



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:04 PM UTC

PDB ID : 6NH5 / pdb_00006nh5
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-fluoro-5-(2-((2R,4S)-4-fluoro-1-methylpyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine
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Deposited on : 2018-12-21
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

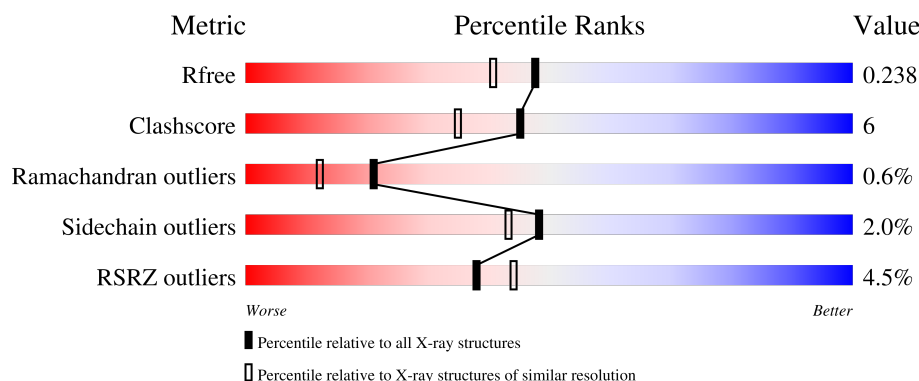
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

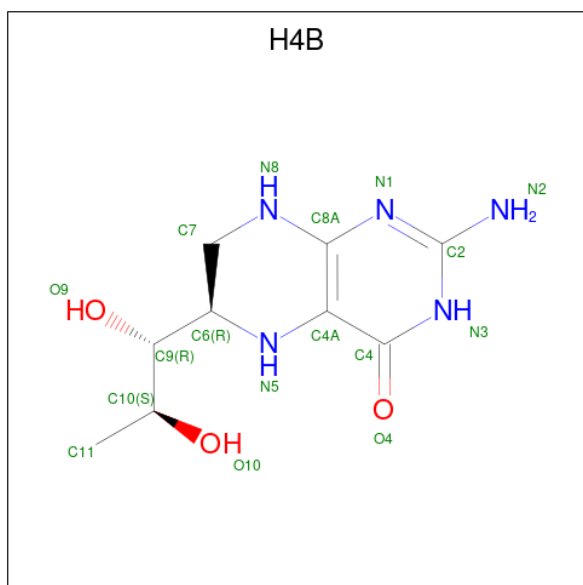
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	440	10% 76% 15% • 8%
1	B	440	% 84% 7% • 8%
1	C	440	4% 79% 12% • 9%
1	D	440	% 83% 8% 8%

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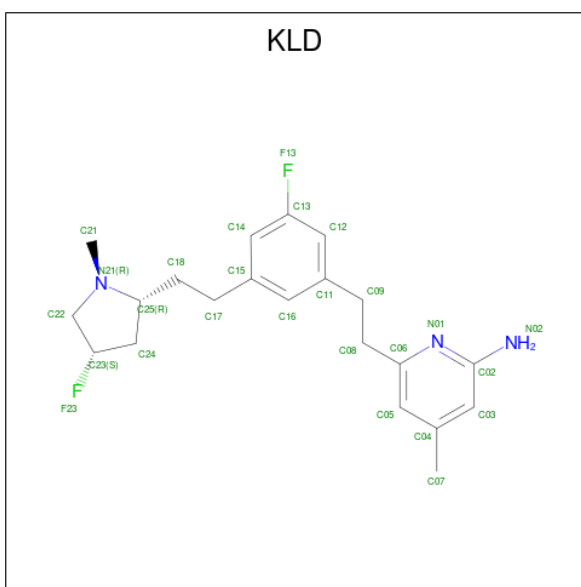
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



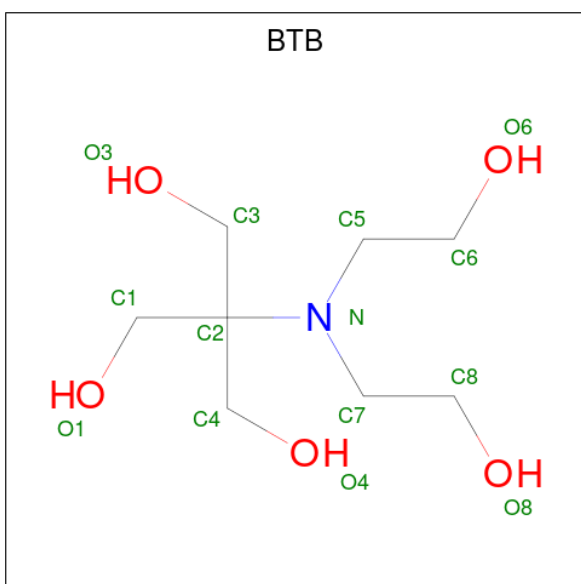
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[2-(3-fluoro-5-{2-[(2R,4S)-4-fluoro-1-methylpyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (CCD ID: KLD) (formula: $C_{21}H_{27}F_2N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			26	21	2	3		
4	B	1	Total	C	F	N	0	0
			26	21	2	3		
4	C	1	Total	C	F	N	0	0
			26	21	2	3		
4	D	1	Total	C	F	N	0	0
			26	21	2	3		

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



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0
6	C	2	Total Zn 2 2	0	0

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

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

- Molecule 9 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

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

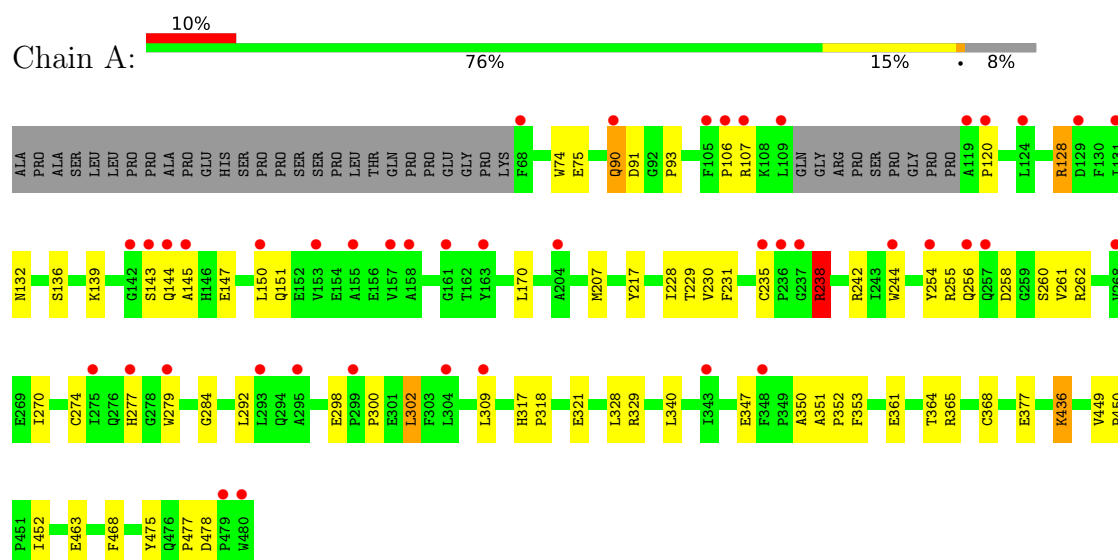
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	102	Total 102	O 102	0	0
10	B	183	Total 183	O 183	0	0
10	C	128	Total 128	O 128	0	0
10	D	195	Total 195	O 195	0	0

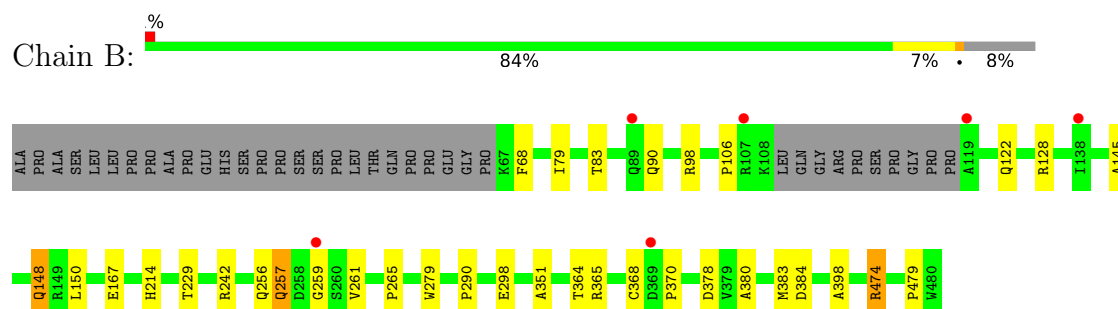
3 Residue-property plots [i](#)

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

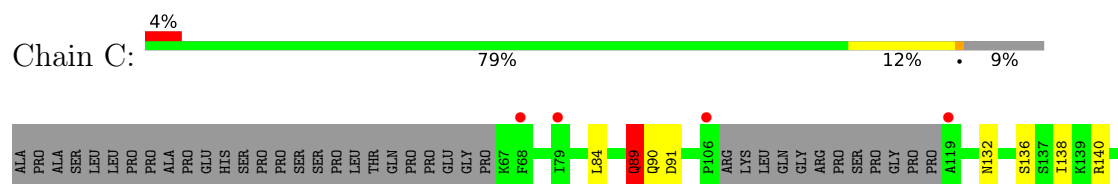
- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A

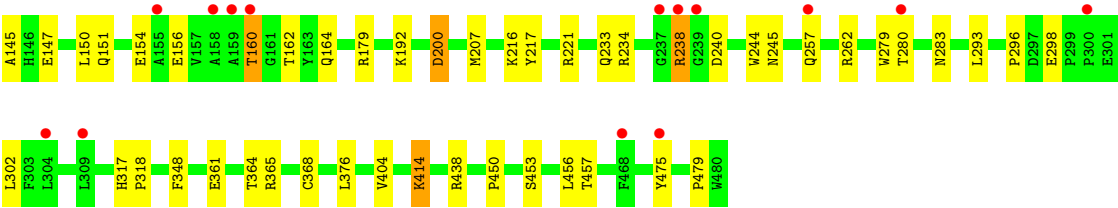


- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A

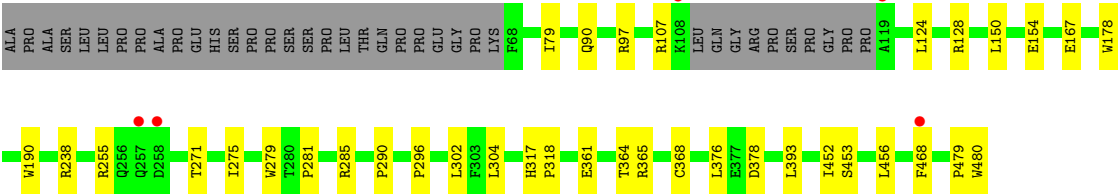
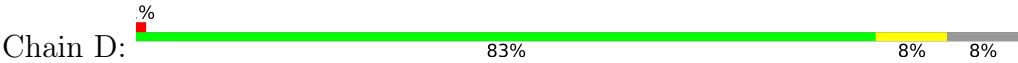


- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A





● Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.53Å 152.76Å 108.98Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	88.71 – 1.96 88.71 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.6 (88.71-1.96) 99.9 (88.71-1.96)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.197 , 0.241 0.193 , 0.238	Depositor DCC
R_{free} test set	7032 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14078	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: BTB, ZN, GD, KLD, H4B, CL, HEM, GOL

