



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:41 AM UTC

PDB ID : 6NH4 / pdb_00006nh4
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-fluoro-5-(2-((2R,4S)-4-fluoropyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine
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Deposited on : 2018-12-21
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

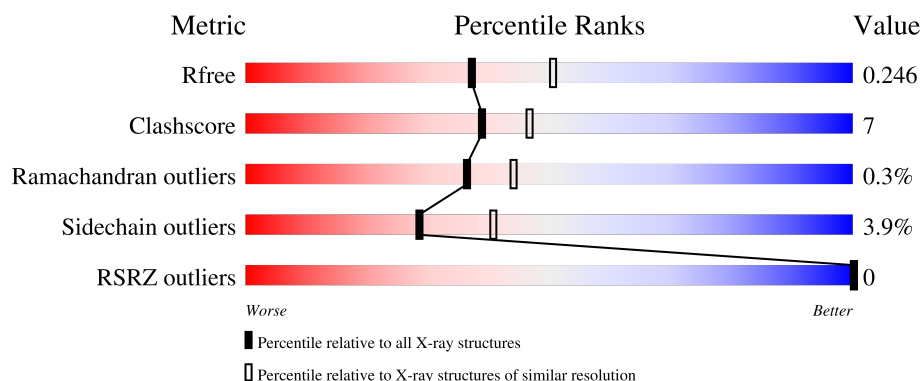
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	 72% 18% • 8%
1	B	440	 80% 11% 9%
1	C	440	 77% 13% • 9%
1	D	440	 77% 15% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	C	511	-	-	X	-

2 Entry composition [i](#)

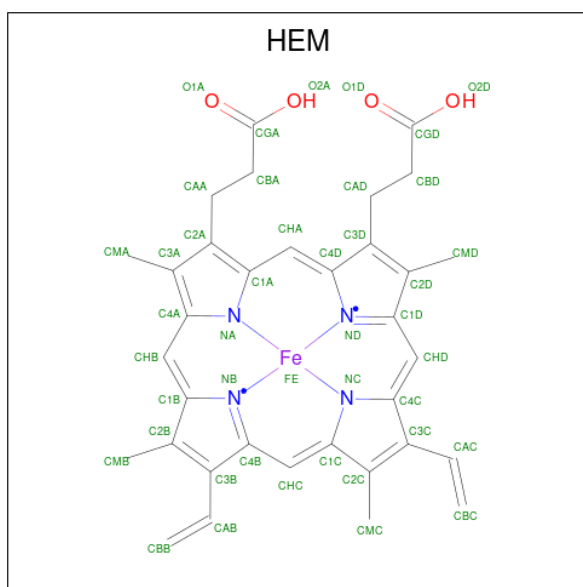
There are 10 unique types of molecules in this entry. The entry contains 14013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothelial nitric oxide synthase splice variant eNOS13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	404	Total	C	N	O	S	0	3	0
			3241	2063	572	589	17			

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



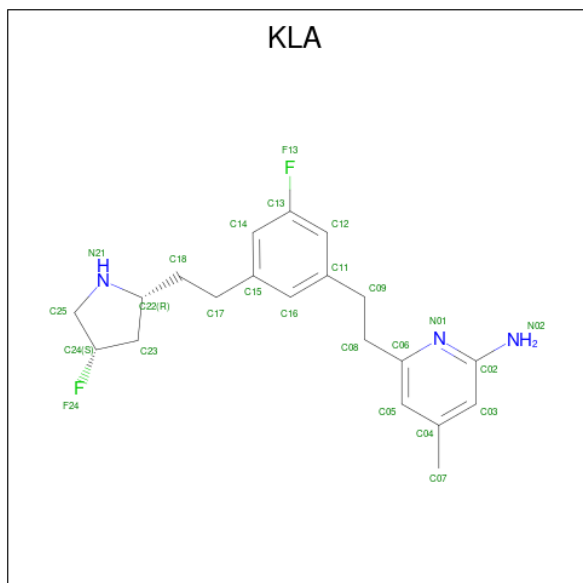
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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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 6-[2-(3-fluoro-5-{2-[(2R,4S)-4-fluoropyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (CCD ID: KLA) (formula: $C_{20}H_{25}F_2N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			25	20	2	3		
3	A	1	Total	C	F	N	0	0
			25	20	2	3		
3	B	1	Total	C	F	N	0	0
			25	20	2	3		
3	C	1	Total	C	F	N	0	0
			25	20	2	3		
3	D	1	Total	C	F	N	0	0
			25	20	2	3		
3	D	1	Total	C	F	N	0	0
			25	20	2	3		

- Molecule 4 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
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	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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	C	3	Total	Zn	0	0
			3	3		

