



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:05 am BST

PDB ID : 6AV6
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-Fluoro-5-(3-(methylamino)propyl)phenethyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2017-09-01
Resolution : 2.08 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

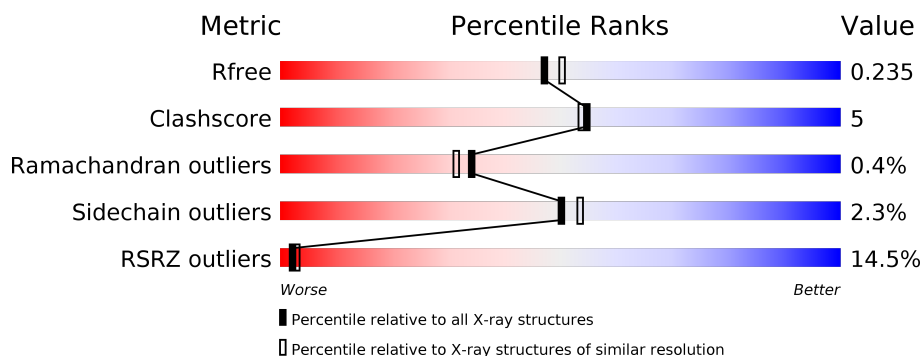
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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>21%</div> <div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	440	<div> <div>8%</div> <div> <div>79%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	440	<div> <div>17%</div> <div> <div>80%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	440	<div> <div>7%</div> <div> <div>82%</div> <div>10%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13659 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	401	Total	C	N	O	S	0	2	0
			3215	2047	566	586	16			
1	B	401	Total	C	N	O	S	0	3	0
			3212	2045	564	586	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: $C_{34}H_{32}FeN_4O_4$).



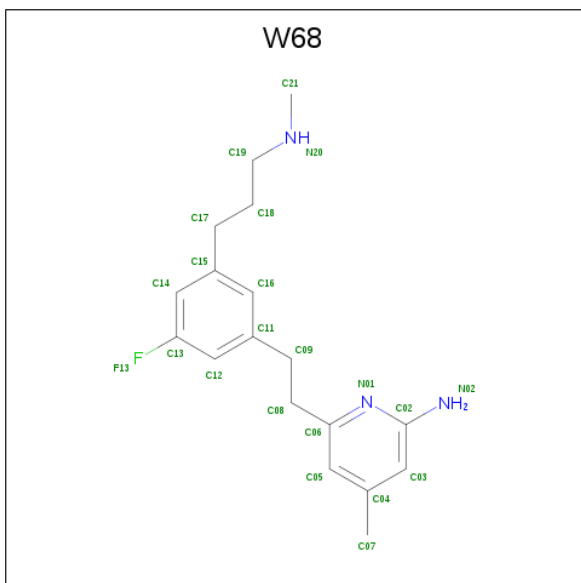
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

Continued on next page...

Continued from previous page...

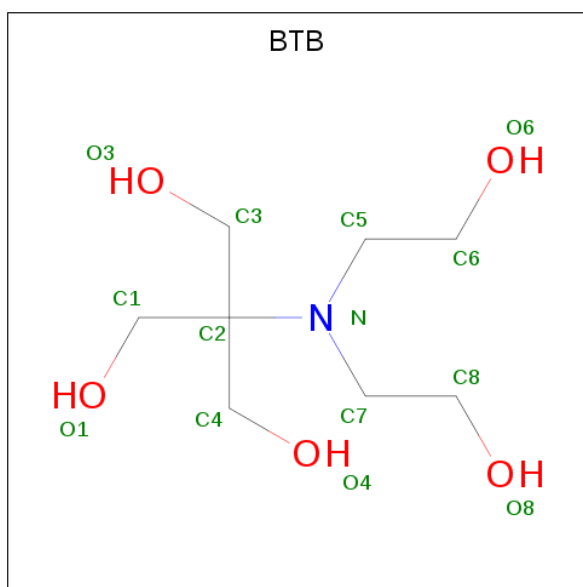
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 6-(2-{3-fluoro-5-[3-(methylamino)propyl]phenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: W68) (formula: C₁₈H₂₄FN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N		
			22	18	1	3		
3	B	1	Total	C	F	N		
			22	18	1	3		
3	C	1	Total	C	F	N		
			22	18	1	3		
3	D	1	Total	C	F	N		
			22	18	1	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

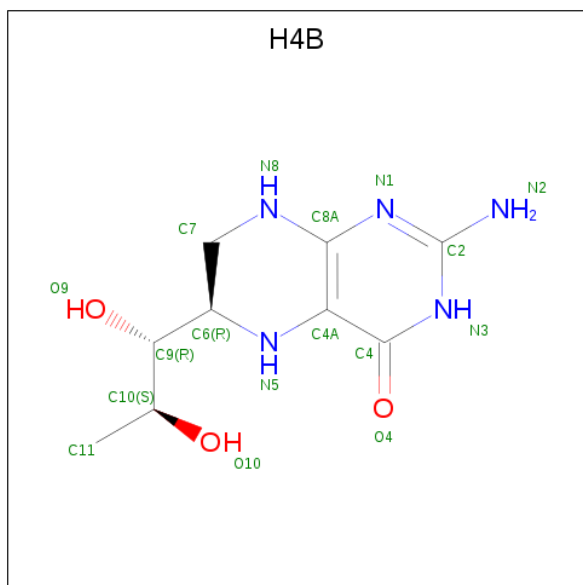
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Gd	0	0
			1	1		
8	A	1	Total	Gd	0	0
			1	1		
8	D	1	Total	Gd	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 9 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

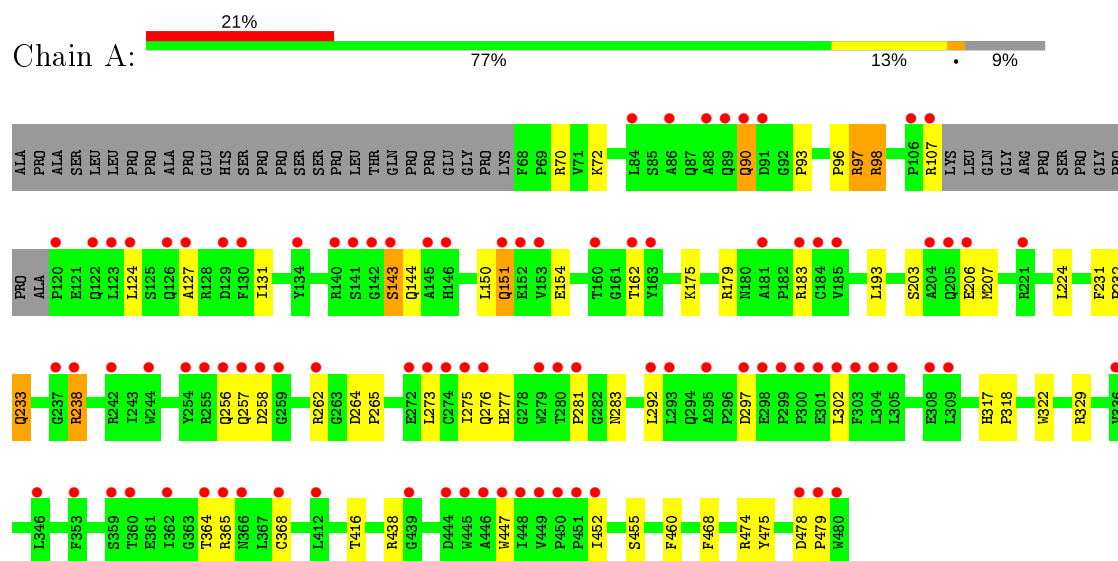
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	47	Total	O	0	0
			47	47		
10	B	112	Total	O	0	0
			112	112		
10	C	66	Total	O	0	0
			66	66		
10	D	101	Total	O	0	0
			101	101		

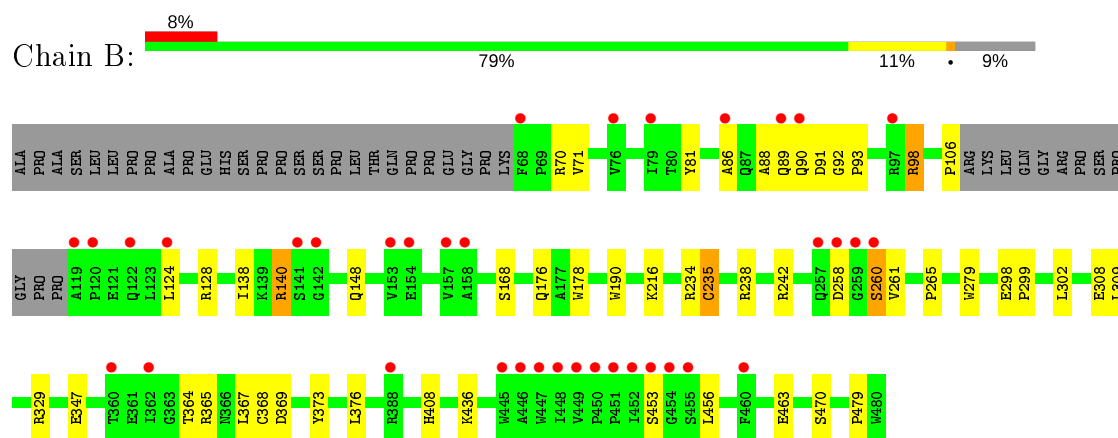
3 Residue-property plots [i](#)

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.

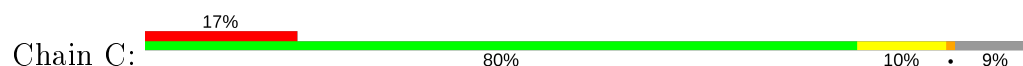
- Molecule 1: Nitric oxide synthase, endothelial

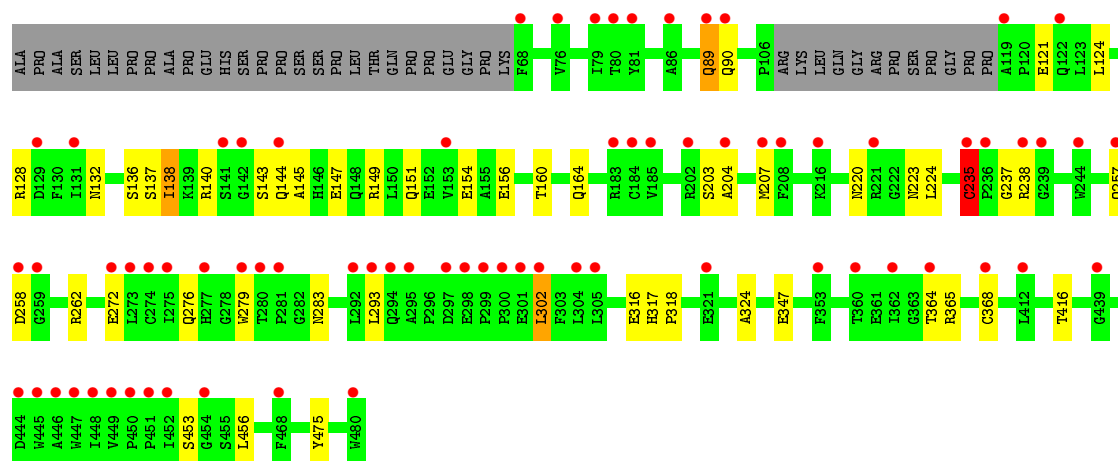


- Molecule 1: Nitric oxide synthase, endothelial

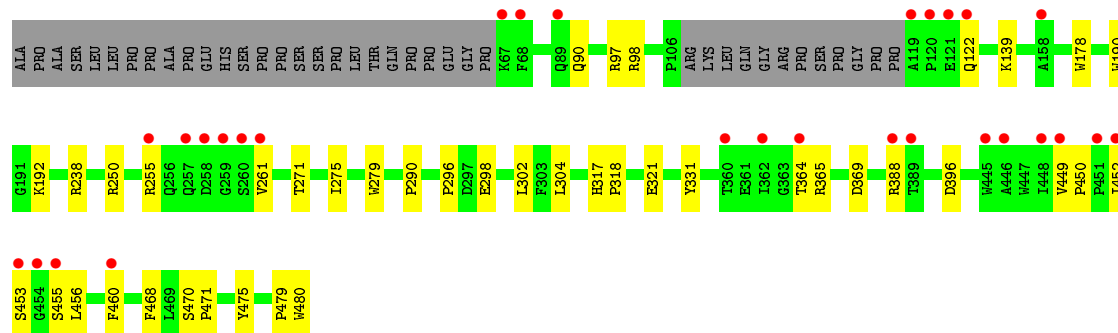
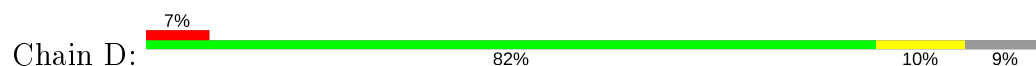