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	0.28	0/3335	0.49	0/4543
1	B	0.34	0/3339	0.51	0/4548
1	C	0.28	0/3307	0.48	0/4506
1	D	0.36	0/3330	0.51	0/4537
All	All	0.32	0/13311	0.50	0/18134

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	238	ARG	Peptide

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	43	0
1	B	3241	0	3152	24	0
1	C	3212	0	3116	32	0
1	D	3232	0	3139	25	1
2	A	43	0	30	5	0
2	B	43	0	30	6	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
3	C	34	0	30	2	0
4	A	26	0	0	2	0
4	B	26	0	0	1	0
4	C	26	0	0	2	0
4	D	26	0	0	0	0
5	A	56	0	76	9	0
5	B	56	0	74	12	1
5	C	28	0	38	3	0
5	D	42	0	55	7	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	1	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	102	0	0	0	0
10	B	183	0	0	1	1
10	C	128	0	0	1	0
10	D	195	0	0	2	1
All	All	14078	0	12992	156	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (156) 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:84:LEU:HD22	1:C:438:ARG:HG3	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:NH2	1:A:477:PRO:O	2.19	0.74
2:A:501:HEM:CGA	3:A:502:H4B:HN22	2.00	0.74
5:D:503:BTB:O8	5:D:503:BTB:H62	1.91	0.70
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.73	0.68
1:C:262:ARG:NH1	1:C:283:ASN:O	2.27	0.67
1:B:378:ASP:OD1	5:B:506:BTB:O4	2.12	0.67
1:A:93:PRO:HG3	1:A:106:PRO:HB3	1.76	0.67
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.76	0.66
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.77	0.66
2:C:501:HEM:CGA	3:C:502:H4B:HN22	2.08	0.66
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.78	0.65
1:B:128:ARG:HG2	1:B:150:LEU:HD22	1.76	0.65
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.33	0.64
2:C:501:HEM:O2A	4:C:503:KLD:F13	2.07	0.62
1:C:279:TRP:HB2	1:C:302:LEU:HD21	1.81	0.62
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.13	0.62
1:B:380:ALA:HA	1:B:383:MET:HE2	1.83	0.61
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.14	0.61
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.81	0.61
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.84	0.60
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.84	0.58
1:A:270:ILE:HD11	1:A:292:LEU:HD13	1.86	0.58
1:C:91:ASP:OD1	1:D:97:ARG:NH2	2.35	0.58
5:A:511:BTB:O4	5:A:511:BTB:O3	2.15	0.58
1:A:279:TRP:HB2	1:A:302:LEU:HD21	1.85	0.58
1:A:128:ARG:O	1:A:132:ASN:ND2	2.38	0.57
1:B:380:ALA:HA	1:B:383:MET:CE	2.34	0.57
5:A:511:BTB:O8	5:A:511:BTB:O6	2.22	0.57
1:A:132:ASN:O	1:A:136:SER:OG	2.22	0.56
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.19	0.56
1:A:361:GLU:OE2	4:A:503:KLD:N02	2.39	0.56
1:D:271:THR:O	1:D:275:ILE:HG12	2.05	0.56
1:D:128:ARG:HG2	1:D:150:LEU:HD22	1.87	0.56
1:A:91:ASP:O	1:A:107:ARG:NH2	2.30	0.55
1:A:228:ILE:HD13	1:A:353:PHE:HB3	1.88	0.55
1:A:321:GLU:H	1:A:321:GLU:CD	2.13	0.55
1:C:361:GLU:OE2	4:C:503:KLD:N02	2.41	0.54
2:A:501:HEM:O2A	4:A:503:KLD:F13	2.16	0.54
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.89	0.53
1:D:107:ARG:HH22	1:D:468:PHE:HB2	1.72	0.53
1:A:256:GLN:OE1	1:A:258:ASP:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:CYS:HB3	1:A:238:ARG:HD3	1.91	0.53
1:C:150:LEU:O	1:C:154:GLU:HG3	2.09	0.53
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.92	0.52
2:B:501:HEM:HBA2	4:B:503:KLD:C12	2.39	0.52
1:B:474:ARG:HD2	10:B:753:HOH:O	2.08	0.52
1:C:234:ARG:NH1	1:C:240:ASP:OD2	2.37	0.52
1:A:90:GLN:HB3	1:A:468:PHE:CD1	2.45	0.51
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.51
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.92	0.51
2:B:501:HEM:CGA	3:B:502:H4B:HN22	2.24	0.51
1:D:124:LEU:HD21	1:D:154:GLU:HG2	1.93	0.50
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.47	0.50
1:A:340:LEU:HD11	1:A:347:GLU:HB3	1.94	0.50
1:C:89:GLN:O	1:D:97:ARG:NH2	2.45	0.49
1:A:244:TRP:HB2	1:A:292:LEU:HB2	1.93	0.49
1:B:365:ARG:HH12	2:B:501:HEM:CGA	2.26	0.49
1:C:200:ASP:OD1	1:C:200:ASP:N	2.40	0.49
1:D:365:ARG:NH1	2:D:501:HEM:O2A	2.46	0.49
1:C:216:LYS:HG3	1:C:217:TYR:N	2.28	0.48
5:C:505:BTB:H51	5:C:505:BTB:H42	1.50	0.48
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.48	0.48
1:D:364:THR:O	1:D:368:CYS:HB2	2.13	0.48
5:B:505:BTB:O3	5:B:505:BTB:H51	2.14	0.47
1:C:179:ARG:NH2	1:C:438:ARG:HD2	2.28	0.47
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.95	0.47
1:C:156:GLU:OE1	1:C:164:GLN:N	2.47	0.47
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.96	0.47
1:C:160:THR:HG23	1:C:162:THR:H	1.80	0.47
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.97	0.47
5:A:511:BTB:H12	5:A:511:BTB:H51	1.55	0.46
1:B:68:PHE:CD1	1:B:83:THR:HA	2.50	0.46
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.31	0.46
5:B:509:BTB:H51	5:B:509:BTB:H41	1.33	0.46
1:B:364:THR:O	1:B:368:CYS:HB2	2.15	0.46
1:C:364:THR:O	1:C:368:CYS:HB2	2.16	0.46
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.97	0.46
5:A:504:BTB:H71	5:A:504:BTB:H41	1.81	0.46
5:D:503:BTB:H32	5:D:503:BTB:H51	1.59	0.46
1:D:107:ARG:HD2	1:D:107:ARG:N	2.30	0.46
1:A:254:TYR:O	1:A:261:VAL:HA	2.16	0.46
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:OE2	5:B:505:BTB:N	2.49	0.45
5:A:506:BTB:H32	5:A:506:BTB:H51	1.46	0.45
1:D:275:ILE:HD11	1:D:281:PRO:HB3	1.98	0.45
1:C:414:LYS:HD2	1:C:414:LYS:HA	1.69	0.45
1:D:361:GLU:HB3	1:D:365:ARG:NH2	2.31	0.45
5:D:504:BTB:H81	5:D:504:BTB:H52	1.58	0.45
1:B:145:ALA:O	1:B:148:GLN:HG3	2.16	0.45
1:B:298:GLU:OE1	5:B:505:BTB:H31	2.17	0.45
1:B:383:MET:HE1	1:B:398:ALA:HA	1.97	0.45
5:B:506:BTB:H72	5:B:506:BTB:H12	1.72	0.45
1:C:132:ASN:O	1:C:136:SER:OG	2.31	0.45
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.99	0.45
1:C:404:VAL:HG23	1:D:393:LEU:HD12	1.99	0.45
1:A:377:GLU:OE2	5:A:505:BTB:H11	2.17	0.45
5:A:504:BTB:H51	5:A:504:BTB:H12	1.51	0.45
5:D:504:BTB:H51	5:D:504:BTB:H32	1.25	0.45
1:B:384:ASP:OD2	5:B:509:BTB:O6	2.31	0.44
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.53	0.44
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.44
1:A:207:MET:HG2	1:A:231:PHE:CE1	2.53	0.44
1:A:231:PHE:HB2	1:A:350:ALA:O	2.18	0.44
1:A:298:GLU:HG2	5:A:506:BTB:H32	2.00	0.44
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.18	0.43
1:A:74:TRP:HE1	1:A:463:GLU:CD	2.26	0.43
1:B:257:GLN:C	1:B:259:GLY:H	2.25	0.43
1:A:144:GLN:HG2	1:A:145:ALA:N	2.34	0.43
1:A:151:GLN:OE1	1:A:151:GLN:N	2.52	0.43
1:C:245:ASN:OD1	1:C:245:ASN:N	2.51	0.43
1:C:138:ILE:O	1:C:140:ARG:HG2	2.19	0.43
1:A:75:GLU:HG3	1:B:370:PRO:HG2	2.01	0.43
1:D:124:LEU:HD12	1:D:124:LEU:HA	1.84	0.43
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.59	0.43
1:A:229:THR:O	1:A:351:ALA:HA	2.19	0.42
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.93	0.42
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.54	0.42
1:C:262:ARG:HD3	1:C:283:ASN:O	2.19	0.42
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.59	0.42
1:A:262:ARG:HE	1:A:284:GLY:HA2	1.85	0.42
5:C:505:BTB:O4	5:C:505:BTB:O1	2.31	0.42
1:A:228:ILE:HD12	1:A:352:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:HE2	1:A:436:LYS:HB3	1.89	0.42
1:A:478:ASP:OD1	1:A:478:ASP:N	2.52	0.42
5:B:509:BTB:H81	5:B:509:BTB:H52	1.56	0.42
1:C:244:TRP:CD1	1:C:479:PRO:HG3	2.55	0.42
5:D:504:BTB:H61	10:D:601:HOH:O	2.19	0.42
1:A:274:CYS:SG	1:A:292:LEU:HD11	2.59	0.41
1:C:453:SER:HB3	1:C:456:LEU:HD12	2.02	0.41
1:D:238:ARG:HG3	1:D:296:PRO:HB3	2.02	0.41
1:A:170:LEU:HD11	1:A:230:VAL:HG21	2.03	0.41
1:B:214:HIS:CD2	1:B:214:HIS:C	2.98	0.41
1:B:229:THR:O	1:B:351:ALA:HA	2.21	0.41
1:D:285:ARG:HD3	10:D:672:HOH:O	2.20	0.41
1:A:277:HIS:CD2	1:A:300:PRO:HG2	2.56	0.41
1:A:328:LEU:C	1:A:329:ARG:HG3	2.45	0.41
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.28	0.41
1:B:365:ARG:NH1	2:B:501:HEM:CGA	2.83	0.41
5:D:504:BTB:H71	5:D:504:BTB:H11	1.36	0.41
5:A:505:BTB:H72	5:A:505:BTB:H41	1.64	0.41
1:C:376:LEU:HB2	10:C:635:HOH:O	2.20	0.41
1:A:255:ARG:HA	1:A:260:SER:O	2.21	0.41
5:B:505:BTB:H42	5:B:505:BTB:H72	1.96	0.41
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.56	0.41
1:A:217:TYR:CD1	1:A:217:TYR:C	2.98	0.41
5:B:504:BTB:H32	5:B:504:BTB:H51	1.79	0.41
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.03	0.41
1:B:365:ARG:NH2	8:B:507:CL:CL	2.91	0.41
1:C:156:GLU:O	1:C:160:THR:HG22	2.21	0.41
1:C:298:GLU:OE1	5:C:505:BTB:O6	2.18	0.41
1:B:383:MET:HE3	1:B:383:MET:HB2	1.69	0.40
1:B:384:ASP:OD2	5:B:509:BTB:O8	2.34	0.40
5:B:506:BTB:H32	5:B:506:BTB:H51	1.84	0.40
1:D:378:ASP:OD1	5:D:505:BTB:H41	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:OE1	5:B:505:BTB:O8[1_554]	2.13	0.07
10:B:612:HOH:O	10:D:608:HOH:O[1_456]	2.15	0.05