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

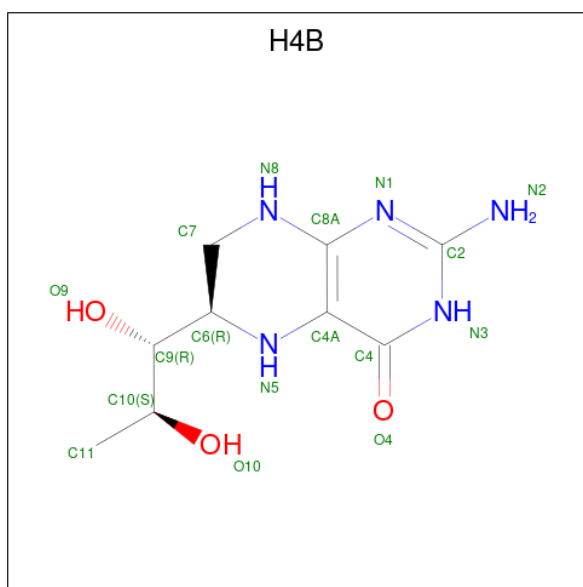


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	2	Total	Cl	0	0
			2	2		
7	C	3	Total	Cl	0	0
			3	3		
7	D	1	Total	Cl	0	0
			1	1		

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



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

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

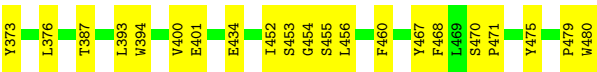
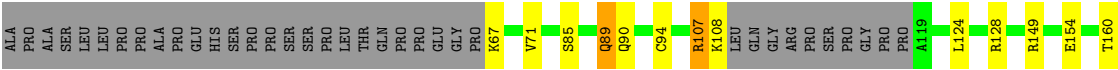
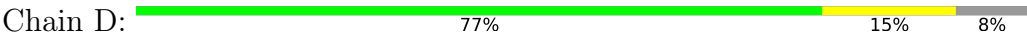
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Gd	0	0
			1	1		
9	C	2	Total	Gd	0	0
			2	2		
9	D	1	Total	Gd	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	114	Total	O	0	0
			114	114		
10	B	174	Total	O	0	0
			174	174		
10	C	145	Total	O	0	0
			145	145		
10	D	175	Total	O	0	0
			175	175		



● 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	59.71Å 152.55Å 109.14Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	39.98 – 2.27 39.98 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.3 (39.98-2.27) 94.3 (39.98-2.27)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.192 , 0.251 0.186 , 0.246	Depositor DCC
R_{free} test set	4242 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14013	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: CL, GD, GOL, BTB, HEM, H4B, ZN, KLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3335	0.52	0/4543
1	B	0.36	0/3319	0.55	0/4523
1	C	0.33	0/3307	0.52	0/4507
1	D	0.37	0/3339	0.57	0/4548
All	All	0.34	0/13300	0.54	0/18121

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	D	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	D	89	GLN	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	49	1
1	B	3221	0	3126	31	0
1	C	3209	0	3108	38	0
1	D	3241	0	3152	44	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
3	A	50	0	0	1	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	50	0	0	0	0
4	A	28	0	36	6	0
4	B	42	0	56	8	0
4	C	14	0	19	1	0
4	D	28	0	36	6	1
5	A	3	0	0	0	0
5	C	3	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	2	0	0	1	0
7	C	3	0	0	2	0
7	D	1	0	0	0	0
8	B	17	0	15	1	0
8	C	17	0	15	1	0
9	B	1	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
10	A	114	0	0	7	0
10	B	174	0	0	6	0
10	C	145	0	0	6	0
10	D	175	0	0	4	0
All	All	14013	0	12845	179	1

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 7.