- Molecule 1: Nitric oxide synthase, endothelial





- 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	59.64Å 152.78Å 108.88Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	39.13 – 2.08 39.13 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.13-2.08) 99.3 (39.13-2.08)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.239 0.194 , 0.235	Depositor DCC
R_{free} test set	5827 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.991	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13659	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, ZN, H4B, CL, W68, 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	0.34	0/3313	0.49	0/4513
1	B	0.39	0/3310	0.51	0/4512
1	C	0.34	0/3307	0.49	0/4507
1	D	0.42	0/3319	0.53	0/4523
All	All	0.37	0/13249	0.51	0/18055

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	3215	0	3118	40	0
1	B	3212	0	3113	38	0
1	C	3209	0	3109	27	0
1	D	3221	0	3126	21	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	22	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
4	A	28	0	38	4	0
4	B	56	0	74	4	0
4	C	14	0	19	2	0
4	D	28	0	38	5	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	6	0	8	0	0
6	C	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	B	34	0	30	1	0
9	C	17	0	15	2	0
9	D	17	0	15	0	0
10	A	47	0	0	2	0
10	B	112	0	0	2	0
10	C	66	0	0	1	0
10	D	101	0	0	0	0
All	All	13659	0	12831	136	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 5.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:O	1:A:98:ARG:NH2	2.11	0.84
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.11	0.83
1:B:365:ARG:NH2	1:B:369:ASP:OD2	2.21	0.73
1:C:235:CYS:O	1:C:238:ARG:NH1	2.24	0.70
1:C:128:ARG:NH2	1:C:154:GLU:OE2	2.24	0.70
1:A:107:ARG:HH12	1:B:70:ARG:HB3	1.56	0.70
1:A:162:THR:OG1	1:A:233:GLN:NE2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.11	0.68
4:A:503:BTB:O4	10:A:601:HOH:O	2.10	0.68
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.68
1:A:107:ARG:HH12	1:B:70:ARG:H	1.44	0.66
1:A:277:HIS:HB3	1:A:302:LEU:HD11	1.78	0.65
4:B:510:BTB:O3	4:B:510:BTB:O4	2.07	0.65
1:B:408:HIS:ND1	10:B:601:HOH:O	2.28	0.65
1:A:97:ARG:NH2	1:B:86:ALA:O	2.29	0.65
1:A:257:GLN:NE2	10:A:602:HOH:O	2.29	0.64
2:B:502:HEM:HBB2	2:B:502:HEM:HHC	1.78	0.64
1:B:138:ILE:HG13	1:B:140:ARG:HG3	1.80	0.62
1:A:256:GLN:HG2	1:A:257:GLN:H	1.65	0.61
1:C:128:ARG:O	1:C:132:ASN:ND2	2.33	0.61
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.81	0.61
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.83	0.61
1:C:347:GLU:OE2	10:C:601:HOH:O	2.15	0.61
1:A:127:ALA:O	1:A:131:ILE:HG12	2.01	0.60
1:A:143:SER:OG	1:A:144:GLN:N	2.31	0.60
1:B:124:LEU:O	1:B:128:ARG:HG3	2.02	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.84	0.59
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.84	0.59
1:B:298:GLU:OE2	4:B:506:BTB:N	2.34	0.59
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.84	0.58
1:A:107:ARG:NH1	1:B:70:ARG:H	2.01	0.58
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.13	0.57
1:D:321:GLU:OE2	4:D:504:BTB:O3	2.20	0.57
1:A:96:PRO:O	1:B:92:GLY:N	2.35	0.56
1:A:97:ARG:NH1	1:B:88:ALA:O	2.39	0.55
1:C:149:ARG:NH2	1:C:164:GLN:O	2.33	0.55
4:B:510:BTB:HO3	4:B:510:BTB:HO4	1.51	0.55
1:B:234:ARG:NH1	1:B:347:GLU:OE1	2.39	0.55
1:C:151:GLN:HA	1:C:154:GLU:HG3	1.89	0.54
1:A:262:ARG:NE	1:A:283:ASN:O	2.41	0.54
4:D:504:BTB:O6	4:D:504:BTB:H82	2.08	0.54
1:A:273:LEU:HA	1:A:276:GLN:HG2	1.90	0.53
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.43	0.53
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.90	0.52
1:C:132:ASN:O	1:C:136:SER:OG	2.22	0.52
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.91	0.52
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.45	0.52
1:B:70:ARG:HB2	1:B:81:TYR:CE2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HD12	1:C:140:ARG:HB2	1.92	0.51
1:D:238:ARG:HD2	1:D:296:PRO:HB3	1.91	0.51
1:B:258:ASP:HB2	1:B:260:SER:HB3	1.93	0.51
1:D:364:THR:HG21	1:D:452:ILE:HG23	1.94	0.50
1:B:89:GLN:OE1	1:B:470:SER:N	2.36	0.50
1:A:90:GLN:HB3	1:A:468:PHE:CD2	2.47	0.50
1:C:143:SER:O	1:C:145:ALA:N	2.45	0.50
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.93	0.50
1:C:147:GLU:N	1:C:147:GLU:OE1	2.45	0.49
1:D:238:ARG:HD2	1:D:296:PRO:CB	2.42	0.49
1:A:224:LEU:HB2	1:A:416:THR:HB	1.95	0.49
1:B:90:GLN:OE1	1:B:91:ASP:N	2.46	0.49
1:A:365:ARG:HH12	9:B:501:H4B:C4	2.26	0.49
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.95	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.48
1:D:271:THR:O	1:D:275:ILE:HG12	2.12	0.48
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.49	0.48
1:C:365:ARG:HH12	9:C:502:H4B:C4	2.27	0.48
4:D:505:BTB:H61	4:D:505:BTB:H72	1.69	0.48
1:C:203:SER:OG	1:C:204:ALA:N	2.47	0.48
1:C:235:CYS:H	1:C:238:ARG:HD3	1.79	0.48
1:A:256:GLN:HG2	1:A:257:GLN:N	2.28	0.48
1:D:298:GLU:OE2	4:D:505:BTB:O3	2.19	0.48
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.28	0.48
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.49	0.48
1:A:322:TRP:CD1	4:A:503:BTB:H82	2.49	0.47
1:A:70:ARG:HH21	1:A:72:LYS:HD2	1.78	0.47
4:B:506:BTB:H71	4:B:506:BTB:H42	1.58	0.47
1:C:156:GLU:O	1:C:160:THR:HG22	2.14	0.47
1:A:207:MET:HG2	1:A:231:PHE:CE1	2.49	0.47
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.96	0.47
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.50	0.47
1:B:124:LEU:HD13	1:B:128:ARG:HH21	1.80	0.47
1:D:455:SER:HA	1:D:460:PHE:CG	2.50	0.47
1:B:308:GLU:N	1:B:308:GLU:OE1	2.43	0.46
1:A:364:THR:O	1:A:368:CYS:HB2	2.16	0.46
1:B:235[B]:CYS:SG	1:B:238:ARG:NE	2.88	0.46
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.98	0.45
1:A:179:ARG:NH2	1:A:438:ARG:HG3	2.31	0.45
1:C:262:ARG:NH1	1:C:283:ASN:O	2.50	0.45
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.52	0.45
1:A:151:GLN:O	1:A:154:GLU:HG3	2.15	0.45
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.99	0.45
1:A:107:ARG:HH22	1:B:70:ARG:N	2.14	0.45
4:C:504:BTB:H72	4:C:504:BTB:H61	1.37	0.45
1:A:478:ASP:OD1	1:A:479:PRO:HD2	2.18	0.44
1:C:121:GLU:O	1:C:124:LEU:HG	2.18	0.44
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.99	0.44
1:C:89:GLN:HB2	1:C:90:GLN:H	1.69	0.44
1:D:250:ARG:NH2	1:D:331:TYR:OH	2.37	0.44
1:B:260:SER:OG	1:B:261:VAL:N	2.51	0.44
4:A:503:BTB:O4	4:A:503:BTB:O3	2.35	0.43
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.43
1:B:365:ARG:HH21	1:B:369:ASP:CG	2.21	0.43
1:C:207:MET:HG2	1:C:293:LEU:HD13	2.00	0.43
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.00	0.42
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.59	0.42
1:B:71:VAL:HG13	1:B:463:GLU:HB2	2.02	0.42
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.88	0.42
1:B:364:THR:O	1:B:368:CYS:HB2	2.19	0.42
4:C:504:BTB:H32	4:C:504:BTB:H71	1.44	0.42
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.42
1:C:224:LEU:HB2	1:C:416:THR:HB	2.01	0.42
4:A:504:BTB:O6	4:A:504:BTB:O3	2.29	0.42
1:D:139:LYS:HB3	1:D:139:LYS:HE3	1.80	0.42
2:C:501:HEM:CGA	9:C:502:H4B:HN22	2.33	0.41
1:A:256:GLN:HB3	1:A:258:ASP:OD1	2.20	0.41
1:A:107:ARG:HA	1:A:107:ARG:HD3	1.89	0.41
1:B:367:LEU:HA	1:B:373:TYR:HB2	2.02	0.41
1:C:220:ASN:HB3	1:C:223:ASN:O	2.21	0.41
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.55	0.41
1:A:150:LEU:O	1:A:154:GLU:HG2	2.20	0.41
1:C:272:GLU:O	1:C:276:GLN:HG3	2.21	0.41
4:D:504:BTB:H42	4:D:504:BTB:H71	1.79	0.41
1:B:235[B]:CYS:SG	1:B:238:ARG:HB3	2.60	0.41
1:A:231:PHE:HB3	1:A:232:PRO:CD	2.49	0.41
1:B:436:LYS:HB3	1:B:436:LYS:HE3	1.77	0.41
1:D:255:ARG:HA	1:D:261:VAL:HG22	2.03	0.41
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.03	0.41
1:C:453:SER:HB3	1:C:456:LEU:HD12	2.03	0.41
1:B:216:LYS:HB2	1:B:309:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PRO:HB3	10:B:620:HOH:O	2.20	0.40
1:B:93:PRO:O	1:B:98:ARG:NH2	2.51	0.40
1:D:470:SER:HA	1:D:471:PRO:C	2.41	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.93	0.40
1:A:175:LYS:NZ	1:A:193:LEU:O	2.53	0.40
1:D:449:VAL:HA	1:D:450:PRO:HD3	1.94	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	399/440 (91%)	375 (94%)	21 (5%)	3 (1%)	19	14
1	B	400/440 (91%)	393 (98%)	7 (2%)	0	100	100
1	C	399/440 (91%)	379 (95%)	16 (4%)	4 (1%)	15	10
1	D	401/440 (91%)	393 (98%)	8 (2%)	0	100	100
All	All	1599/1760 (91%)	1540 (96%)	52 (3%)	7 (0%)	34	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	A	90	GLN
1	C	144	GLN
1	C	237	GLY
1	A	238	ARG
1	A	297	ASP
1	C	235	CYS