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%)	376 (94%)	22 (6%)	4 (1%)	12	5
1	B	403/440 (92%)	394 (98%)	8 (2%)	1 (0%)	43	36
1	C	399/440 (91%)	385 (96%)	10 (2%)	4 (1%)	12	5
1	D	402/440 (91%)	395 (98%)	7 (2%)	0	100	100
All	All	1606/1760 (91%)	1550 (96%)	47 (3%)	9 (1%)	21	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	ALA
1	A	90	GLN
1	A	120	PRO
1	A	143	SER
1	A	238	ARG
1	B	106	PRO
1	C	238	ARG
1	C	89	GLN
1	C	296	PRO

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%)	339 (98%)	6 (2%)	53	49
1	B	346/373 (93%)	337 (97%)	9 (3%)	40	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	342/373 (92%)	331 (97%)	11 (3%)	34	25
1	D	345/373 (92%)	343 (99%)	2 (1%)	78	79
All	All	1378/1492 (92%)	1350 (98%)	28 (2%)	48	43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	139	LYS
1	A	238	ARG
1	A	302	LEU
1	A	309	LEU
1	A	436	LYS
1	B	79	ILE
1	B	90	GLN
1	B	98	ARG
1	B	122	GLN
1	B	148	GLN
1	B	167	GLU
1	B	256	GLN
1	B	257	GLN
1	B	474	ARG
1	C	89	GLN
1	C	90	GLN
1	C	147	GLU
1	C	151	GLN
1	C	160	THR
1	C	192	LYS
1	C	200	ASP
1	C	221	ARG
1	C	257	GLN
1	C	280	THR
1	C	414	LYS
1	D	79	ILE
1	D	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN

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Mol	Chain	Res	Type
1	A	276	GLN
1	A	277	HIS
1	C	133	GLN
1	C	476	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	501	1	50,50,50	1.66	7 (14%)	67,82,82	1.46	9 (13%)
5	BTB	B	505	-	13,13,13	0.49	0	7,16,16	1.16	1 (14%)
5	BTB	C	505	-	13,13,13	0.33	0	7,16,16	0.41	0
5	BTB	B	506	-	13,13,13	0.37	0	7,16,16	0.67	0
4	KLD	A	503	-	28,28,28	0.43	0	32,39,39	1.63	8 (25%)
5	BTB	C	504	-	13,13,13	0.51	0	7,16,16	1.30	1 (14%)
5	BTB	A	511	-	13,13,13	0.70	0	7,16,16	2.06	2 (28%)
5	BTB	D	503	9	13,13,13	0.41	0	7,16,16	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	A	502	-	17,18,18	0.78	0	14,26,26	2.14	7 (50%)
4	KLD	B	503	-	28,28,28	0.48	0	32,39,39	1.81	7 (21%)
3	H4B	C	509	-	17,18,18	0.79	0	14,26,26	1.74	5 (35%)
2	HEM	B	501	1	50,50,50	1.84	9 (18%)	67,82,82	1.54	17 (25%)
5	BTB	B	509	-	13,13,13	0.56	0	7,16,16	0.89	0
7	GOL	A	508	-	5,5,5	0.35	0	5,5,5	0.37	0
2	HEM	A	501	1	50,50,50	1.62	7 (14%)	67,82,82	1.22	7 (10%)
7	GOL	C	507	-	5,5,5	0.37	0	5,5,5	0.34	0
2	HEM	D	501	1	50,50,50	1.82	8 (16%)	67,82,82	1.39	11 (16%)
5	BTB	D	504	-	13,13,13	0.66	0	7,16,16	0.86	0
5	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.45	0
5	BTB	B	504	9	13,13,13	0.50	0	7,16,16	0.76	0
5	BTB	A	506	-	13,13,13	0.34	0	7,16,16	0.50	0
5	BTB	D	505	-	13,13,13	0.43	0	7,16,16	0.43	0
4	KLD	D	502	-	28,28,28	0.67	0	32,39,39	2.06	6 (18%)
4	KLD	C	503	-	28,28,28	0.52	0	32,39,39	1.83	8 (25%)
5	BTB	A	504	-	13,13,13	0.36	0	7,16,16	0.85	0
3	H4B	B	502	-	17,18,18	0.86	0	14,26,26	1.80	3 (21%)
3	H4B	C	502	-	17,18,18	0.82	0	14,26,26	1.86	5 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	2/14/54/54	-
5	BTB	B	505	-	-	3/21/21/21	-
5	BTB	C	505	-	-	6/21/21/21	-
5	BTB	B	506	-	-	4/21/21/21	-
4	KLD	A	503	-	-	4/10/22/22	0/3/3/3
5	BTB	C	504	-	-	7/21/21/21	-
5	BTB	A	511	-	-	10/21/21/21	-
5	BTB	D	503	9	-	11/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
4	KLD	B	503	-	-	5/10/22/22	0/3/3/3
3	H4B	C	509	-	-	3/8/17/17	0/2/2/2
2	HEM	B	501	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	B	509	-	-	14/21/21/21	-
7	GOL	A	508	-	-	3/4/4/4	-
2	HEM	A	501	1	-	2/14/54/54	-
7	GOL	C	507	-	-	4/4/4/4	-
2	HEM	D	501	1	-	2/14/54/54	-
5	BTB	D	504	-	-	16/21/21/21	-
5	BTB	A	505	-	-	4/21/21/21	-
5	BTB	B	504	9	-	2/21/21/21	-
5	BTB	A	506	-	-	9/21/21/21	-
5	BTB	D	505	-	-	12/21/21/21	-
4	KLD	D	502	-	-	6/10/22/22	0/3/3/3
4	KLD	C	503	-	-	3/10/22/22	0/3/3/3
5	BTB	A	504	-	-	8/21/21/21	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NC	6.28	2.15	1.95
2	D	501	HEM	FE-NB	6.08	2.13	1.94
2	D	501	HEM	FE-NC	5.74	2.14	1.95
2	B	501	HEM	FE-NB	5.49	2.11	1.94
2	C	501	HEM	FE-NB	5.05	2.10	1.94
2	A	501	HEM	FE-NB	5.01	2.10	1.94
2	A	501	HEM	FE-NC	4.26	2.09	1.95
2	C	501	HEM	FE-ND	4.26	2.08	1.94
2	B	501	HEM	FE-NA	4.13	2.08	1.95
2	C	501	HEM	FE-NA	4.06	2.08	1.95
2	D	501	HEM	FE-NA	4.06	2.08	1.95
2	C	501	HEM	FE-NC	4.00	2.08	1.95
2	A	501	HEM	FE-ND	3.61	2.06	1.94
2	A	501	HEM	FE-NA	3.51	2.06	1.95
2	D	501	HEM	FE-ND	3.45	2.05	1.94
2	B	501	HEM	CAC-C3C	3.22	1.56	1.47
2	C	501	HEM	CAB-C3B	3.15	1.55	1.47
2	A	501	HEM	CAB-C3B	3.06	1.55	1.47
2	A	501	HEM	CAC-C3C	3.06	1.55	1.47
2	B	501	HEM	CAB-C3B	2.89	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-ND	2.87	2.03	1.94
2	D	501	HEM	CAB-C3B	2.81	1.54	1.47
2	C	501	HEM	CAC-C3C	2.77	1.54	1.47
2	D	501	HEM	CAC-C3C	2.70	1.54	1.47
2	B	501	HEM	CMA-C3A	2.64	1.56	1.50
2	C	501	HEM	CMC-C2C	2.33	1.55	1.50
2	B	501	HEM	CMD-C2D	2.30	1.55	1.50
2	D	501	HEM	CMD-C2D	2.26	1.55	1.50
2	B	501	HEM	CMB-C2B	2.16	1.55	1.50
2	A	501	HEM	CMC-C2C	2.12	1.55	1.50
2	D	501	HEM	C4A-C3A	2.05	1.47	1.43

