505	14/14	0.92	0.24	65,74,78,79	0
7	GOL	A	507	6/6	0.93	0.20	64,72,77,80	0
2	HEM	A	501	43/43	0.95	0.15	39,50,73,80	0
2	HEM	C	501	43/43	0.95	0.15	35,54,73,86	0
8	CL	C	507	1/1	0.95	0.09	71,71,71,71	0

Continued on next page...

Continued from previous page...

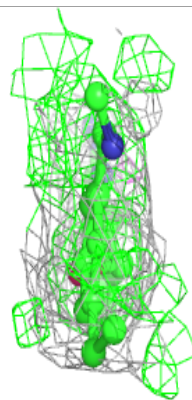
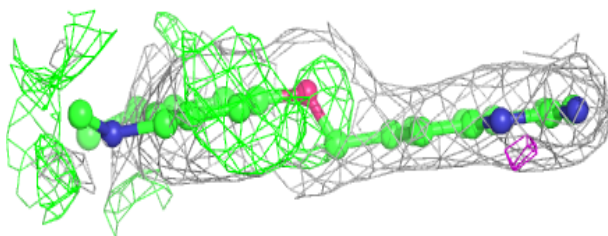
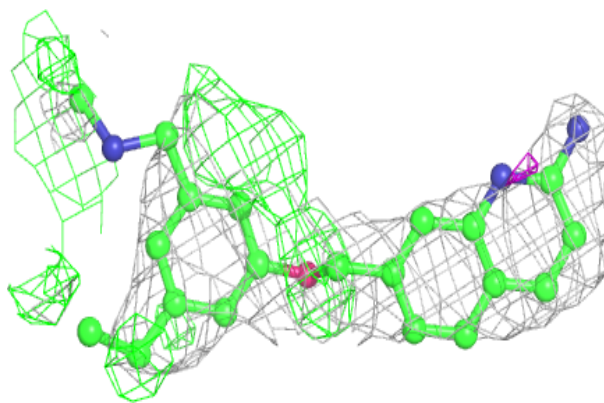
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	D	501	43/43	0.96	0.15	31,41,68,71	0
8	CL	D	510	1/1	0.96	0.19	79,79,79,79	0
8	CL	B	508	1/1	0.96	0.07	50,50,50,50	0
2	HEM	B	501	43/43	0.96	0.14	30,38,61,67	0
8	CL	A	508	1/1	0.97	0.09	67,67,67,67	0
6	ZN	C	505	1/1	0.98	0.13	45,45,45,45	0
11	MG	D	509	1/1	0.98	0.20	35,35,35,35	0
8	CL	D	508	1/1	0.98	0.06	47,47,47,47	0
9	GD	B	509	1/1	0.99	0.18	52,52,52,52	0
10	CA	A	510	1/1	0.99	0.22	37,37,37,37	0
6	ZN	A	506	1/1	0.99	0.13	46,46,46,46	0
9	GD	D	507	1/1	1.00	0.15	51,51,51,51	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.

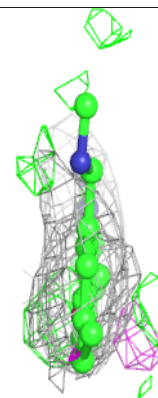
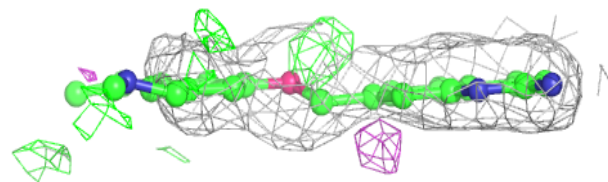
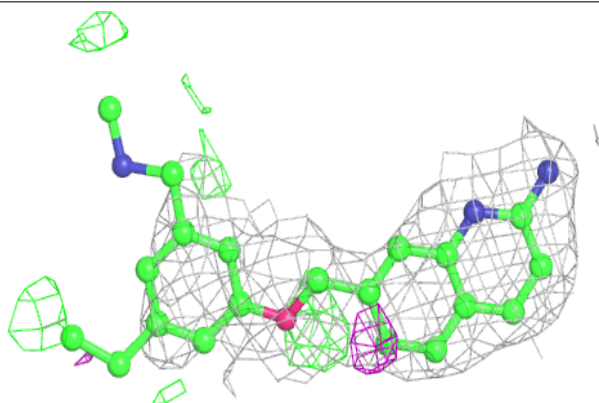


Electron density around 8J4 C 503:

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

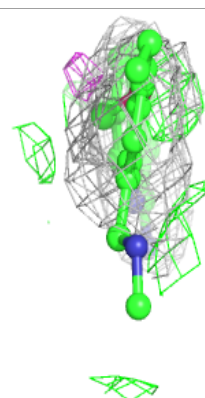
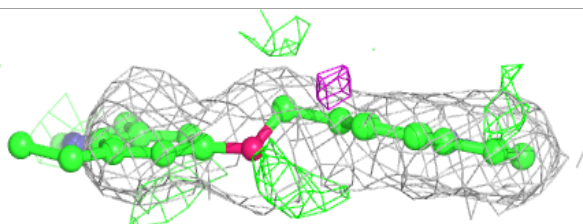
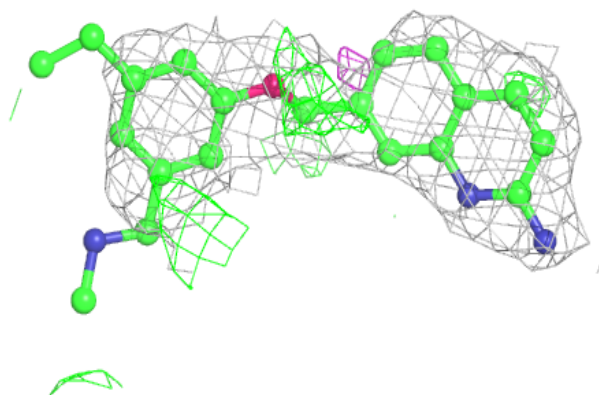
**Electron density around 8J4 B 503:**

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

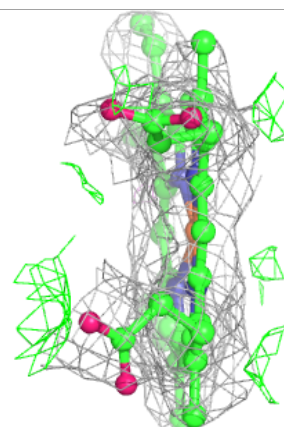
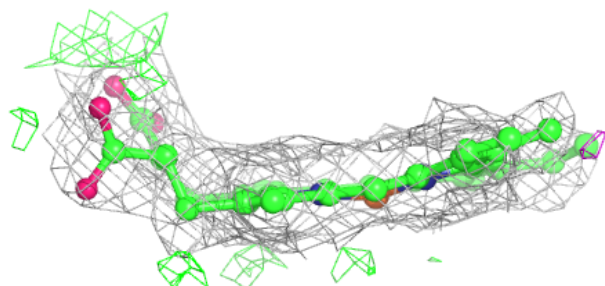
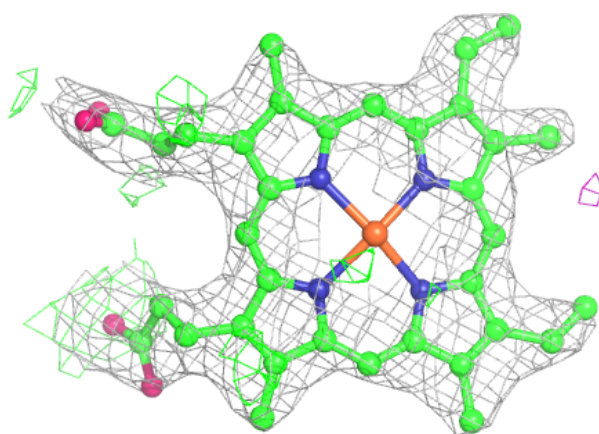


Electron density around 8J4 D 503:

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

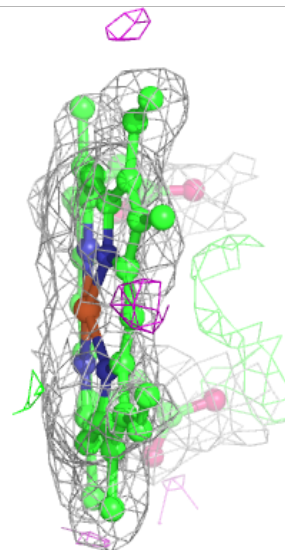
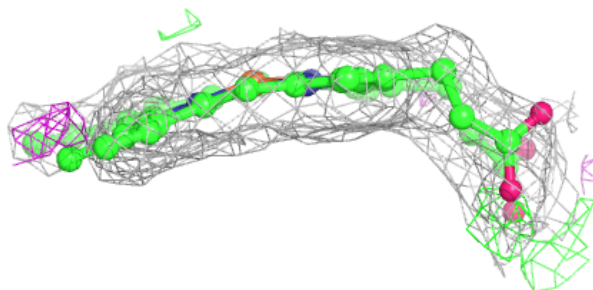
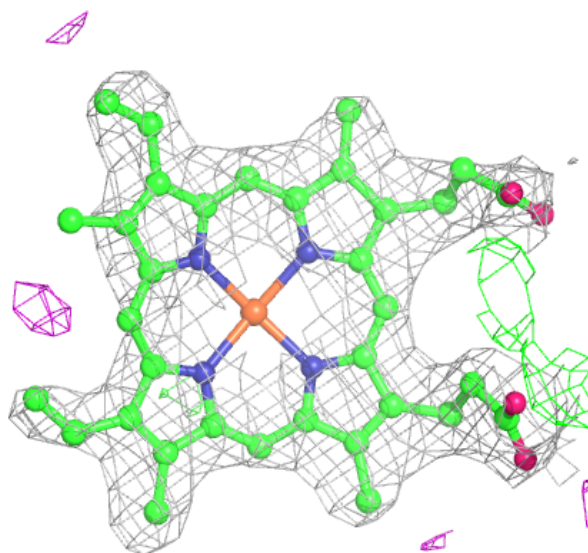
**Electron density around HEM A 501:**

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



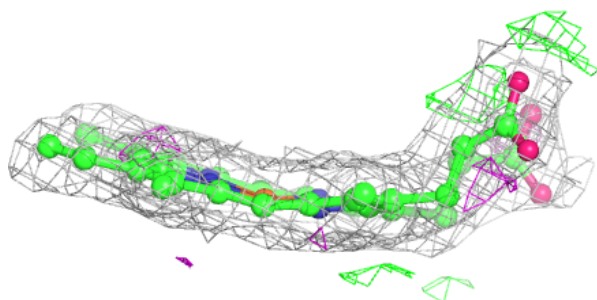
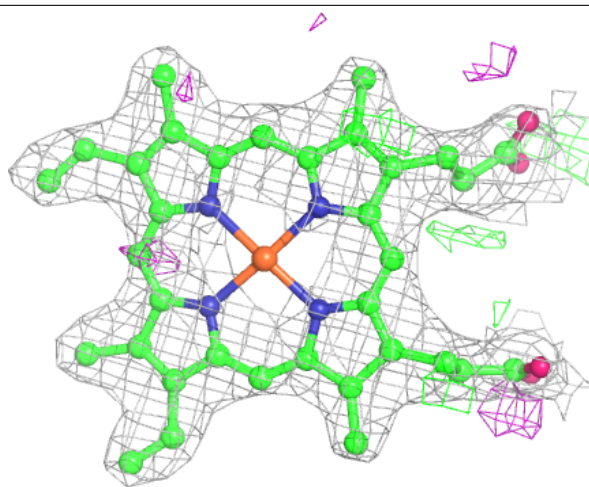
Electron density around HEM C 501:

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



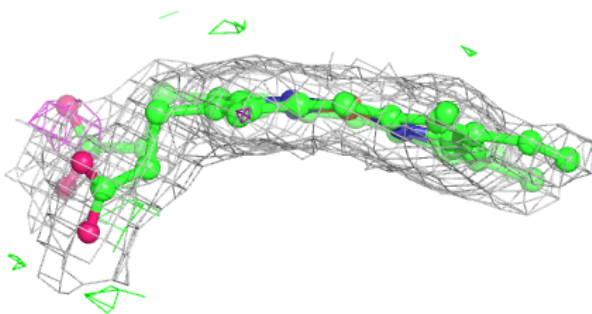
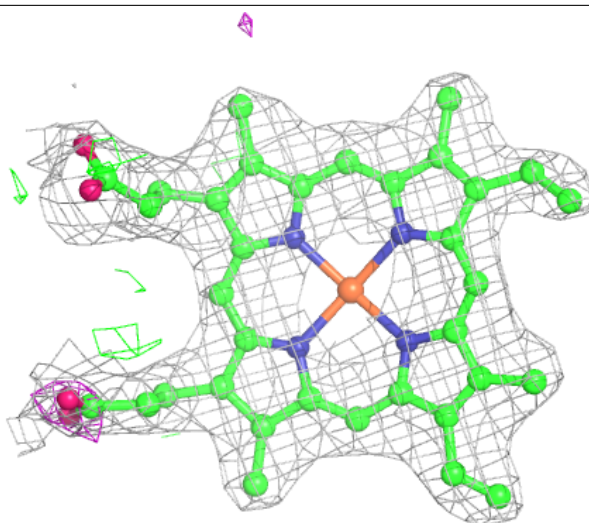
Electron density around HEM D 501:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.