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	343/373 (92%)	332 (97%)	11 (3%)	39	40
1	B	343/373 (92%)	333 (97%)	10 (3%)	42	44
1	C	342/373 (92%)	336 (98%)	6 (2%)	59	63
1	D	344/373 (92%)	338 (98%)	6 (2%)	60	65
All	All	1372/1492 (92%)	1339 (98%)	33 (2%)	50	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	98	ARG
1	A	124	LEU
1	A	143	SER
1	A	151	GLN
1	A	203	SER
1	A	206	GLU
1	A	233	GLN
1	A	238	ARG
1	A	329	ARG
1	A	474	ARG
1	B	98	ARG
1	B	140	ARG
1	B	148	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	176	GLN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	260	SER
1	B	329	ARG
1	C	137	SER
1	C	138	ILE
1	C	235	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	257	GLN
1	C	258	ASP
1	C	302	LEU
1	D	97	ARG
1	D	98	ARG
1	D	122	GLN
1	D	192	LYS
1	D	388	ARG
1	D	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	233	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BTB	B	506	-	13,13,13	0.38	0	7,16,16	0.68	0
9	H4B	B	501	-	16,18,18	0.88	0	11,26,26	2.60	6 (54%)
4	BTB	B	505	8	13,13,13	0.46	0	7,16,16	0.45	0
3	W68	A	502	-	23,23,23	0.48	0	30,30,30	1.64	3 (10%)
4	BTB	C	504	-	13,13,13	0.51	0	7,16,16	0.45	0
2	HEM	D	501	1	27,50,50	2.06	7 (25%)	17,82,82	2.10	7 (41%)
4	BTB	D	504	8	13,13,13	0.35	0	7,16,16	0.79	0
3	W68	B	504	-	23,23,23	0.65	0	30,30,30	1.82	4 (13%)
4	BTB	B	509	8	13,13,13	0.39	0	7,16,16	0.78	0
2	HEM	A	501	1	27,50,50	2.15	6 (22%)	17,82,82	1.52	5 (29%)
4	BTB	D	505	-	13,13,13	0.57	0	7,16,16	0.72	0
3	W68	D	503	-	23,23,23	0.73	0	30,30,30	1.87	6 (20%)
3	W68	C	503	-	23,23,23	0.67	0	30,30,30	2.02	6 (20%)
4	BTB	A	503	8	13,13,13	0.40	0	7,16,16	0.29	0
2	HEM	B	502	1	27,50,50	2.10	5 (18%)	17,82,82	1.61	4 (23%)
6	GOL	C	506	-	5,5,5	0.32	0	5,5,5	0.33	0
9	H4B	C	502	-	16,18,18	0.89	0	11,26,26	2.74	6 (54%)
4	BTB	B	510	-	13,13,13	0.59	0	7,16,16	1.05	0
4	BTB	A	504	-	13,13,13	0.55	0	7,16,16	0.97	0
6	GOL	A	506	-	5,5,5	0.33	0	5,5,5	0.43	0
9	H4B	B	503	-	16,18,18	1.00	0	11,26,26	2.68	6 (54%)
2	HEM	C	501	1	27,50,50	2.17	6 (22%)	17,82,82	1.77	5 (29%)
9	H4B	D	502	-	16,18,18	0.83	0	11,26,26	2.61	5 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	B	506	-	-	5/21/21/21	-
9	H4B	B	501	-	-	3/8/17/17	0/2/2/2
4	BTB	B	505	8	-	1/21/21/21	-
3	W68	A	502	-	-	6/10/10/10	0/2/2/2
4	BTB	C	504	-	-	13/21/21/21	-
2	HEM	D	501	1	-	3/6/54/54	-
4	BTB	D	504	8	-	8/21/21/21	-
3	W68	B	504	-	-	5/10/10/10	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	B	509	8	-	2/21/21/21	-
2	HEM	A	501	1	-	2/6/54/54	-
4	BTB	D	505	-	-	8/21/21/21	-
3	W68	D	503	-	-	5/10/10/10	0/2/2/2
3	W68	C	503	-	-	5/10/10/10	0/2/2/2
4	BTB	A	503	8	-	4/21/21/21	-
2	HEM	B	502	1	-	3/6/54/54	-
6	GOL	C	506	-	-	2/4/4/4	-
9	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	BTB	B	510	-	-	10/21/21/21	-
4	BTB	A	504	-	-	1/21/21/21	-
6	GOL	A	506	-	-	1/4/4/4	-
9	H4B	B	503	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	3/6/54/54	-
9	H4B	D	502	-	-	4/8/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	5.35	1.53	1.37
2	C	501	HEM	C3D-C2D	5.12	1.52	1.37
2	B	502	HEM	C3D-C2D	5.11	1.52	1.37
2	B	502	HEM	C3B-C2B	-5.07	1.33	1.40
2	D	501	HEM	C3D-C2D	5.01	1.52	1.37
2	D	501	HEM	C3B-C2B	-4.61	1.34	1.40
2	C	501	HEM	C3B-C2B	-4.57	1.34	1.40
2	A	501	HEM	C3B-C2B	-4.55	1.34	1.40
2	C	501	HEM	C3B-CAB	4.09	1.56	1.47
2	B	502	HEM	C3C-CAC	3.90	1.55	1.47
2	C	501	HEM	C3C-CAC	3.88	1.55	1.47
2	A	501	HEM	C3C-CAC	3.88	1.55	1.47
2	A	501	HEM	C3B-CAB	3.81	1.55	1.47
2	D	501	HEM	C3B-CAB	3.72	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.68	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.64	1.35	1.40
2	B	502	HEM	C3B-CAB	3.51	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.45	1.35	1.40
2	D	501	HEM	C3C-CAC	3.45	1.54	1.47
2	B	502	HEM	C3C-C2C	-2.91	1.36	1.40
2	C	501	HEM	CAA-C2A	2.62	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C1D-ND	2.61	1.41	1.36
2	A	501	HEM	CAA-C2A	2.24	1.55	1.52
2	D	501	HEM	CAA-C2A	2.03	1.55	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	W68	C02-N01-C06	7.62	123.88	118.10
3	B	504	W68	C02-N01-C06	6.97	123.38	118.10
3	D	503	W68	C02-N01-C06	6.73	123.20	118.10
3	A	502	W68	C02-N01-C06	6.12	122.74	118.10
9	B	503	H4B	C4-C4A-C8A	5.57	119.52	114.57
9	C	502	H4B	C4-C4A-C8A	5.43	119.39	114.57
9	B	501	H4B	C4-C4A-C8A	5.29	119.27	114.57
3	C	503	W68	C05-C06-N01	-4.85	117.76	122.90
9	D	502	H4B	C4-C4A-C8A	4.76	118.80	114.57
2	B	502	HEM	CBD-CAD-C3D	-4.24	104.66	112.48
2	D	501	HEM	CMA-C3A-C4A	-4.17	122.06	128.46
2	D	501	HEM	CBD-CAD-C3D	-3.99	105.12	112.48
3	B	504	W68	C05-C06-N01	-3.82	118.85	122.90
3	D	503	W68	C05-C06-N01	-3.76	118.91	122.90
3	A	502	W68	C05-C06-N01	-3.50	119.19	122.90
9	D	502	H4B	C4-C4A-N5	3.50	122.06	119.12
9	B	503	H4B	N3-C2-N1	-3.45	120.01	125.42
2	C	501	HEM	CBD-CAD-C3D	-3.30	106.40	112.48
9	C	502	H4B	C4-C4A-N5	3.29	121.88	119.12
9	C	502	H4B	N3-C2-N1	-3.26	120.31	125.42
9	D	502	H4B	N3-C2-N1	-3.23	120.35	125.42
3	D	503	W68	C08-C06-C05	3.22	125.48	121.22
9	B	501	H4B	N3-C2-N1	-3.20	120.39	125.42
9	D	502	H4B	C4-N3-C2	3.17	120.96	115.93
9	C	502	H4B	C4-N3-C2	3.11	120.88	115.93
2	C	501	HEM	CMA-C3A-C4A	-3.05	123.77	128.46
9	B	503	H4B	C2-N1-C8A	3.00	121.26	114.54
2	D	501	HEM	C4A-C3A-C2A	2.98	109.07	107.00
9	B	501	H4B	C4-N3-C2	2.97	120.65	115.93
9	B	503	H4B	C4-N3-C2	2.93	120.59	115.93
2	C	501	HEM	C4A-C3A-C2A	2.88	109.00	107.00
3	B	504	W68	C12-C13-C14	-2.88	119.88	123.52
2	D	501	HEM	CMC-C2C-C3C	2.86	130.03	124.68
9	B	501	H4B	C4-C4A-N5	2.79	121.46	119.12
9	B	501	H4B	C2-N1-C8A	2.79	120.78	114.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	W68	C12-C13-C14	-2.77	120.02	123.52
9	C	502	H4B	C2-N1-C8A	2.76	120.73	114.54
2	C	501	HEM	C1D-C2D-C3D	-2.74	105.09	107.00
2	A	501	HEM	CBD-CAD-C3D	-2.74	107.44	112.48
2	A	501	HEM	C4A-C3A-C2A	2.71	108.88	107.00
3	D	503	W68	C09-C08-C06	2.68	119.00	112.99
9	D	502	H4B	C2-N1-C8A	2.68	120.54	114.54
3	D	503	W68	C12-C13-C14	-2.62	120.21	123.52
2	B	502	HEM	CMC-C2C-C3C	2.55	129.45	124.68
2	D	501	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
2	C	501	HEM	CMC-C2C-C3C	2.37	129.11	124.68
2	A	501	HEM	CMC-C2C-C3C	2.36	129.10	124.68
9	B	503	H4B	C4-C4A-N5	2.31	121.06	119.12
3	C	503	W68	C08-C06-C05	2.27	124.23	121.22
3	C	503	W68	C12-C13-C14	-2.25	120.67	123.52
3	B	504	W68	C19-C18-C17	-2.25	108.94	112.95
9	C	502	H4B	N2-C2-N3	2.24	120.74	117.25
2	A	501	HEM	CMA-C3A-C4A	-2.20	125.09	128.46
9	B	503	H4B	N2-C2-N1	2.18	120.64	117.25
3	C	503	W68	N02-C02-N01	2.17	119.93	116.49
2	B	502	HEM	C1D-C2D-C3D	-2.16	105.50	107.00
2	B	502	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
2	D	501	HEM	CMA-C3A-C2A	2.08	128.87	124.94
3	C	503	W68	C09-C08-C06	2.08	117.66	112.99
2	A	501	HEM	C1D-C2D-C3D	-2.07	105.56	107.00
9	B	501	H4B	N2-C2-N3	2.06	120.45	117.25
3	D	503	W68	C11-C12-C13	2.04	120.67	118.81
2	D	501	HEM	CAA-CBA-CGA	-2.03	109.26	112.67