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	502	KLD	C02-N01-C06	8.06	124.10	118.07
4	C	503	KLD	C02-N01-C06	5.21	121.97	118.07
4	B	503	KLD	C21-N21-C22	-4.72	106.16	112.48
4	A	503	KLD	C02-N01-C06	4.54	121.46	118.07
3	C	502	H4B	C2-N1-C8A	4.23	120.83	113.36
3	A	502	H4B	C2-N1-C8A	4.07	120.54	113.36
3	B	502	H4B	C2-N1-C8A	4.04	120.50	113.36
5	A	511	BTB	O8-C8-C7	-3.95	94.93	111.22
4	D	502	KLD	C05-C06-N01	-3.93	118.25	122.73
2	C	501	HEM	CAA-CBA-CGA	-3.92	103.27	113.67
4	B	503	KLD	C02-N01-C06	3.91	121.00	118.07
3	C	509	H4B	C2-N1-C8A	3.85	120.16	113.36
4	B	503	KLD	C14-C13-C12	-3.82	118.86	123.50
4	C	503	KLD	C08-C06-N01	3.46	121.30	116.06
4	D	502	KLD	C08-C06-C05	3.45	126.65	121.65
3	A	502	H4B	C11-C10-C9	-3.43	107.92	112.11
2	C	501	HEM	CBD-CAD-C3D	-3.38	103.18	112.53
4	A	503	KLD	C09-C08-C06	-3.33	105.60	113.01
2	C	501	HEM	C2A-C1A-NA	-3.30	106.49	110.15
4	A	503	KLD	C14-C13-C12	-3.26	119.54	123.50
2	B	501	HEM	CBA-CAA-C2A	-3.20	103.69	112.53
4	D	502	KLD	C14-C13-C12	-3.12	119.70	123.50
5	A	511	BTB	C8-C7-N	-3.12	99.40	111.59
2	A	501	HEM	C3B-C2B-C1B	3.06	108.71	106.41
5	C	504	BTB	O3-C3-C2	-3.06	104.19	111.40
2	B	501	HEM	C4D-ND-C1D	3.06	108.83	105.21
4	C	503	KLD	N02-C02-N01	3.00	121.41	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C2B-C1B	2.92	108.60	106.41
4	D	502	KLD	C11-C12-C13	2.90	121.28	118.75
2	D	501	HEM	C4A-NA-C1A	2.90	110.54	105.82
4	C	503	KLD	C05-C06-N01	-2.85	119.48	122.73
2	A	501	HEM	CAA-CBA-CGA	-2.82	106.20	113.67
4	B	503	KLD	C11-C12-C13	2.80	121.19	118.75
2	B	501	HEM	C3B-C2B-C1B	2.79	108.51	106.41
2	C	501	HEM	C3D-C4D-ND	-2.79	107.11	110.17
4	C	503	KLD	C14-C13-C12	-2.79	120.11	123.50
2	C	501	HEM	C3B-C2B-C1B	2.73	108.46	106.41
3	A	502	H4B	C2-N3-C4	-2.72	120.17	125.11
4	B	503	KLD	C08-C09-C11	-2.72	103.97	113.23
4	C	503	KLD	F23-C23-C24	2.71	112.02	108.89
3	A	502	H4B	O4-C4-C4A	-2.69	120.78	127.26
2	C	501	HEM	C3B-C4B-NB	-2.68	107.54	109.47
2	B	501	HEM	C3D-C4D-ND	-2.67	107.24	110.17
2	D	501	HEM	C1B-NB-C4B	2.65	108.34	105.21
3	B	502	H4B	O4-C4-C4A	-2.65	120.88	127.26
2	D	501	HEM	CBD-CAD-C3D	-2.63	105.25	112.53
4	C	503	KLD	C11-C12-C13	2.63	121.05	118.75
2	B	501	HEM	C2A-C1A-NA	-2.59	107.27	110.15
2	B	501	HEM	CMC-C2C-C1C	-2.58	120.19	124.73
2	A	501	HEM	C1B-NB-C4B	2.56	108.24	105.21
3	C	509	H4B	C4A-C4-N3	2.55	119.13	112.13
4	B	503	KLD	C09-C08-C06	-2.54	107.37	113.01
2	D	501	HEM	C2A-C1A-NA	-2.53	107.34	110.15
2	B	501	HEM	C2D-C1D-ND	-2.53	106.98	109.90
2	B	501	HEM	C1B-NB-C4B	2.51	108.18	105.21
3	B	502	H4B	C4A-C4-N3	2.50	119.00	112.13
2	D	501	HEM	CHC-C1C-NC	2.50	127.17	124.45
3	A	502	H4B	C4A-C4-N3	2.48	118.94	112.13
3	C	509	H4B	O4-C4-C4A	-2.46	121.32	127.26
3	C	502	H4B	C4A-C4-N3	2.46	118.88	112.13
2	A	501	HEM	C2A-C1A-NA	-2.43	107.46	110.15
2	A	501	HEM	C3B-C4B-NB	-2.41	107.74	109.47
4	B	503	KLD	F23-C23-C24	2.40	111.67	108.89
2	B	501	HEM	CHA-C4D-ND	2.40	127.33	124.37
2	B	501	HEM	C4A-NA-C1A	2.39	109.72	105.82
4	A	503	KLD	C05-C06-N01	-2.39	120.01	122.73
2	B	501	HEM	C3B-C4B-NB	-2.39	107.75	109.47
3	A	502	H4B	N2-C2-N3	2.38	121.78	116.76
3	C	509	H4B	C2-N3-C4	-2.38	120.80	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3D-C4D-ND	-2.36	107.58	110.17
2	D	501	HEM	C4C-NC-C1C	2.34	109.63	105.82
3	C	502	H4B	O4-C4-C4A	-2.30	121.72	127.26
4	A	503	KLD	C21-N21-C22	-2.27	109.44	112.48
2	D	501	HEM	C3A-C4A-NA	-2.25	106.53	110.14
3	C	502	H4B	C4-C4A-N5	2.25	122.40	116.27
4	D	502	KLD	C05-C04-C03	2.25	120.61	118.11
2	B	501	HEM	O2A-CGA-CBA	2.24	121.08	114.00
2	B	501	HEM	CHC-C1C-NC	2.22	126.87	124.45
2	B	501	HEM	CHD-C1D-ND	2.21	126.81	124.42
2	C	501	HEM	C4D-ND-C1D	2.21	107.82	105.21
4	C	503	KLD	C21-N21-C22	-2.19	109.55	112.48
5	B	505	BTB	O4-C4-C2	-2.19	106.25	111.40
4	A	503	KLD	C08-C06-N01	2.18	119.37	116.06
2	C	501	HEM	C1B-NB-C4B	2.18	107.79	105.21
2	D	501	HEM	C3B-C4B-NB	-2.18	107.90	109.47
2	D	501	HEM	C4D-ND-C1D	2.17	107.78	105.21
2	B	501	HEM	C4C-NC-C1C	2.15	109.32	105.82
2	A	501	HEM	CBD-CAD-C3D	-2.14	106.61	112.53
2	A	501	HEM	C4D-ND-C1D	2.13	107.73	105.21
3	A	502	H4B	C4-C4A-N5	2.12	122.06	116.27
3	C	509	H4B	C4-C4A-N5	2.11	122.02	116.27
2	C	501	HEM	C4A-NA-C1A	2.07	109.20	105.82
2	B	501	HEM	O1A-CGA-CBA	-2.07	116.54	123.09
4	A	503	KLD	C17-C15-C16	-2.06	117.07	120.54
2	B	501	HEM	CMA-C3A-C4A	-2.05	122.30	125.42
4	A	503	KLD	C11-C12-C13	2.05	120.54	118.75
3	C	502	H4B	N2-C2-N3	2.01	121.01	116.76

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	C	509	H4B	C7-C6-C9-O9
3	C	509	H4B	C7-C6-C9-C10
4	A	503	KLD	C17-C18-C25-N21
4	B	503	KLD	C17-C18-C25-N21
4	D	502	KLD	C17-C18-C25-N21

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Mol	Chain	Res	Type	Atoms
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	C4-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	O1-C1-C2-C3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	506	BTB	C1-C2-C3-O3
5	A	511	BTB	O1-C1-C2-C3
5	A	511	BTB	O1-C1-C2-C4
5	A	511	BTB	O1-C1-C2-N
5	A	511	BTB	C1-C2-C3-O3
5	A	511	BTB	C4-C2-C3-O3
5	A	511	BTB	N-C2-C3-O3
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-N
5	B	509	BTB	C1-C2-C3-O3
5	B	509	BTB	C4-C2-C3-O3
5	B	509	BTB	N-C2-C3-O3
5	B	509	BTB	C1-C2-C4-O4
5	B	509	BTB	C3-C2-C4-O4
5	B	509	BTB	N-C2-C4-O4
5	B	509	BTB	C1-C2-N-C5
5	B	509	BTB	C1-C2-N-C7
5	B	509	BTB	C3-C2-N-C7
5	B	509	BTB	C4-C2-N-C7
5	B	509	BTB	C8-C7-N-C5
5	C	504	BTB	C1-C2-N-C5
5	C	504	BTB	C1-C2-N-C7
5	C	504	BTB	C3-C2-N-C5
5	C	504	BTB	C3-C2-N-C7
5	C	504	BTB	C4-C2-N-C5
5	C	504	BTB	C4-C2-N-C7
5	C	505	BTB	C1-C2-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	D	503	BTB	O1-C1-C2-C3
5	D	503	BTB	O1-C1-C2-C4
5	D	503	BTB	O1-C1-C2-N
5	D	503	BTB	C1-C2-C4-O4
5	D	503	BTB	C3-C2-C4-O4
5	D	503	BTB	N-C2-C4-O4
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-C3-O3
5	D	504	BTB	C4-C2-C3-O3
5	D	504	BTB	N-C2-C3-O3
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C1-C2-N-C7
5	D	504	BTB	C3-C2-N-C5
5	D	504	BTB	C3-C2-N-C7
5	D	504	BTB	C4-C2-N-C5
5	D	504	BTB	C4-C2-N-C7
5	D	504	BTB	C8-C7-N-C5
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C5
7	A	508	GOL	O1-C1-C2-C3
7	C	507	GOL	O1-C1-C2-C3
7	C	507	GOL	C1-C2-C3-O3
5	D	503	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
5	A	511	BTB	N-C5-C6-O6
5	B	509	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
5	C	504	BTB	N-C5-C6-O6
5	B	506	BTB	N-C7-C8-O8
5	D	504	BTB	N-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	511	BTB	N-C7-C8-O8
7	A	508	GOL	O1-C1-C2-O2
7	C	507	GOL	O1-C1-C2-O2
4	C	503	KLD	C15-C17-C18-C25
2	B	501	HEM	C2A-CAA-CBA-CGA
5	A	506	BTB	N-C5-C6-O6
7	C	507	GOL	O2-C2-C3-O3
5	B	504	BTB	O1-C1-C2-C3
7	A	508	GOL	O2-C2-C3-O3
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
3	B	502	H4B	N5-C6-C9-O9
3	C	509	H4B	N5-C6-C9-O9
5	A	506	BTB	C1-C2-N-C5
5	A	506	BTB	C1-C2-N-C7
5	A	506	BTB	C3-C2-N-C5
5	A	506	BTB	C4-C2-N-C7
5	A	511	BTB	C4-C2-N-C7
5	B	509	BTB	C3-C2-N-C5
5	B	509	BTB	C4-C2-N-C5
5	D	503	BTB	C1-C2-N-C5
5	D	503	BTB	C3-C2-N-C5
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C7
4	A	503	KLD	C17-C18-C25-C24
4	B	503	KLD	C17-C18-C25-C24
4	D	502	KLD	C17-C18-C25-C24
3	C	502	H4B	C7-C6-C9-C10
5	A	505	BTB	N-C7-C8-O8
5	B	505	BTB	C3-C2-C4-O4
5	B	506	BTB	O1-C1-C2-C4
4	D	502	KLD	C08-C09-C11-C12
4	A	503	KLD	C14-C15-C17-C18
4	D	502	KLD	C08-C09-C11-C16
4	A	503	KLD	C16-C15-C17-C18
3	C	502	H4B	C7-C6-C9-O9
4	B	503	KLD	C14-C15-C17-C18
4	D	502	KLD	C14-C15-C17-C18
2	B	501	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	D	502	KLD	C16-C15-C17-C18
4	B	503	KLD	C15-C17-C18-C25
5	D	503	BTB	N-C7-C8-O8
4	B	503	KLD	C16-C15-C17-C18
2	B	501	HEM	CAA-CBA-CGA-O1A
4	C	503	KLD	C16-C15-C17-C18
4	C	503	KLD	C14-C15-C17-C18
2	D	501	HEM	C2A-CAA-CBA-CGA
3	A	502	H4B	N5-C6-C9-O9
3	C	502	H4B	N5-C6-C9-O9
5	A	504	BTB	N-C2-C3-O3
5	A	506	BTB	N-C2-C3-O3
5	A	506	BTB	C3-C2-N-C7
5	A	506	BTB	C4-C2-N-C5
5	A	511	BTB	C3-C2-N-C7
5	D	503	BTB	C4-C2-N-C5
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	C4-C2-N-C5

There are no ring outliers.