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	506	BTB	C1-C2-C4-O4
4	B	506	BTB	C3-C2-C4-O4
4	B	506	BTB	N-C2-C4-O4
9	B	501	H4B	C7-C6-C9-O9
9	B	501	H4B	C7-C6-C9-C10
4	C	504	BTB	O1-C1-C2-C3
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	O1-C1-C2-N
4	C	504	BTB	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	504	BTB	C4-C2-C3-O3
4	C	504	BTB	C1-C2-N-C5
4	C	504	BTB	C1-C2-N-C7
4	C	504	BTB	C3-C2-N-C5
4	C	504	BTB	C3-C2-N-C7
4	C	504	BTB	C4-C2-N-C5
4	C	504	BTB	C4-C2-N-C7
4	C	504	BTB	C6-C5-N-C7
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C2A-CAA-CBA-CGA
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	O1-C1-C2-N
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
4	D	505	BTB	C1-C2-C3-O3
4	D	505	BTB	C1-C2-C4-O4
4	D	505	BTB	C3-C2-C4-O4
4	D	505	BTB	N-C2-C4-O4
4	D	505	BTB	C6-C5-N-C7
4	A	503	BTB	C1-C2-C3-O3
4	A	503	BTB	C4-C2-C3-O3
4	A	503	BTB	N-C2-C3-O3
6	C	506	GOL	O1-C1-C2-C3
4	B	510	BTB	O1-C1-C2-C3
4	B	510	BTB	O1-C1-C2-C4
4	B	510	BTB	O1-C1-C2-N
4	B	510	BTB	C1-C2-N-C5
4	B	510	BTB	C1-C2-N-C7
4	B	510	BTB	C3-C2-N-C5
4	B	510	BTB	C3-C2-N-C7
4	B	510	BTB	C4-C2-N-C5
4	B	510	BTB	C4-C2-N-C7
9	B	503	H4B	C7-C6-C9-O9
9	B	503	H4B	C7-C6-C9-C10
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C2A-CAA-CBA-CGA
9	D	502	H4B	N5-C6-C9-O9
9	D	502	H4B	C7-C6-C9-O9
9	D	502	H4B	C7-C6-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	503	BTB	N-C7-C8-O8
3	C	503	W68	C17-C18-C19-N20
6	C	506	GOL	O1-C1-C2-O2
4	D	504	BTB	N-C7-C8-O8
4	B	510	BTB	N-C5-C6-O6
6	A	506	GOL	C1-C2-C3-O3
4	B	506	BTB	N-C7-C8-O8
3	C	503	W68	C15-C17-C18-C19
3	A	502	W68	N01-C06-C08-C09
4	A	504	BTB	N-C7-C8-O8
4	B	506	BTB	N-C5-C6-O6
3	A	502	W68	C05-C06-C08-C09
3	A	502	W68	C18-C19-N20-C21
9	B	503	H4B	N5-C6-C9-O9
4	B	505	BTB	O1-C1-C2-N
4	C	504	BTB	N-C2-C3-O3
4	D	504	BTB	C1-C2-N-C5
4	D	504	BTB	C1-C2-N-C7
4	D	504	BTB	C3-C2-N-C7
4	D	504	BTB	C4-C2-N-C7
4	D	505	BTB	O1-C1-C2-N
2	B	502	HEM	C1A-C2A-CAA-CBA
2	B	502	HEM	C3A-C2A-CAA-CBA
3	D	503	W68	C05-C06-C08-C09
3	B	504	W68	C18-C19-N20-C21
9	D	502	H4B	N5-C6-C9-C10
3	D	503	W68	N01-C06-C08-C09
3	A	502	W68	C08-C09-C11-C12
3	B	504	W68	C05-C06-C08-C09
3	C	503	W68	C08-C09-C11-C12
3	A	502	W68	C08-C09-C11-C16
3	B	504	W68	N01-C06-C08-C09
3	C	503	W68	C08-C09-C11-C16
3	D	503	W68	C08-C09-C11-C12
3	D	503	W68	C08-C09-C11-C16
3	B	504	W68	C08-C09-C11-C12
3	B	504	W68	C08-C09-C11-C16
2	B	502	HEM	C2A-CAA-CBA-CGA
9	B	501	H4B	N5-C6-C9-O9
3	D	503	W68	C18-C19-N20-C21
4	B	509	BTB	O1-C1-C2-C3
4	B	509	BTB	O1-C1-C2-C4

Continued on next page...

Continued from previous page...

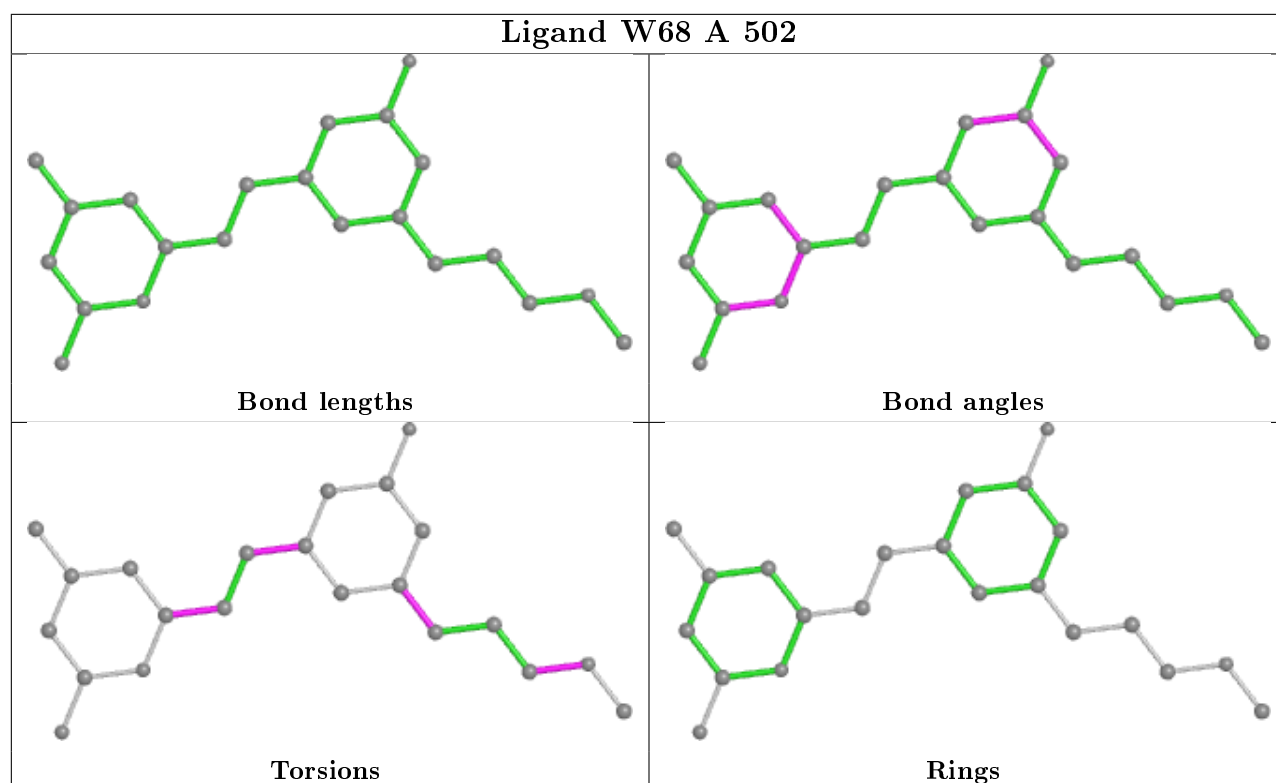
Mol	Chain	Res	Type	Atoms
4	D	505	BTB	O1-C1-C2-C3
4	D	505	BTB	O1-C1-C2-C4
3	C	503	W68	C18-C19-N20-C21
3	A	502	W68	C14-C15-C17-C18

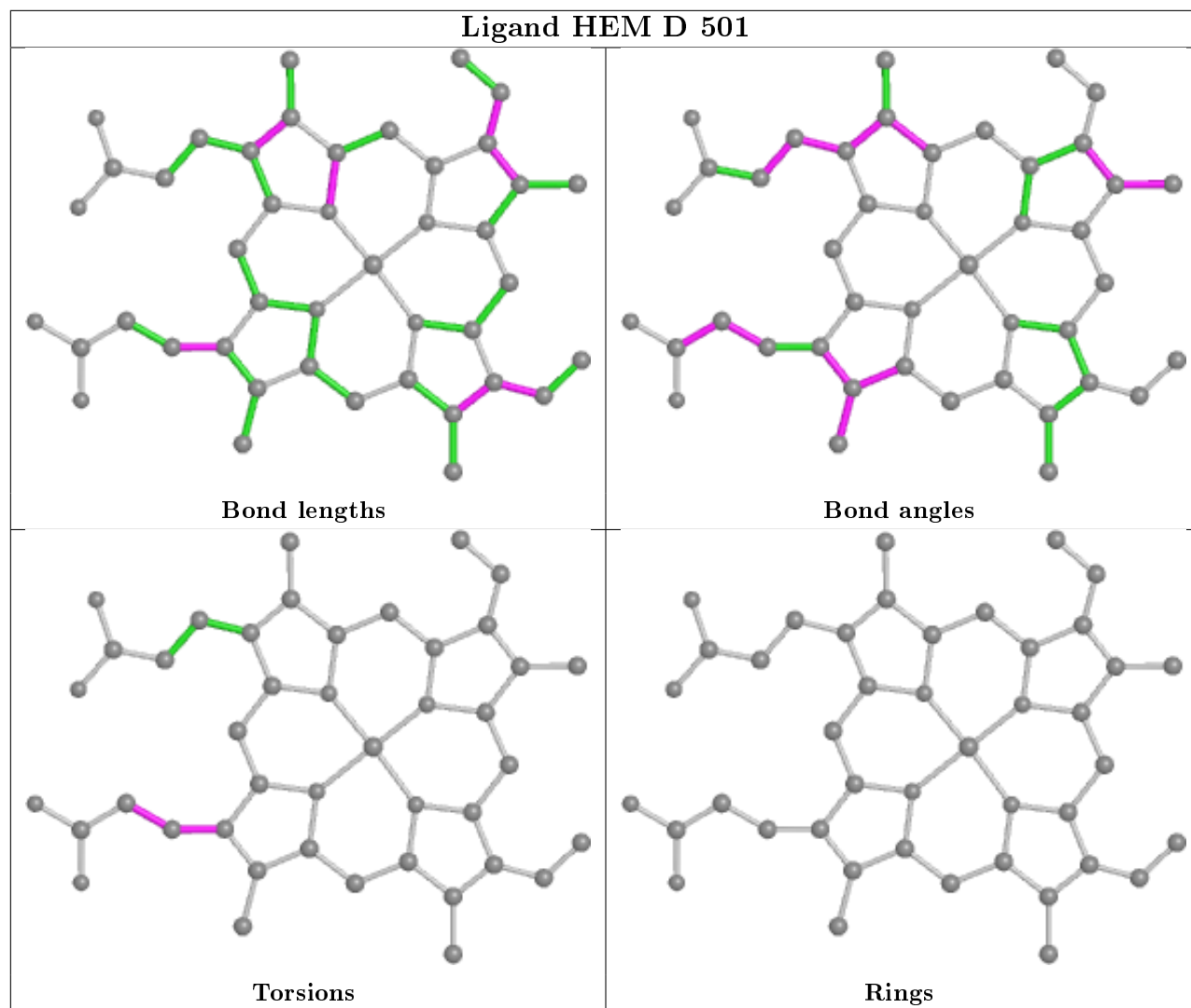
There are no ring outliers.

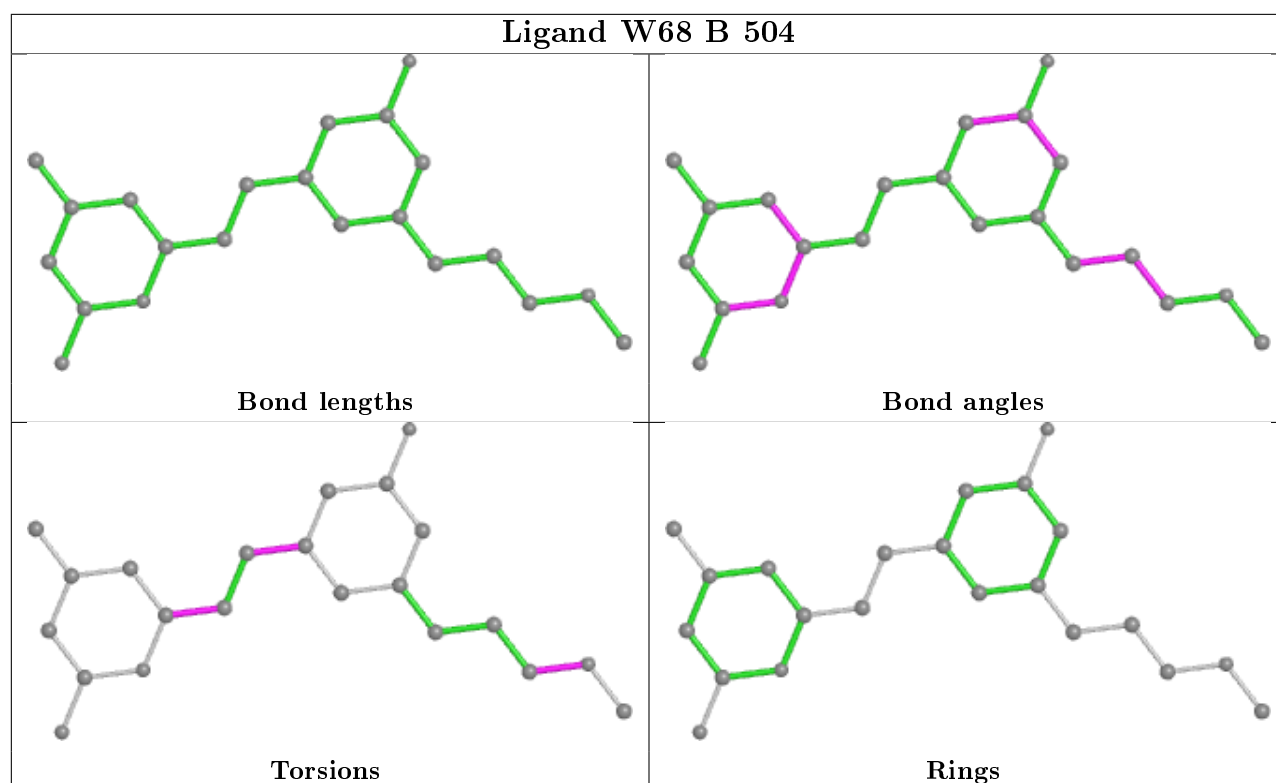
13 monomers are involved in 26 short contacts:

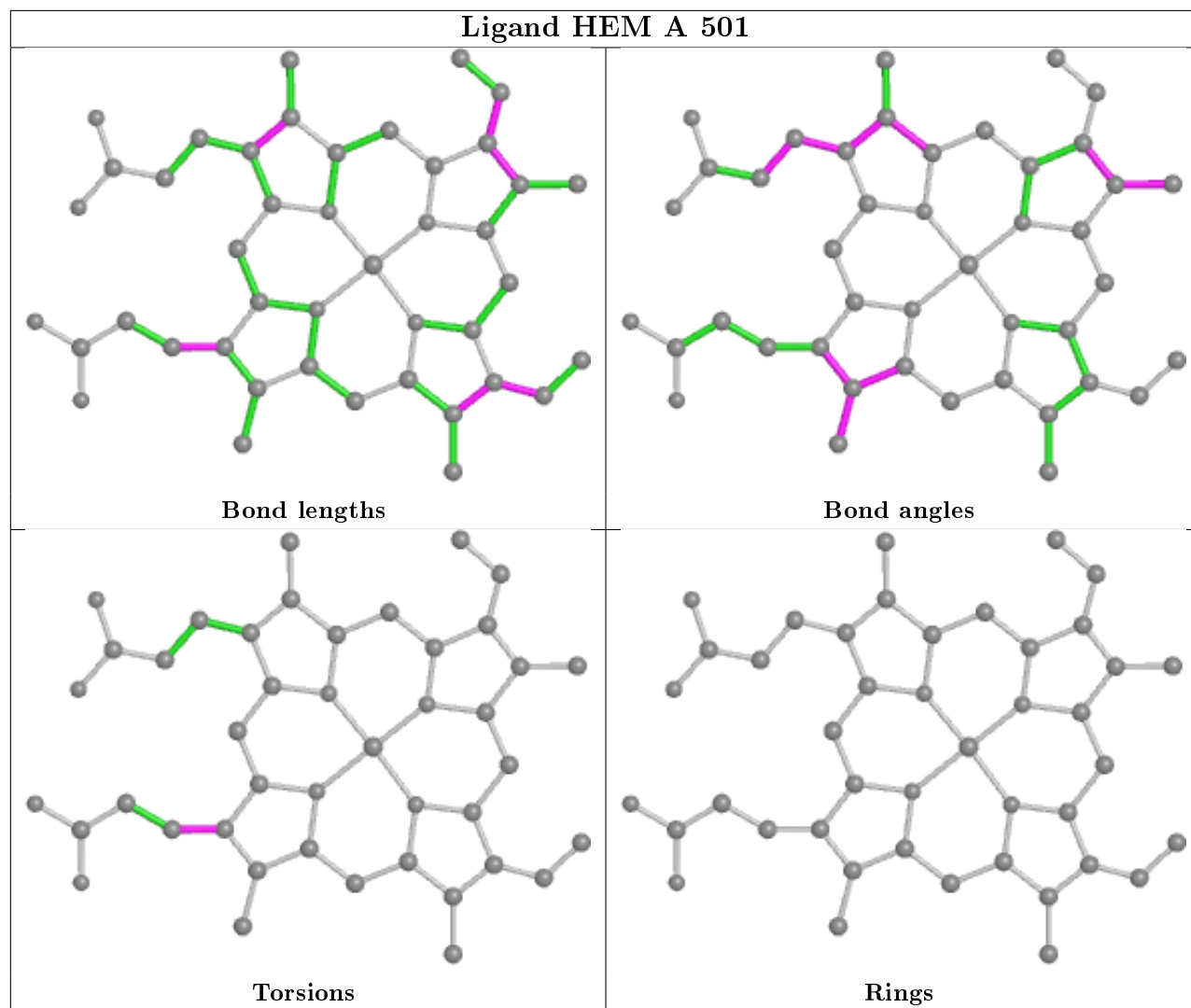
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	BTB	2	0
9	B	501	H4B	1	0
4	C	504	BTB	2	0
2	D	501	HEM	2	0
4	D	504	BTB	3	0
2	A	501	HEM	2	0
4	D	505	BTB	2	0
4	A	503	BTB	3	0
2	B	502	HEM	1	0
9	C	502	H4B	2	0
4	B	510	BTB	2	0
4	A	504	BTB	1	0
2	C	501	HEM	4	0

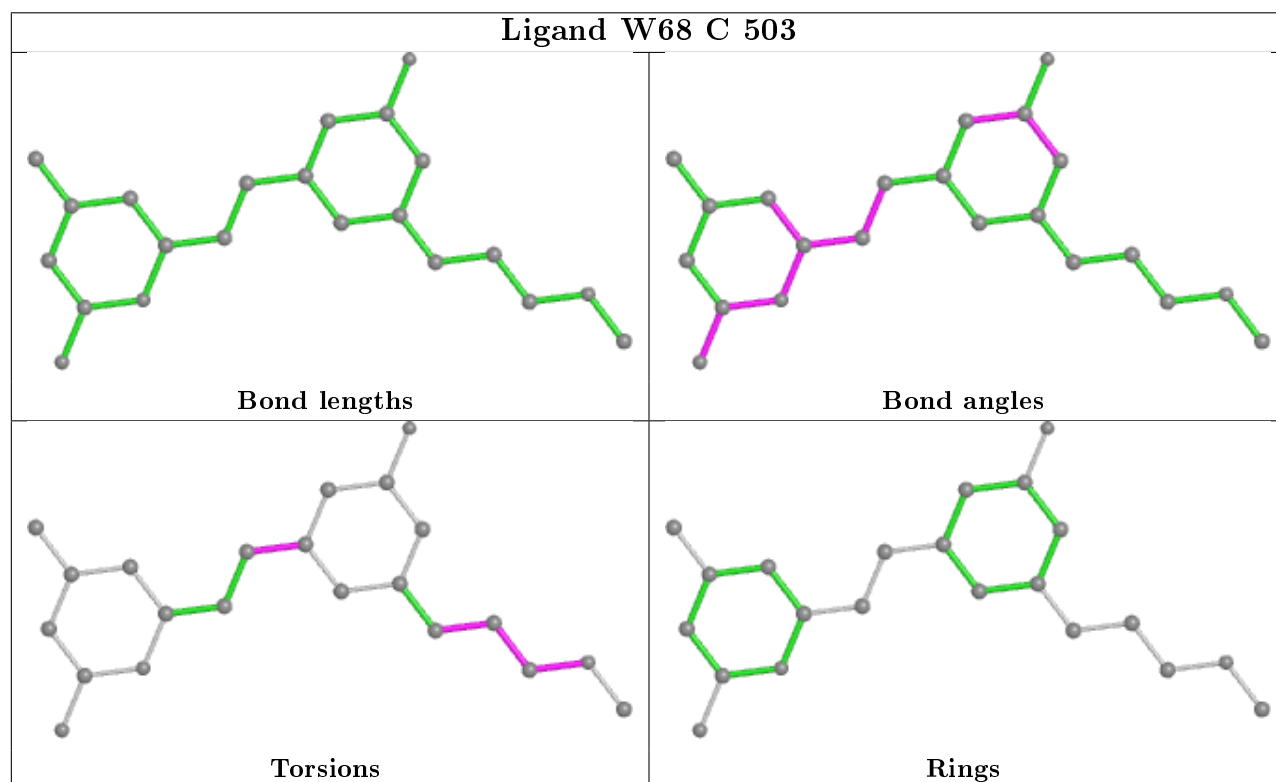
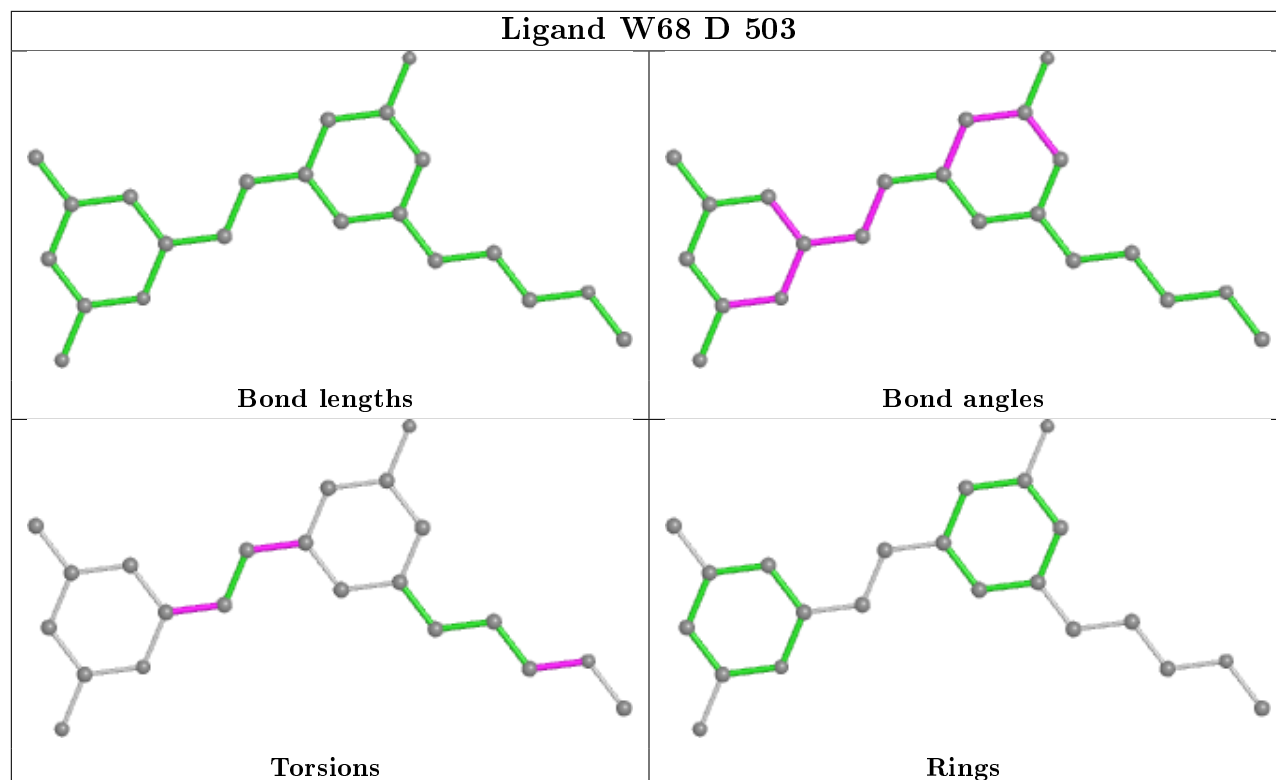
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