22 monomers are involved in 55 short contacts:

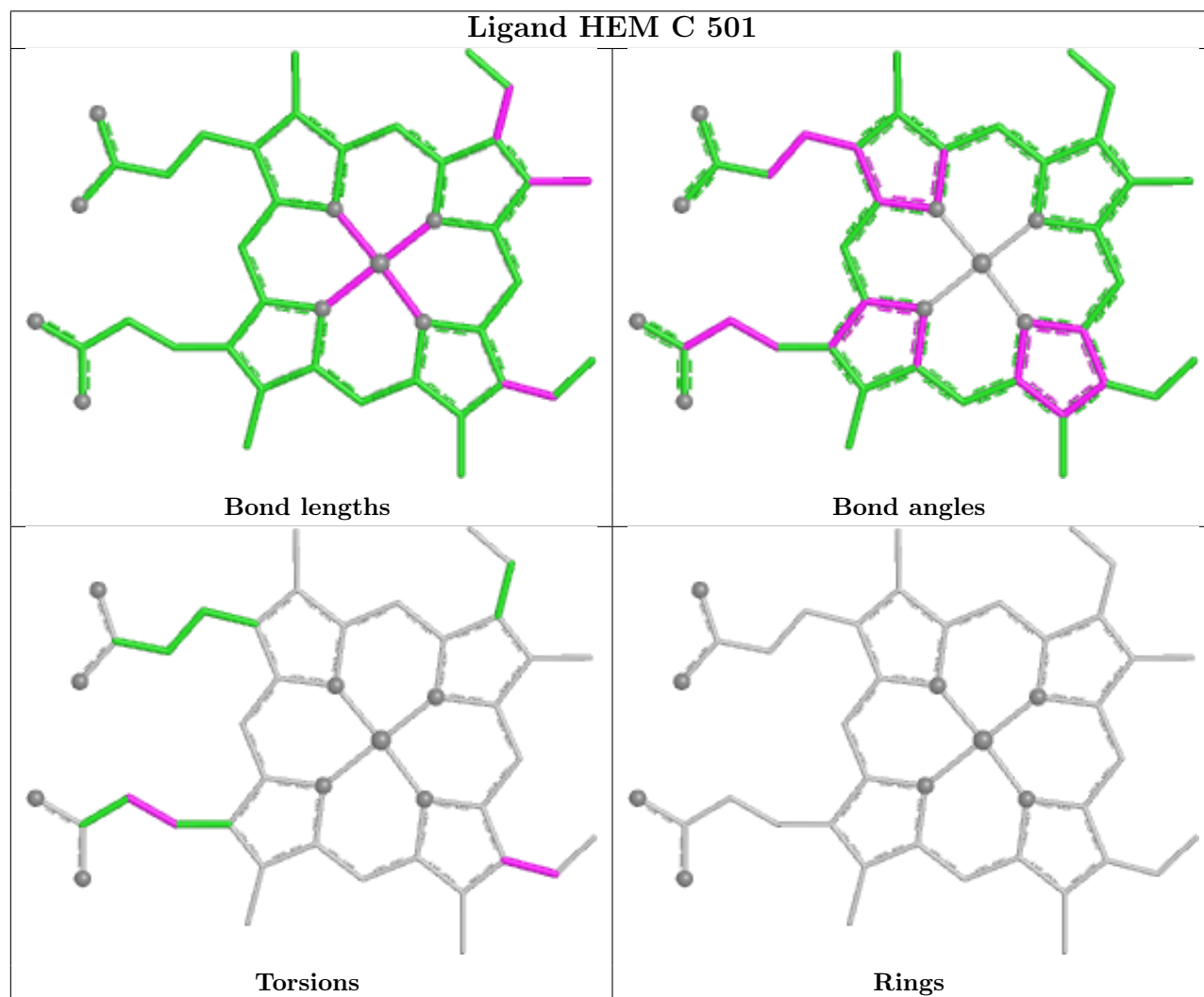
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	5	0
5	B	505	BTB	4	1
5	C	505	BTB	3	0
5	B	506	BTB	3	0
4	A	503	KLD	2	0
5	A	511	BTB	3	0
5	D	503	BTB	2	0
3	A	502	H4B	2	0
4	B	503	KLD	1	0
2	B	501	HEM	6	0
5	B	509	BTB	4	0
2	A	501	HEM	5	0
2	D	501	HEM	3	0
5	D	504	BTB	4	0
5	A	505	BTB	2	0
5	B	504	BTB	1	0
5	A	506	BTB	2	0
5	D	505	BTB	1	0
4	C	503	KLD	2	0

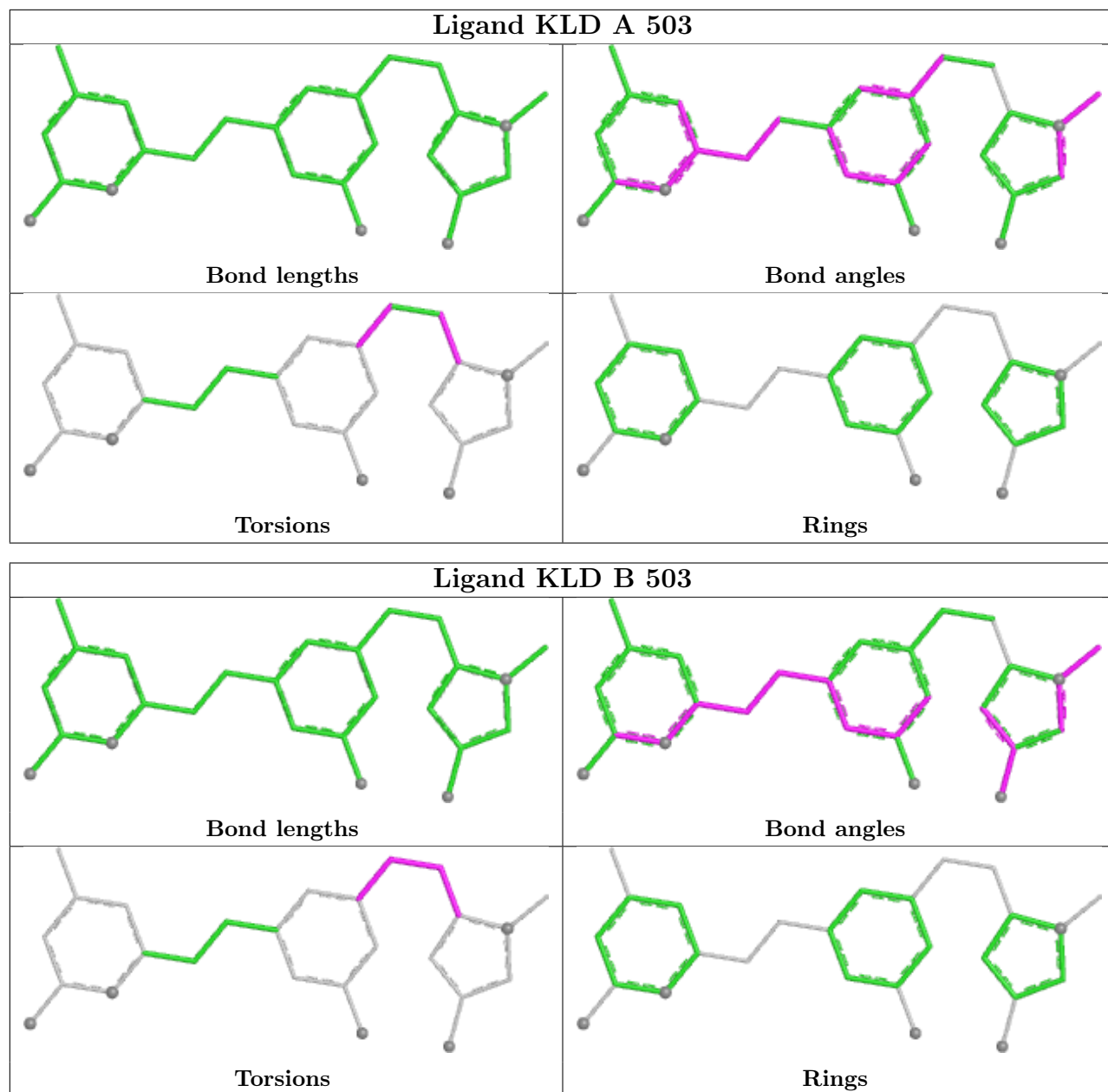
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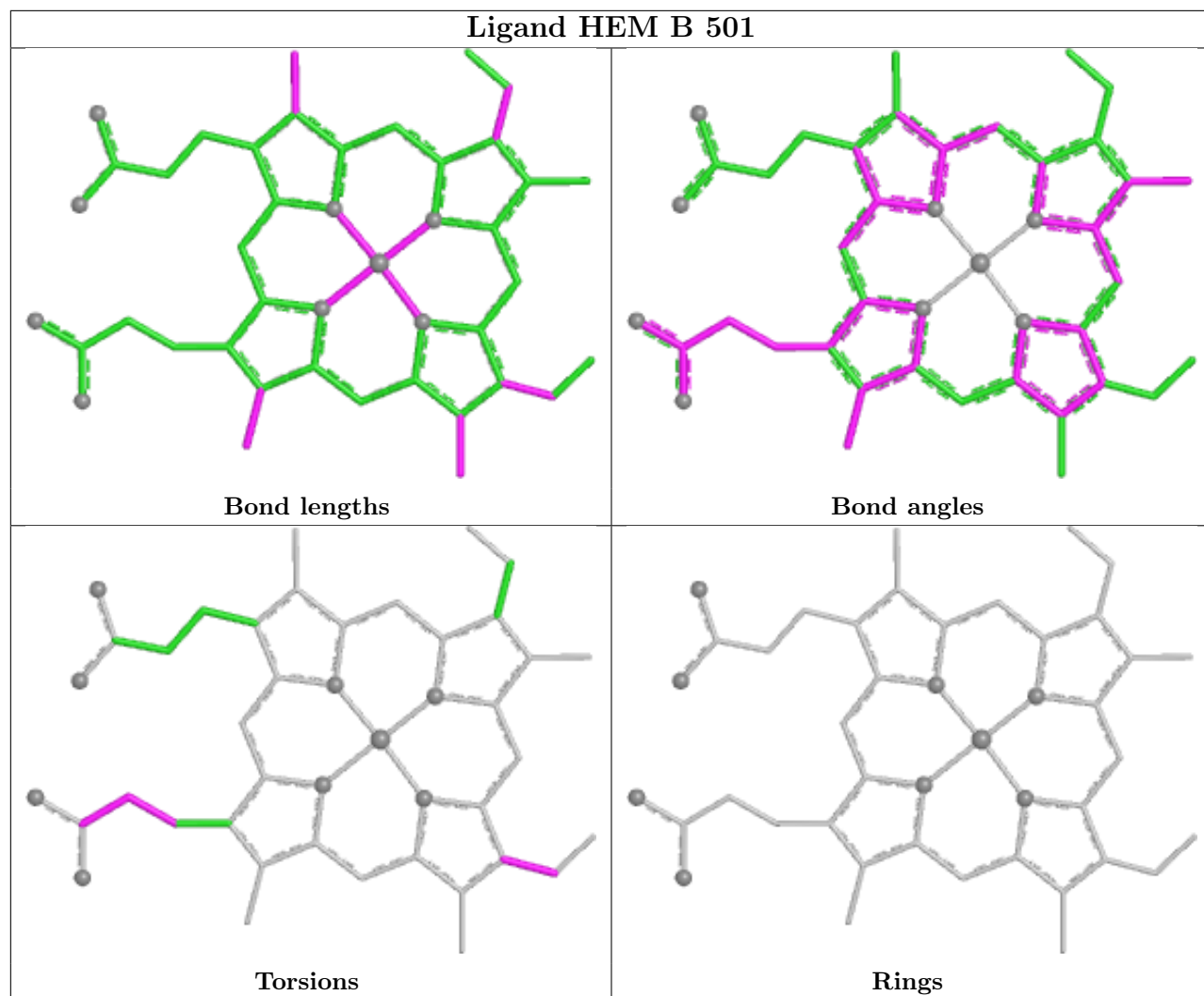
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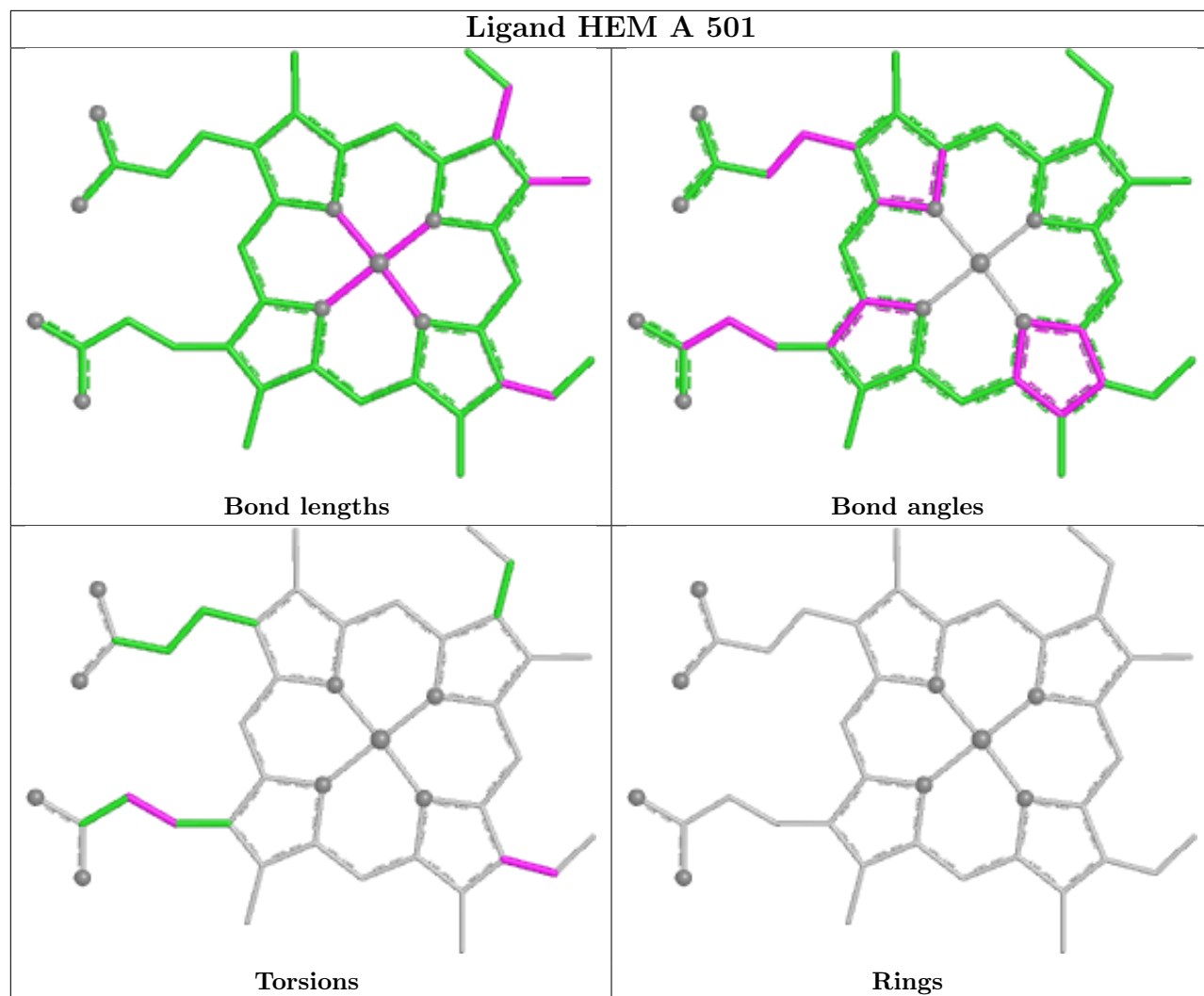
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	2	0
3	B	502	H4B	1	0
3	C	502	H4B	2	0