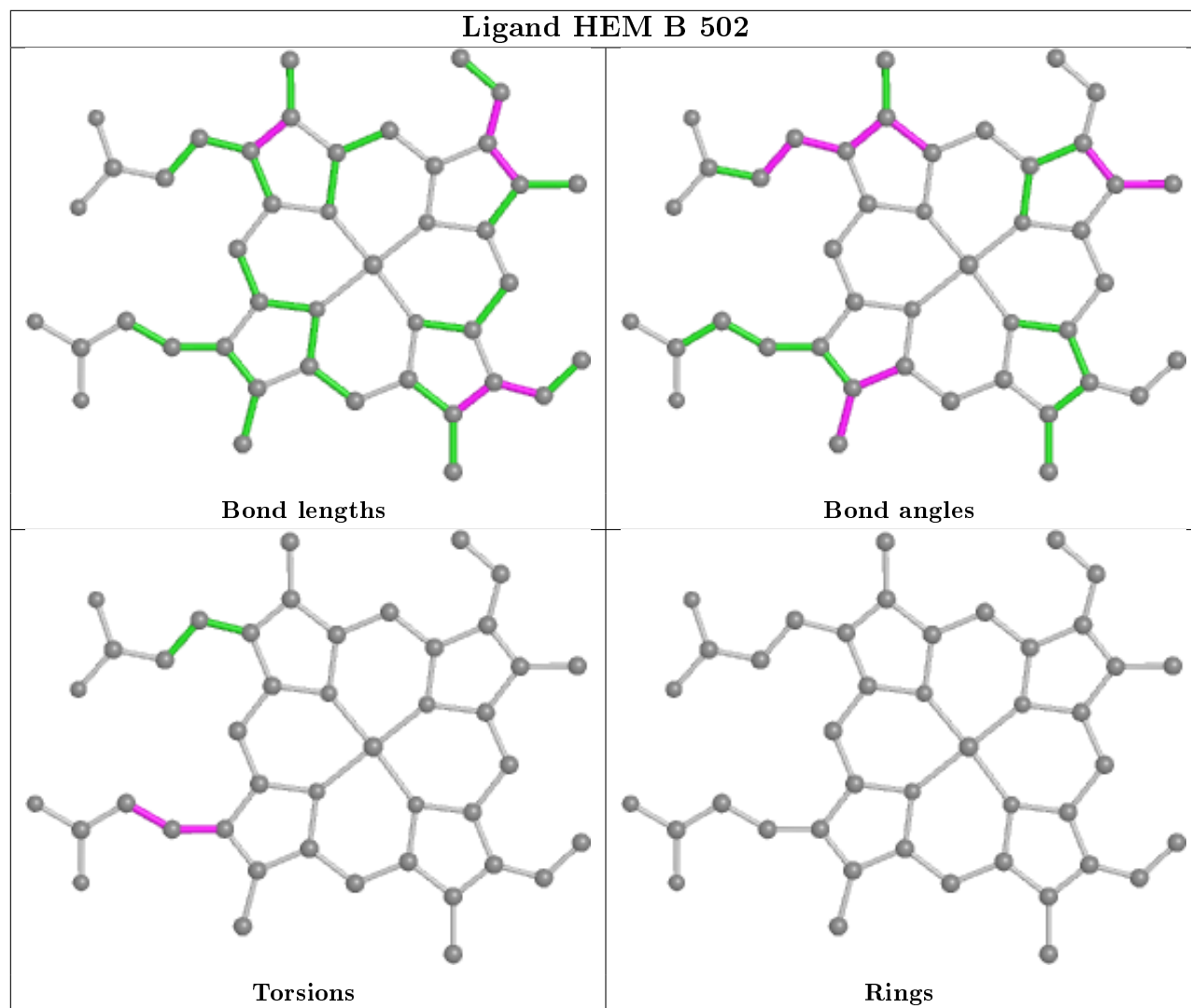


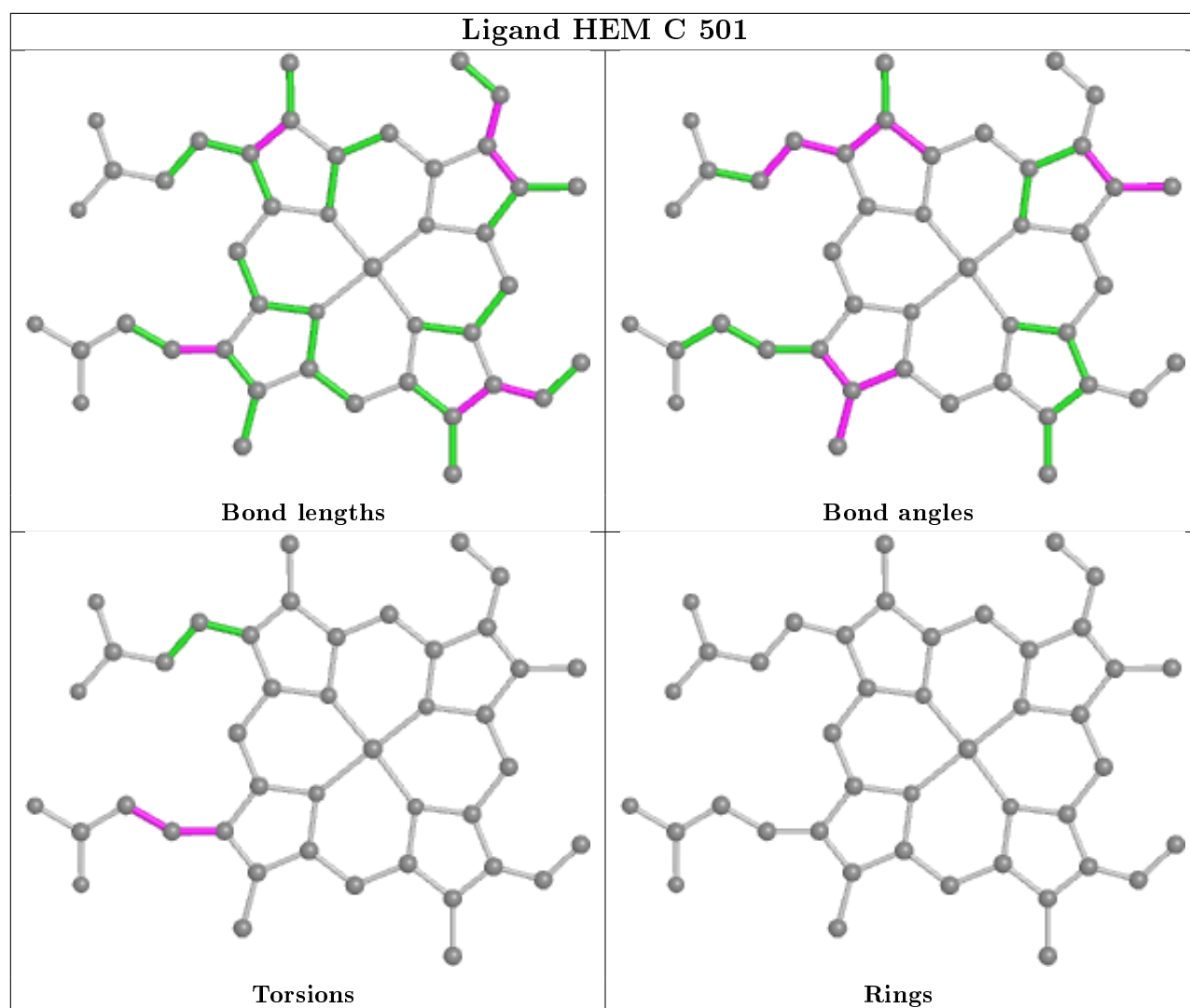












5.7 Other polymers [i](#)

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	401/440 (91%)	1.25	94 (23%) 0 0	34, 70, 131, 163	0
1	B	401/440 (91%)	0.35	36 (8%) 9 11	31, 49, 93, 128	0
1	C	401/440 (91%)	0.90	73 (18%) 1 1	36, 64, 115, 157	0
1	D	402/440 (91%)	0.25	29 (7%) 15 19	29, 47, 81, 124	0
All	All	1605/1760 (91%)	0.69	232 (14%) 2 3	29, 57, 114, 163	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	8.0
1	A	204	ALA	7.8
1	C	142	GLY	6.6
1	C	238	ARG	6.4
1	A	480	TRP	6.2
1	A	142	GLY	6.2
1	A	244	TRP	6.1
1	A	274	CYS	6.0
1	A	293	LEU	5.8
1	A	259	GLY	5.7
1	A	448	ILE	5.5
1	A	88	ALA	5.4
1	A	258	ASP	5.4
1	A	302	LEU	5.2
1	A	280	THR	5.1
1	A	447	TRP	5.0
1	A	120	PRO	5.0
1	C	448	ILE	4.9
1	A	304	LEU	4.8
1	C	239	GLY	4.7
1	C	301	GLU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	67	LYS	4.7
1	B	452	ILE	4.4
1	A	107	ARG	4.3
1	A	303	PHE	4.3
1	C	447	TRP	4.3
1	B	460	PHE	4.2
1	A	89	GLN	4.2
1	B	259	GLY	4.2
1	A	141	SER	4.2
1	A	273	LEU	4.2
1	A	145	ALA	4.2
1	D	257	GLN	4.1
1	C	480	TRP	4.1
1	A	122	GLN	4.1
1	A	275	ILE	4.1
1	D	89	GLN	4.1
1	A	299	PRO	4.1
1	A	254	TYR	4.0
1	A	272	GLU	4.0
1	B	89	GLN	4.0
1	C	68	PHE	4.0
1	A	301	GLU	4.0
1	C	300	PRO	4.0
1	C	304	LEU	4.0
1	A	281	PRO	3.9
1	A	279	TRP	3.9
1	A	479	PRO	3.9
1	B	142	GLY	3.9
1	C	445	TRP	3.8
1	A	452	ILE	3.8
1	C	236	PRO	3.8
1	C	280	THR	3.7
1	A	127	ALA	3.7
1	A	123	LEU	3.7
1	B	257	GLN	3.7
1	A	445	TRP	3.7
1	C	119	ALA	3.6
1	D	452	ILE	3.5
1	C	89	GLN	3.5
1	C	275	ILE	3.5
1	A	257	GLN	3.5
1	A	86	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	256	GLN	3.5
1	A	449	VAL	3.5
1	A	450	PRO	3.5
1	B	449	VAL	3.4
1	D	446	ALA	3.4
1	A	185	VAL	3.4
1	C	446	ALA	3.4
1	A	300	PRO	3.4
1	A	160	THR	3.4
1	B	454	GLY	3.4
1	C	202	ARG	3.4
1	D	68	PHE	3.4
1	A	184	CYS	3.4
1	C	298	GLU	3.3
1	C	450	PRO	3.3
1	A	162	THR	3.3
1	A	305	LEU	3.3
1	D	121	GLU	3.3
1	C	79	ILE	3.3
1	C	449	VAL	3.3
1	A	451	PRO	3.2
1	B	258	ASP	3.2
1	A	129	ASP	3.2
1	C	294	GLN	3.1
1	C	153	VAL	3.1
1	C	185	VAL	3.1
1	A	237	GLY	3.1
1	A	143	SER	3.1
1	B	79	ILE	3.1
1	A	295	ALA	3.1
1	C	302	LEU	3.1
1	A	353	PHE	3.1
1	C	235	CYS	3.1
1	A	360	THR	3.0
1	C	360	THR	3.0
1	A	238	ARG	3.0
1	B	450	PRO	3.0
1	B	76	VAL	3.0
1	B	120	PRO	3.0
1	A	255	ARG	3.0
1	C	292	LEU	3.0
1	C	258	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	GLN	3.0
1	D	454	GLY	3.0
1	A	308	GLU	3.0
1	D	122	GLN	3.0
1	C	204	ALA	3.0
1	C	468	PHE	2.9
1	C	274	CYS	2.9
1	D	255	ARG	2.9
1	C	272	GLU	2.9
1	B	157	VAL	2.9
1	C	90	GLN	2.9
1	C	184	CYS	2.9
1	B	119	ALA	2.9
1	C	144	GLN	2.9
1	A	140	ARG	2.9
1	C	451	PRO	2.9
1	C	281	PRO	2.9
1	C	295	ALA	2.9
1	A	292	LEU	2.9
1	A	106	PRO	2.8
1	C	293	LEU	2.8
1	A	183	ARG	2.8
1	B	446	ALA	2.8
1	A	346	LEU	2.8
1	B	445	TRP	2.8
1	A	365	ARG	2.8
1	D	260	SER	2.8
1	C	299	PRO	2.8
1	D	360	THR	2.8
1	C	76	VAL	2.8
1	C	244	TRP	2.8
1	A	134	TYR	2.7
1	C	412	LEU	2.7
1	B	90	GLN	2.7
1	A	221	ARG	2.7
1	A	446	ALA	2.7
1	B	451	PRO	2.7
1	A	146	HIS	2.7
1	B	360	THR	2.7
1	D	449	VAL	2.6
1	C	452	ILE	2.6
1	C	221	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	158	ALA	2.6
1	C	454	GLY	2.6
1	C	259	GLY	2.6
1	C	279	TRP	2.6
1	D	119	ALA	2.6
1	C	122	GLN	2.6
1	C	444	ASP	2.6
1	C	305	LEU	2.6
1	A	444	ASP	2.6
1	C	183	ARG	2.6
1	A	297	ASP	2.6
1	A	309	LEU	2.6
1	A	163	TYR	2.5
1	C	207	MET	2.5
1	C	439	GLY	2.5
1	D	460	PHE	2.5
1	D	388	ARG	2.5
1	B	68	PHE	2.5
1	C	208	PHE	2.5
1	A	90	GLN	2.5
1	D	258	ASP	2.5
1	B	153	VAL	2.5
1	B	260	SER	2.4
1	A	412	LEU	2.4
1	C	129	ASP	2.4
1	D	455	SER	2.4
1	C	257	GLN	2.4
1	C	297	ASP	2.4
1	D	448	ILE	2.4
1	B	158	ALA	2.4
1	B	122	GLN	2.4
1	A	84	LEU	2.4
1	A	359	SER	2.4
1	B	362	ILE	2.4
1	A	91	ASP	2.4
1	A	130	PHE	2.3
1	B	453	SER	2.3
1	D	364	THR	2.3
1	D	362	ILE	2.3
1	C	80	THR	2.3
1	D	445	TRP	2.3
1	A	336	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	277	HIS	2.3
1	C	321	GLU	2.3
1	B	388	ARG	2.3
1	C	81	TYR	2.3
1	A	152	GLU	2.3
1	D	261	VAL	2.3
1	D	259	GLY	2.2
1	B	447	TRP	2.2
1	D	453	SER	2.2
1	B	97	ARG	2.2
1	B	86	ALA	2.2
1	B	448	ILE	2.2
1	A	478	ASP	2.2
1	A	364	THR	2.2
1	A	181	ALA	2.1
1	A	242	ARG	2.1
1	D	451	PRO	2.1
1	A	439	GLY	2.1
1	B	141[A]	SER	2.1
1	B	455	SER	2.1
1	C	131	ILE	2.1
1	C	362	ILE	2.1
1	B	124	LEU	2.1
1	C	353	PHE	2.1
1	D	120	PRO	2.1
1	A	366	ASN	2.1
1	A	126	GLN	2.1
1	A	206	GLU	2.1
1	C	273	LEU	2.1
1	A	262	ARG	2.1
1	A	151	GLN	2.1
1	C	141	SER	2.0
1	C	368	CYS	2.1
1	B	154	GLU	2.0
1	C	216	LYS	2.0
1	A	362	ILE	2.0
1	D	389	THR	2.0
1	A	298	GLU	2.0
1	A	124	LEU	2.0
1	A	368	CYS	2.0
1	C	86	ALA	2.0
1	C	364	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	205	GLN	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(Å ²)	Q<0.9
4	BTB	C	504	14/14	0.74	0.15	80,87,93,94	0
8	GD	A	508	1/1	0.81	0.06	128,128,128,128	0
4	BTB	D	504	14/14	0.82	0.22	42,69,84,86	0
4	BTB	D	505	14/14	0.83	0.21	66,75,84,90	0
9	H4B	C	502	17/17	0.84	0.26	66,75,88,97	0
4	BTB	A	504	14/14	0.85	0.14	70,81,89,95	0
4	BTB	B	506	14/14	0.86	0.23	47,65,81,85	0
4	BTB	B	510	14/14	0.86	0.17	55,75,88,90	0
9	H4B	B	501	17/17	0.87	0.32	77,86,100,107	0
9	H4B	D	502	17/17	0.88	0.26	37,72,93,99	0
9	H4B	B	503	17/17	0.89	0.24	58,68,92,98	0
3	W68	C	503	22/22	0.89	0.32	46,74,99,104	0
4	BTB	B	505	14/14	0.90	0.14	40,66,86,97	0
6	GOL	A	506	6/6	0.91	0.22	53,69,84,88	0
3	W68	D	503	22/22	0.92	0.23	23,78,97,107	0
3	W68	B	504	22/22	0.92	0.23	30,73,97,108	0
3	W68	A	502	22/22	0.92	0.41	55,101,117,123	0
4	BTB	B	509	14/14	0.93	0.24	35,85,98,103	0
4	BTB	A	503	14/14	0.93	0.25	62,91,102,107	0
7	CL	A	507	1/1	0.94	0.22	67,67,67,67	0
8	GD	C	508	1/1	0.95	0.08	114,114,114,114	0
6	GOL	C	506	6/6	0.95	0.22	44,52,67,71	0

Continued on next page...

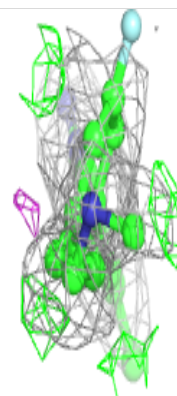
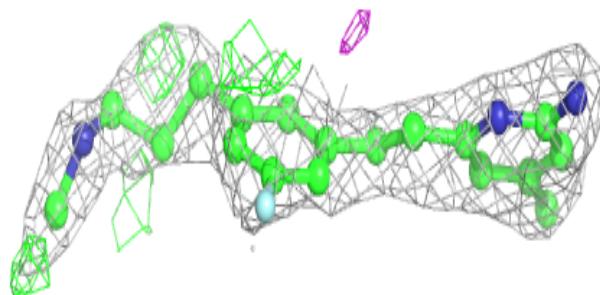
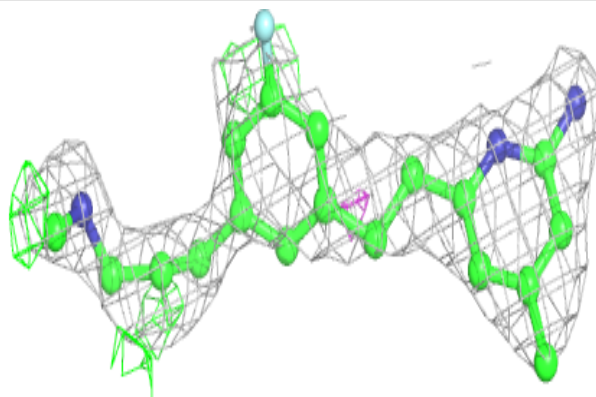
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	501	43/43	0.96	0.27	52,72,89,99	0
2	HEM	C	501	43/43	0.96	0.22	35,54,83,98	0
7	CL	D	507	1/1	0.96	0.12	46,46,46,46	0
8	GD	D	506	1/1	0.97	0.16	57,57,57,57	0
2	HEM	B	502	43/43	0.97	0.15	25,38,77,103	0
7	CL	B	507	1/1	0.97	0.13	50,50,50,50	0
7	CL	C	507	1/1	0.97	0.26	61,61,61,61	0
2	HEM	D	501	43/43	0.97	0.13	26,34,77,92	0
5	ZN	A	505	1/1	0.98	0.10	52,52,52,52	0
8	GD	B	508	1/1	0.98	0.14	53,53,53,53	0
5	ZN	C	505	1/1	0.99	0.10	42,42,42,42	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.

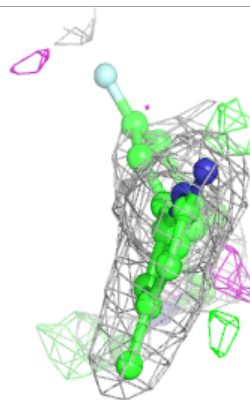
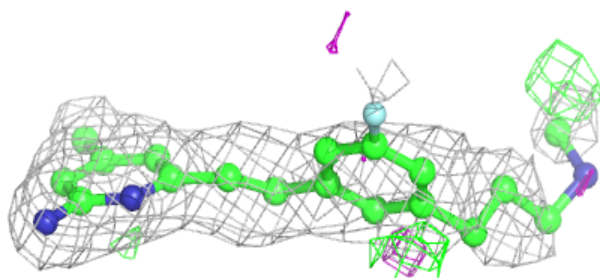
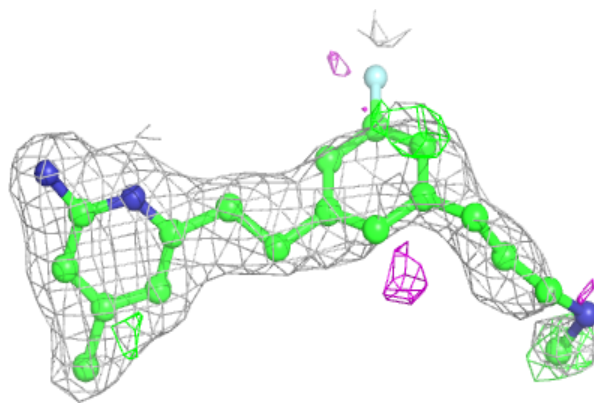
Electron density around W68 C 503:

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

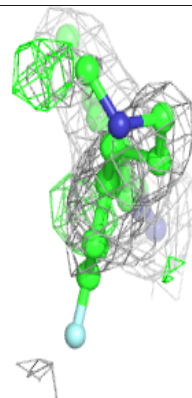
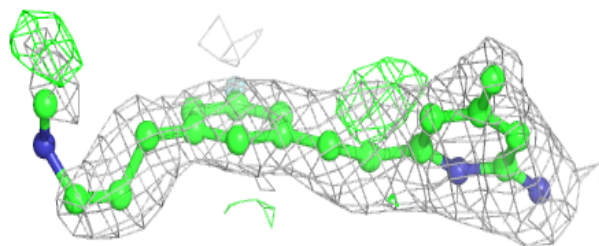
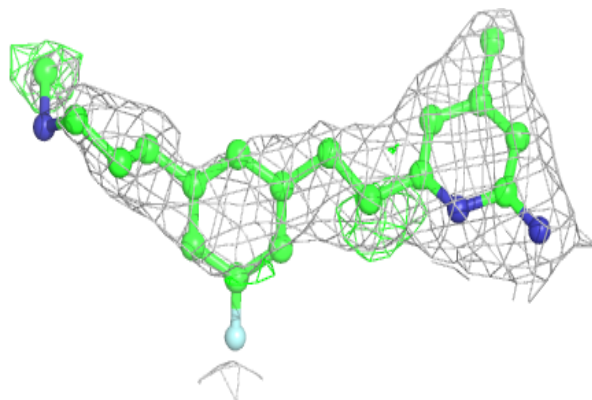


Electron density around W68 D 503:

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

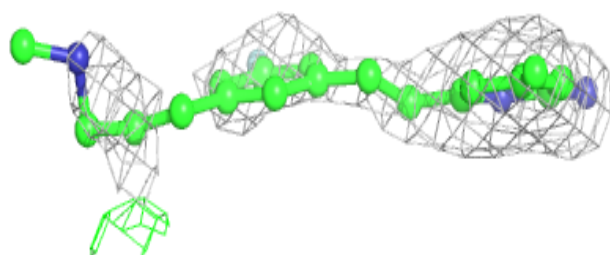
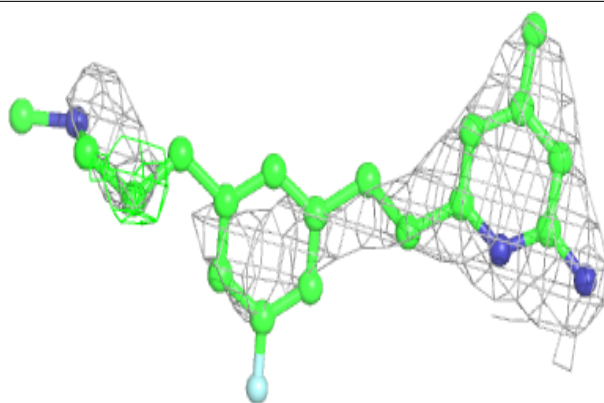
**Electron density around W68 B 504:**

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

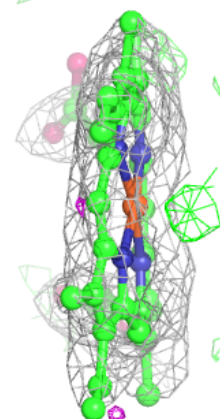
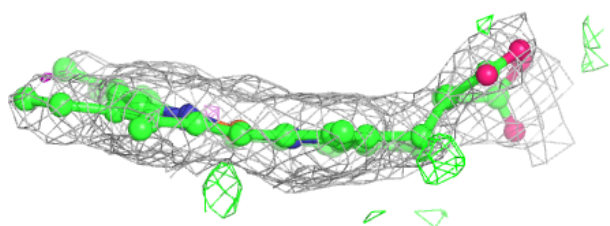
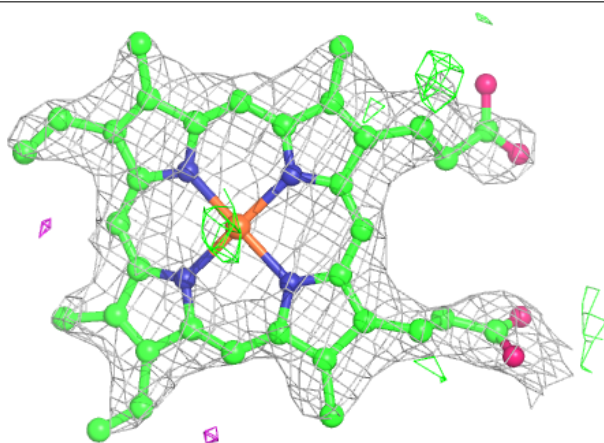


Electron density around W68 A 502:

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

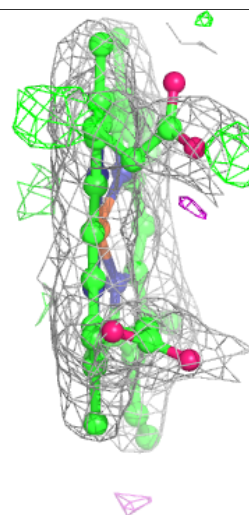
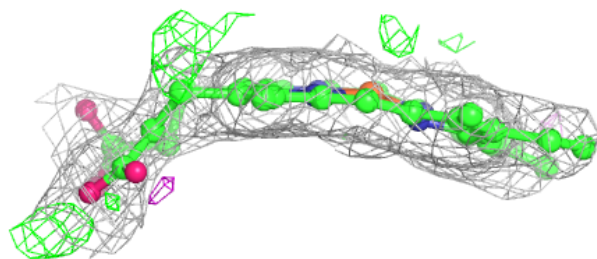
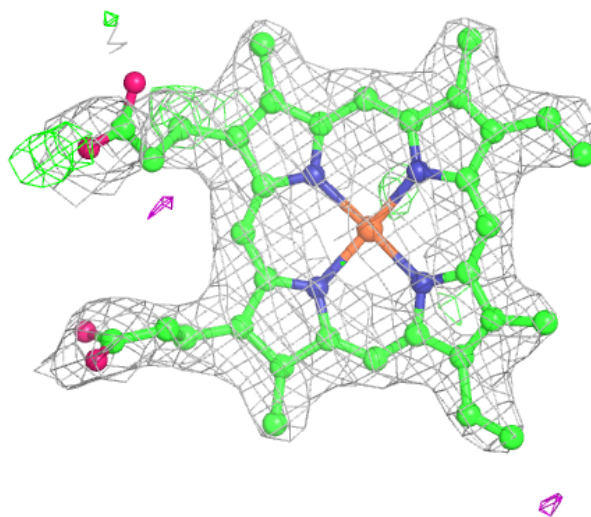
**Electron density around HEM A 501:**

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



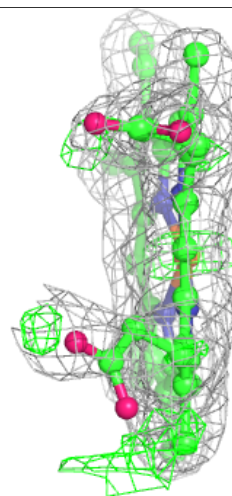
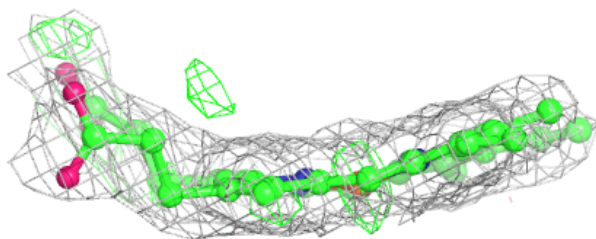
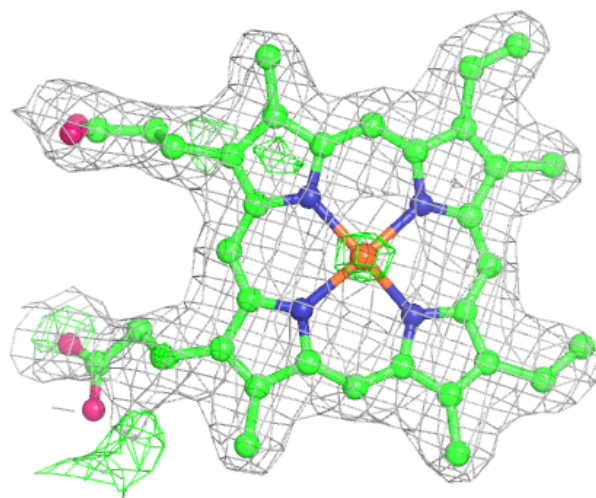
Electron density around HEM C 501:

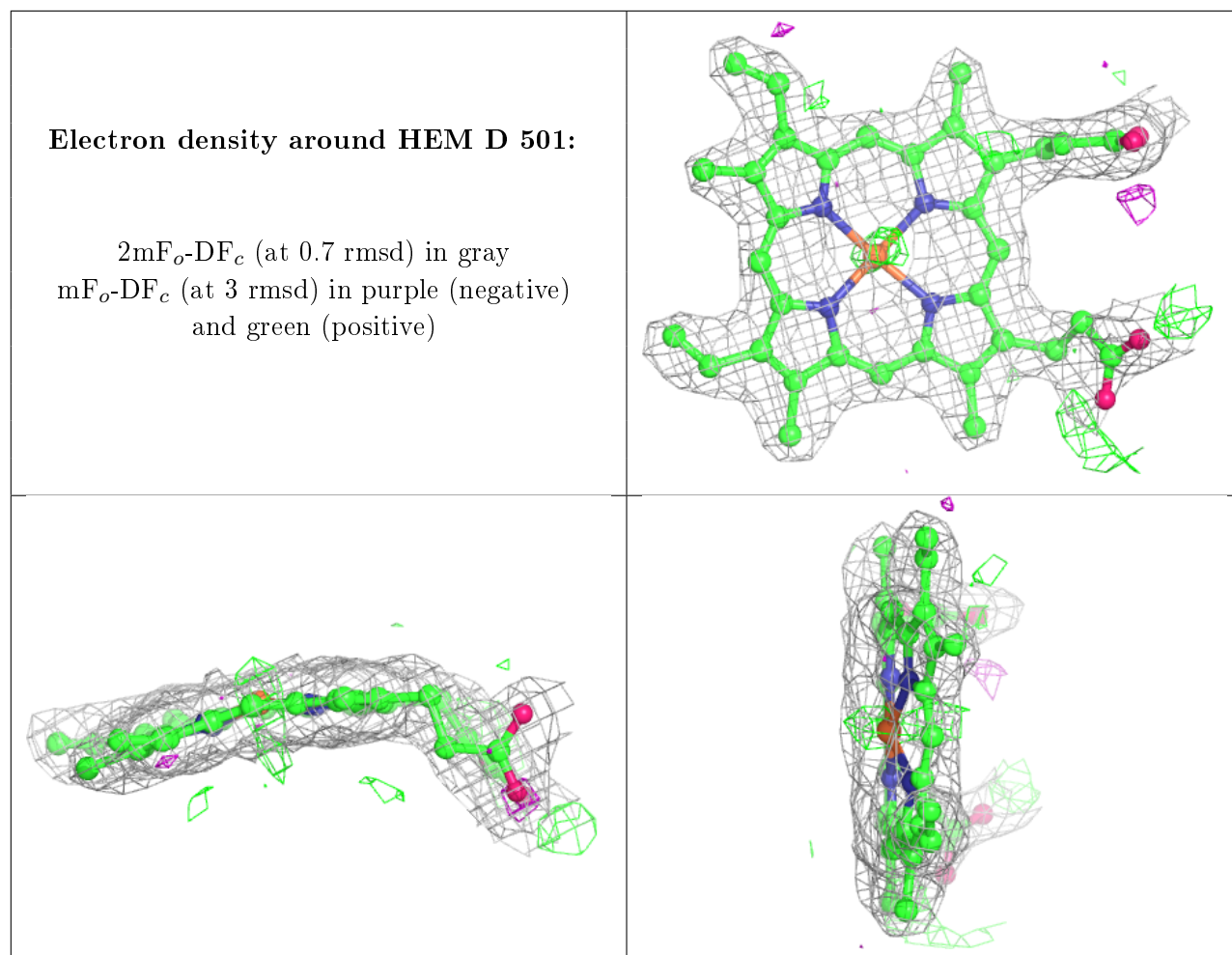
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.