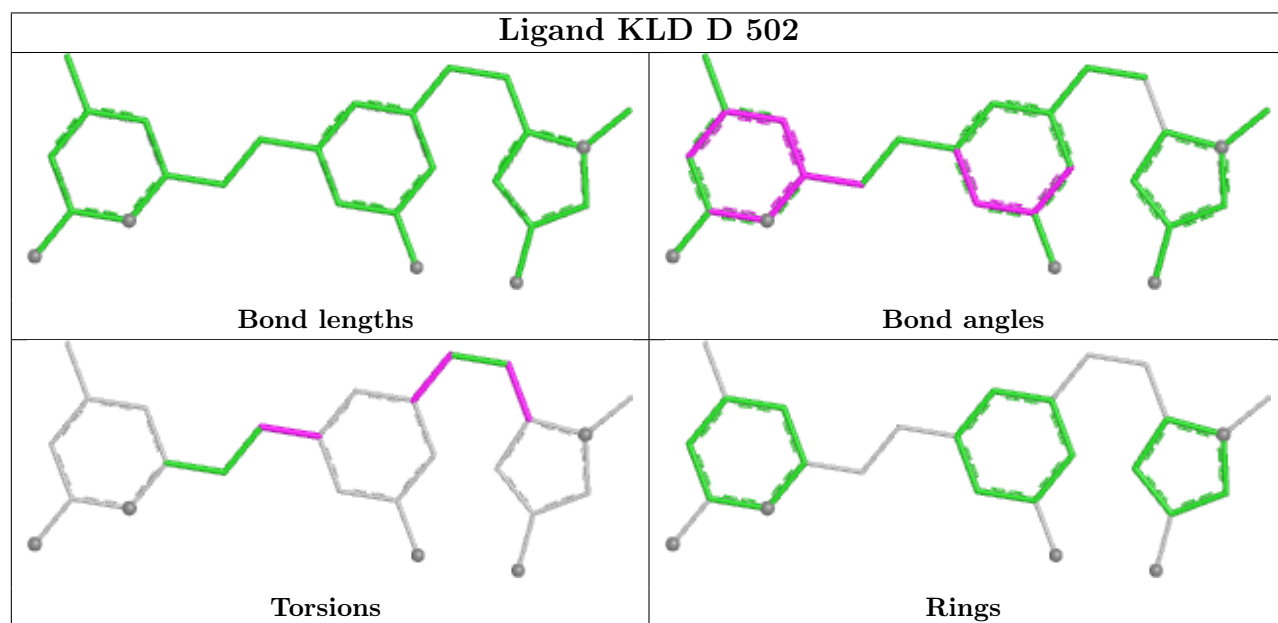
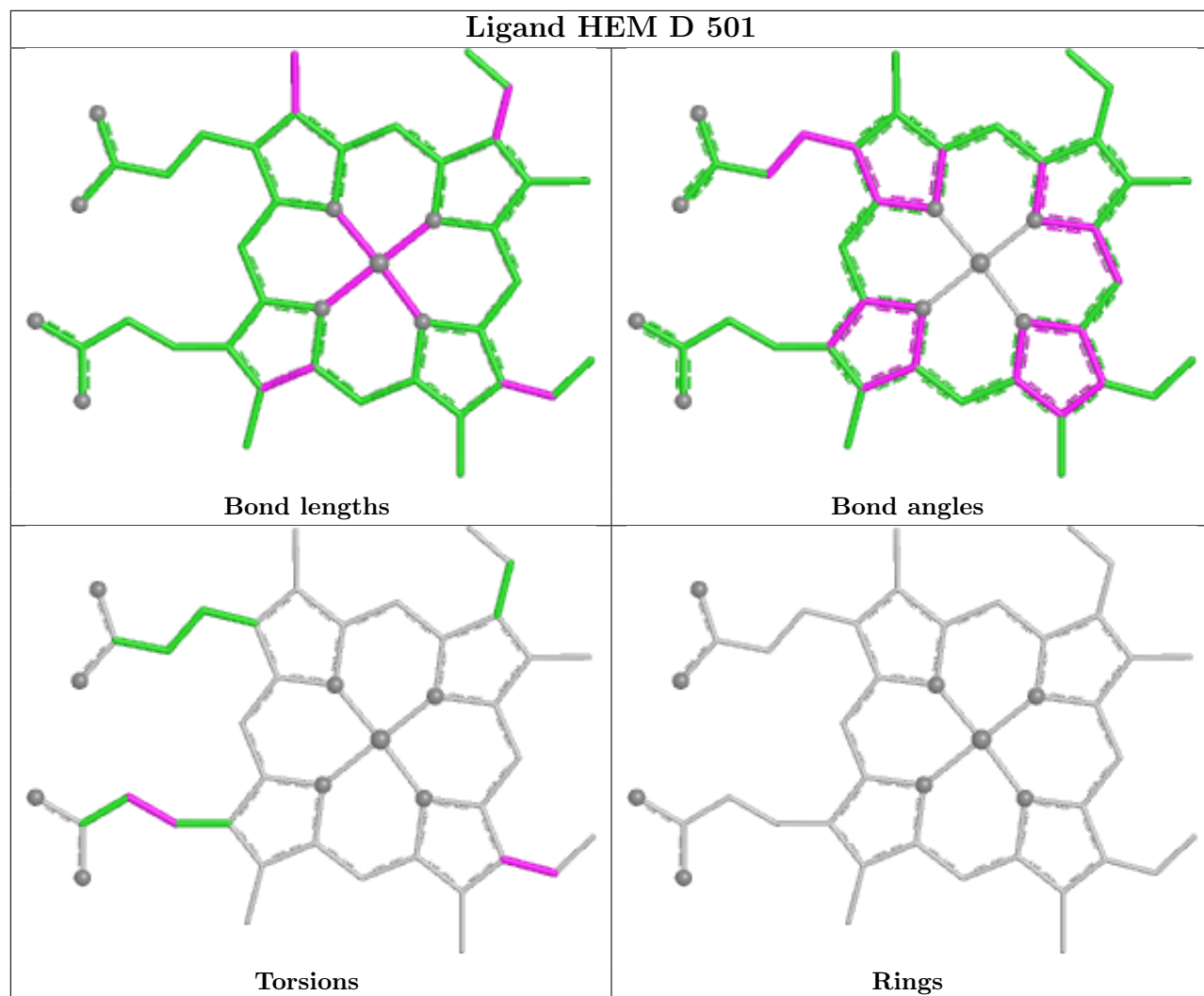
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

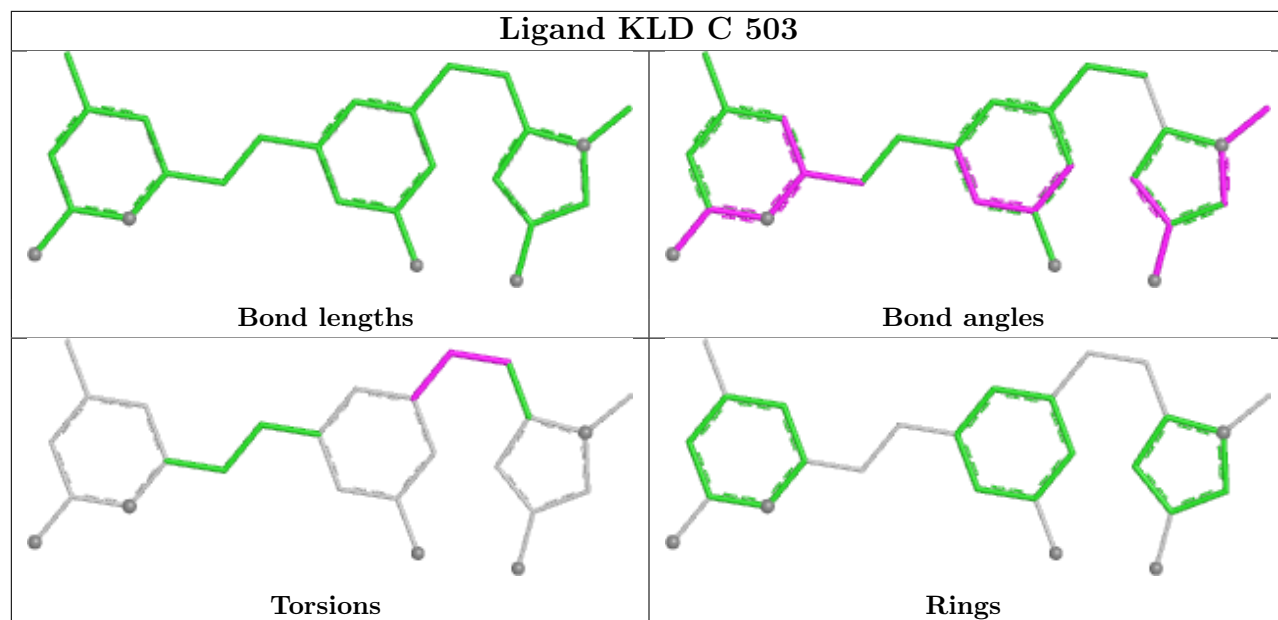












5.7 Other polymers [i](#)

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%)	0.72	43 (10%) 11 13	25, 62, 116, 143	2 (0%)
1	B	404/440 (91%)	0.06	6 (1%) 72 78	24, 42, 79, 117	3 (0%)
1	C	402/440 (91%)	0.47	18 (4%) 38 44	27, 56, 97, 118	1 (0%)
1	D	403/440 (91%)	0.01	5 (1%) 76 82	22, 40, 69, 109	3 (0%)
All	All	1613/1760 (91%)	0.32	72 (4%) 38 44	22, 48, 99, 143	9 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	4.6
1	A	145	ALA	4.1
1	D	119	ALA	4.1
1	A	257	GLN	3.9
1	C	237	GLY	3.2
1	A	480	TRP	3.2
1	A	119	ALA	3.1
1	C	119	ALA	3.1
1	C	155	ALA	3.1
1	C	106	PRO	3.1
1	A	124	LEU	2.9
1	A	129	ASP	2.8
1	A	237	GLY	2.8
1	B	138	ILE	2.7
1	A	236	PRO	2.7
1	A	158	ALA	2.7
1	A	106	PRO	2.7
1	A	155	ALA	2.7
1	A	142	GLY	2.7
1	A	157	VAL	2.7
1	A	254	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	468	PHE	2.6
1	A	143	SER	2.6
1	A	150	LEU	2.6
1	C	239	GLY	2.6
1	A	304	LEU	2.6
1	A	204	ALA	2.6
1	A	244	TRP	2.6
1	B	259	GLY	2.6
1	A	153	VAL	2.5
1	C	68	PHE	2.5
1	C	309	LEU	2.5
1	A	348	PHE	2.5
1	A	109	LEU	2.4
1	C	280	THR	2.4
1	A	479	PRO	2.4
1	C	257	GLN	2.4
1	C	304	LEU	2.4
1	C	238	ARG	2.3
1	C	158	ALA	2.3
1	A	299	PRO	2.3
1	A	268	VAL	2.3
1	A	279	TRP	2.3
1	A	295	ALA	2.3
1	C	159	ALA	2.3
1	A	144	GLN	2.3
1	D	257	GLN	2.3
1	A	309	LEU	2.3
1	A	275	ILE	2.2
1	D	108	LYS	2.2
1	A	131	ILE	2.2
1	C	160	THR	2.2
1	A	293	LEU	2.2
1	A	107	ARG	2.2
1	A	68	PHE	2.1
1	A	343	ILE	2.1
1	B	369	ASP	2.1
1	A	90	GLN	2.1
1	A	105	PHE	2.1
1	A	163	TYR	2.1
1	C	79	ILE	2.1
1	A	161	GLY	2.1
1	C	300	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	119	ALA	2.1
1	B	107	ARG	2.1
1	C	468	PHE	2.0
1	B	89	GLN	2.0
1	A	235	CYS	2.0
1	D	258	ASP	2.0
1	A	256	GLN	2.0
1	A	277	HIS	2.0
1	C	475	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	D	505	14/14	0.67	0.16	74,82,95,96	0
5	BTB	C	505	14/14	0.70	0.15	79,110,121,124	0
5	BTB	A	506	14/14	0.70	0.15	104,115,128,130	0
5	BTB	A	504	14/14	0.72	0.27	97,107,111,112	0
5	BTB	C	504	14/14	0.74	0.27	80,106,136,143	0
5	BTB	D	504	14/14	0.76	0.16	60,75,87,89	0
5	BTB	B	506	14/14	0.76	0.14	85,111,117,118	0
6	ZN	A	510	1/1	0.76	0.25	140,140,140,140	0
5	BTB	B	505	14/14	0.77	0.15	42,62,74,80	0
5	BTB	B	509	14/14	0.80	0.20	39,67,82,87	0
5	BTB	A	505	14/14	0.80	0.15	60,72,81,85	0
4	KLD	A	503	26/26	0.83	0.19	36,105,115,116	0
3	H4B	C	502	17/17	0.84	0.15	56,70,78,80	0
4	KLD	C	503	26/26	0.85	0.18	36,79,110,112	0

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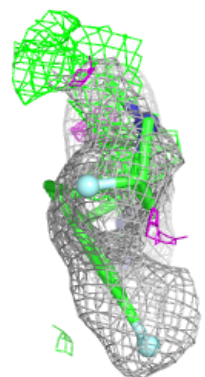
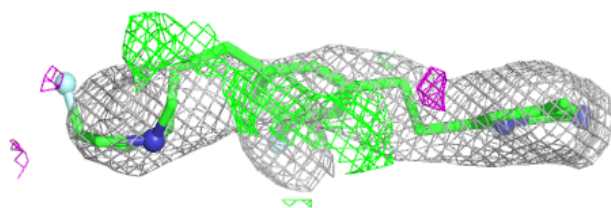
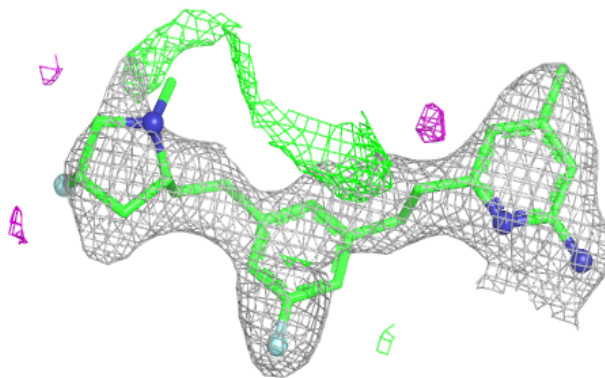
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	H4B	A	502	17/17	0.85	0.16	81,89,98,100	0
5	BTB	D	503	14/14	0.87	0.13	40,66,79,81	0
3	H4B	B	502	17/17	0.87	0.12	47,58,76,83	0
7	GOL	C	507	6/6	0.88	0.10	50,64,73,75	0
3	H4B	C	509	17/17	0.89	0.13	45,67,80,82	0
5	BTB	A	511	14/14	0.89	0.23	10,74,105,106	0
7	GOL	A	508	6/6	0.90	0.09	49,65,78,78	0
4	KLD	B	503	26/26	0.90	0.15	27,81,105,110	0
6	ZN	C	510	1/1	0.91	0.08	37,37,37,37	1
5	BTB	B	504	14/14	0.91	0.12	46,57,78,83	0
4	KLD	D	502	26/26	0.91	0.15	23,73,105,113	0
8	CL	A	509	1/1	0.91	0.13	67,67,67,67	0
2	HEM	A	501	43/43	0.96	0.10	37,58,87,110	0
2	HEM	C	501	43/43	0.97	0.09	27,41,74,101	0
9	GD	D	506	1/1	0.97	0.06	50,50,50,50	0
2	HEM	B	501	43/43	0.98	0.07	19,30,69,96	0
8	CL	B	507	1/1	0.98	0.10	38,38,38,38	0
8	CL	C	508	1/1	0.98	0.10	52,52,52,52	0
9	GD	B	508	1/1	0.98	0.04	44,44,44,44	0
6	ZN	A	507	1/1	0.98	0.03	41,41,41,41	0
2	HEM	D	501	43/43	0.99	0.07	22,29,72,99	0
8	CL	D	507	1/1	0.99	0.06	38,38,38,38	0
6	ZN	C	506	1/1	1.00	0.02	35,35,35,35	0

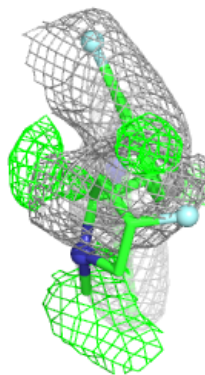
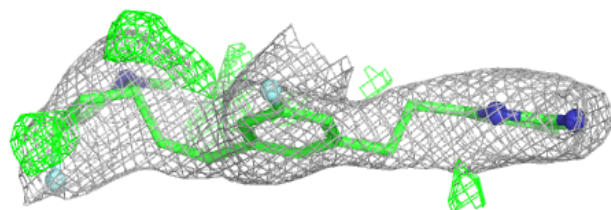
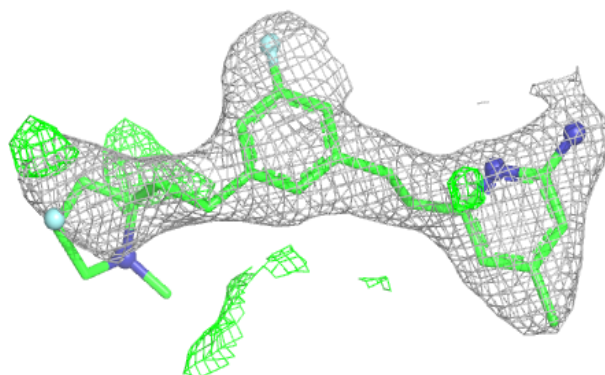
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KLD A 503:

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

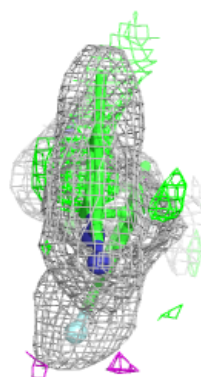
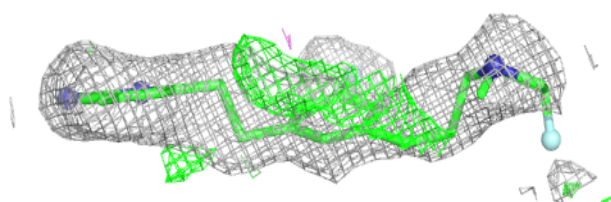
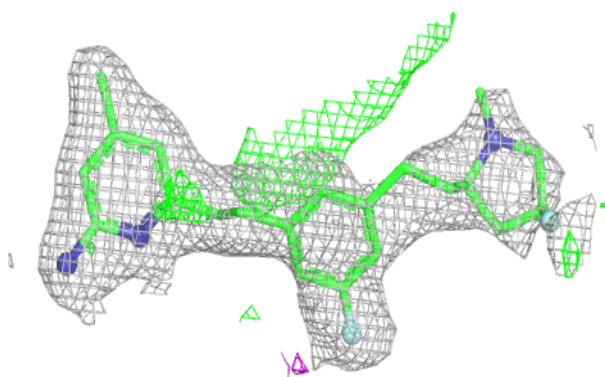
**Electron density around KLD C 503:**

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

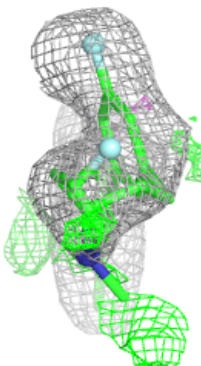
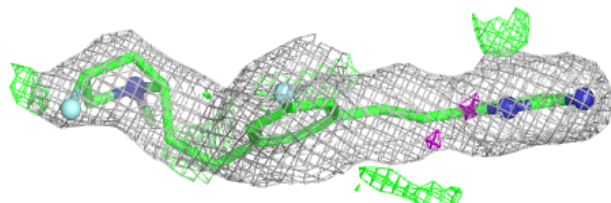
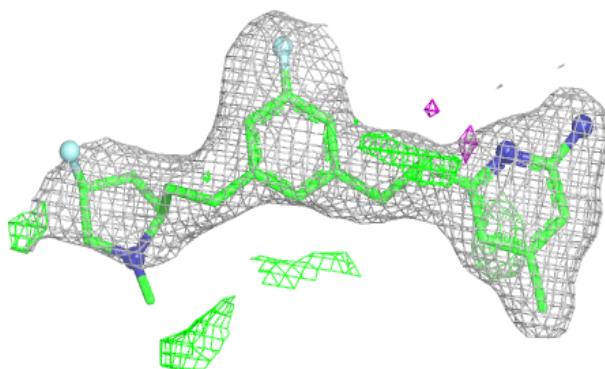


Electron density around KLD B 503:

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

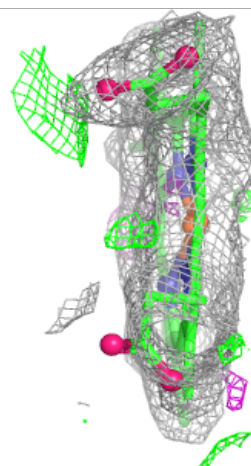
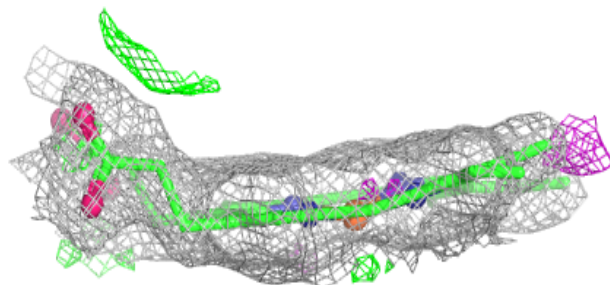
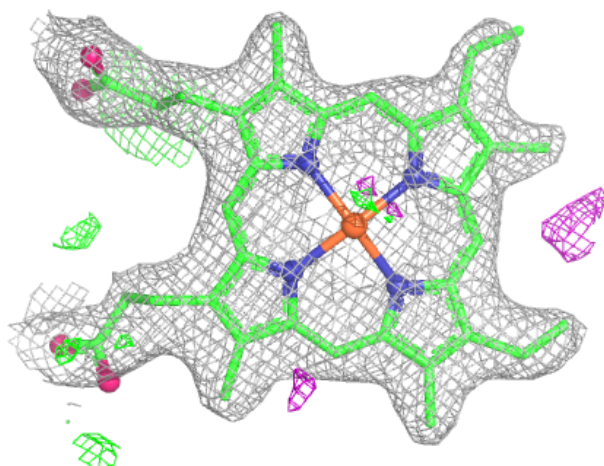
**Electron density around KLD D 502:**

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



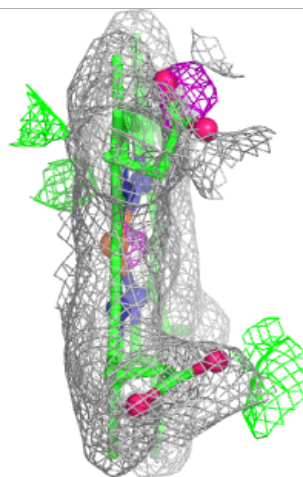
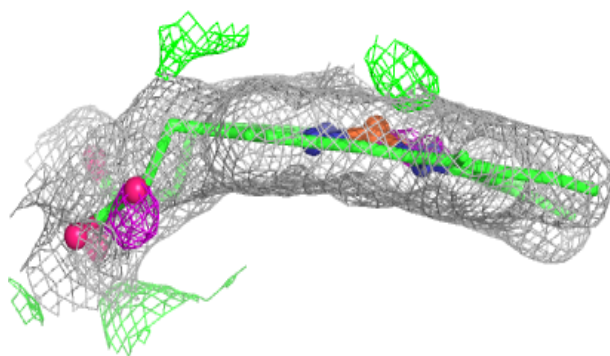
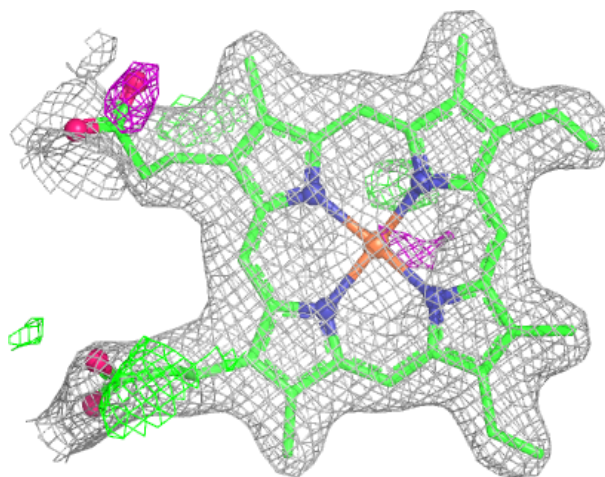
Electron density around HEM A 501:

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



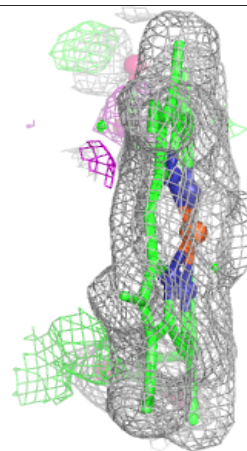
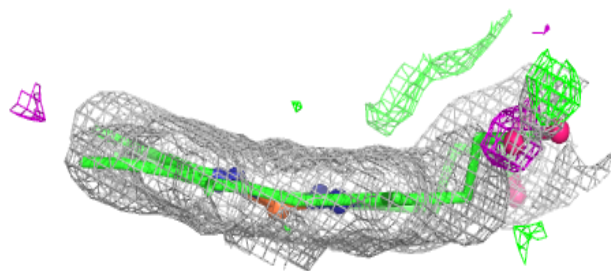
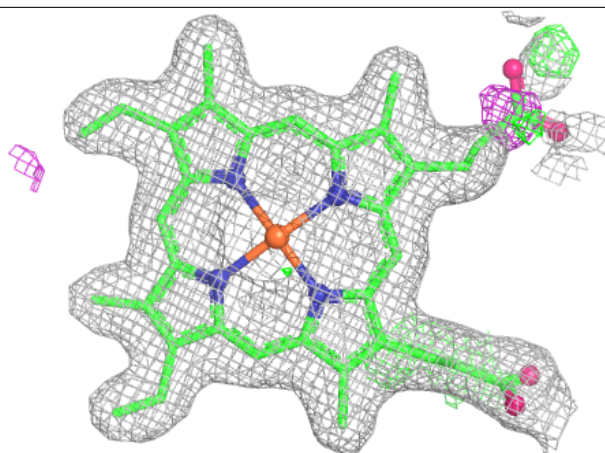
Electron density around HEM C 501:

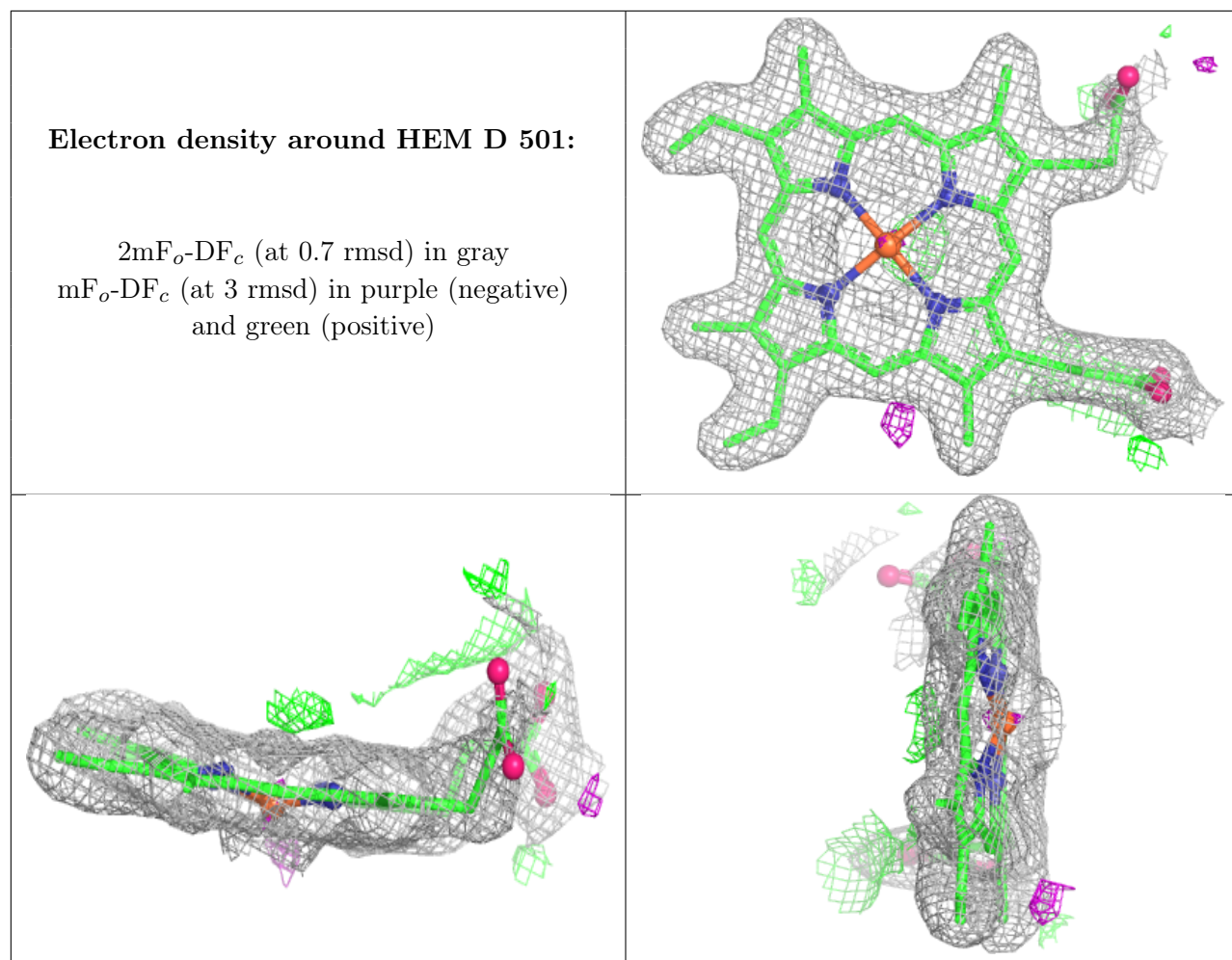
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 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.