All (179) 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:D:365:ARG:NH1	2:D:501:HEM:O2A	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLU:OE2	4:D:504:BTB:O4	1.99	0.79
1:C:365:ARG:NH1	2:C:502:HEM:O2A	2.18	0.77
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.67	0.76
4:A:503:BTB:O8	1:C:257:GLN:OE1	2.04	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.73	0.70
1:C:68:PHE:N	10:C:602:HOH:O	2.23	0.70
1:A:148:GLN:NE2	10:A:603:HOH:O	2.25	0.69
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.75	0.68
1:A:201:CYS:O	1:A:202:ARG:NH1	2.25	0.68
1:A:242:ARG:HD3	1:A:479:PRO:HB3	1.75	0.67
1:A:238:ARG:NH1	10:A:604:HOH:O	2.26	0.67
1:A:86:ALA:O	1:B:97:ARG:NH2	2.28	0.66
1:D:107:ARG:HH12	1:D:475:TYR:HB2	1.60	0.66
1:A:365:ARG:NH1	2:A:501:HEM:O2A	2.30	0.65
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.78	0.65
1:C:384:ASP:HB3	7:C:511:CL:CL	2.34	0.65
1:A:258:ASP:N	1:A:258:ASP:OD1	2.30	0.63
2:A:501:HEM:CGA	8:B:501:H4B:HN22	2.12	0.63
1:C:347:GLU:OE2	10:C:601:HOH:O	2.16	0.63
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.81	0.62
1:A:361:GLU:OE2	3:A:502:KLA:N02	2.33	0.61
1:B:397:LYS:NZ	10:B:601:HOH:O	2.18	0.61
1:A:221:ARG:NH2	10:A:605:HOH:O	2.33	0.60
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.33	0.60
2:C:502:HEM:HBB2	2:C:502:HEM:HHC	1.84	0.60
1:B:361:GLU:HB3	1:B:365:ARG:NH2	2.18	0.59
1:C:200:ASP:OD1	1:C:200:ASP:N	2.36	0.59
2:C:502:HEM:HMC2	2:C:502:HEM:HBC2	1.85	0.58
1:A:128:ARG:O	1:A:132:ASN:ND2	2.36	0.58
1:B:285:ARG:NH2	10:B:608:HOH:O	2.34	0.57
2:B:502:HEM:HBC2	2:B:502:HEM:HMC2	1.85	0.57
1:C:364:THR:O	1:C:368:CYS:HB2	2.04	0.57
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.37	0.57
1:C:149:ARG:NE	1:C:169:GLU:OE2	2.37	0.57
1:A:321:GLU:H	1:A:321:GLU:CD	2.14	0.56
4:A:503:BTB:O3	4:A:503:BTB:O4	2.18	0.56
1:B:90:GLN:HB2	1:B:468:PHE:CD1	2.40	0.56
1:A:340:LEU:HD21	1:A:347:GLU:HG2	1.86	0.56
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.42	0.55
4:A:504:BTB:O3	4:A:504:BTB:O1	2.18	0.55
1:D:271:THR:O	1:D:275:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:NH2	10:B:605:HOH:O	2.30	0.54
1:A:207:MET:HE3	1:A:293:LEU:HB3	1.90	0.53
1:B:106:PRO:O	10:B:602:HOH:O	2.19	0.53
7:B:509:CL:CL	7:C:511:CL:CL	3.00	0.53
1:C:376:LEU:HB2	10:C:630:HOH:O	2.09	0.53
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.91	0.53
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.44	0.52
1:D:107:ARG:NH1	10:D:611:HOH:O	2.42	0.52
1:A:378:ASP:OD1	10:A:601:HOH:O	2.19	0.52
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.40	0.52
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.92	0.52
1:B:298:GLU:HG2	10:B:709:HOH:O	2.10	0.52
1:B:70:ARG:NE	10:B:612:HOH:O	2.42	0.51
1:B:298:GLU:OE2	4:B:505:BTB:N	2.44	0.51
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.93	0.51
1:D:211:ILE:O	1:D:215:ILE:HG13	2.11	0.51
1:A:183:ARG:HG2	1:A:447:TRP:CG	2.46	0.51
1:A:244:TRP:CH2	1:A:300:PRO:HG3	2.46	0.50
1:B:361:GLU:HB3	1:B:365:ARG:HH22	1.76	0.50
1:C:279:TRP:HB2	1:C:302:LEU:HD21	1.94	0.50
1:D:220:ASN:O	1:D:221:ARG:HG2	2.11	0.50
1:A:388:ARG:HG2	4:A:503:BTB:H82	1.93	0.50
1:C:90:GLN:NE2	10:C:610:HOH:O	2.39	0.50
1:D:434:GLU:OE1	10:D:602:HOH:O	2.20	0.50
1:C:455:SER:HA	1:C:460:PHE:CG	2.46	0.49
1:D:67:LYS:NZ	10:D:614:HOH:O	2.45	0.49
1:C:397:LYS:HG3	1:D:400:VAL:HG11	1.94	0.49
1:A:100:LEU:HB3	1:A:103:LEU:HD22	1.94	0.49
1:B:321:GLU:OE1	4:B:504:BTB:H82	2.12	0.49
1:C:257:GLN:HA	10:C:685:HOH:O	2.12	0.49
1:B:358:MET:HE3	1:B:360:THR:OG1	2.13	0.48
1:C:160:THR:HG23	1:C:162:THR:H	1.78	0.48
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.95	0.48
4:D:505:BTB:H32	4:D:505:BTB:H51	1.41	0.48
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.53	0.48
1:B:298:GLU:CD	4:B:505:BTB:H31	2.39	0.48
1:B:298:GLU:OE1	4:B:505:BTB:H31	2.13	0.48
1:D:455:SER:HA	1:D:460:PHE:CG	2.49	0.48
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.95	0.48
1:D:128:ARG:NH2	1:D:154:GLU:OE2	2.46	0.48
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.49	0.47
1:B:165:LEU:HG	1:B:346:LEU:HD12	1.96	0.47
1:C:263:GLY:O	1:C:265:PRO:HD3	2.14	0.47
1:D:342:GLU:OE2	10:D:603:HOH:O	2.20	0.47
2:B:502:HEM:HH3	2:B:502:HEM:HBB2	1.96	0.47
1:D:339:MET:HE3	1:D:475:TYR:CD1	2.50	0.47
1:A:122:GLN:O	1:A:126:GLN:HG3	2.15	0.47
1:A:290:PRO:HB2	1:A:302:LEU:HD22	1.97	0.47
1:C:219:THR:HA	1:C:224:LEU:HD23	1.97	0.46
2:C:502:HEM:CGA	8:C:503:H4B:HN22	2.28	0.46
1:D:387:THR:HA	1:D:394:TRP:CD1	2.50	0.46
1:B:85:SER:HB3	1:B:467:TYR:CE1	2.51	0.46
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.98	0.46
4:D:504:BTB:H32	4:D:504:BTB:H51	1.61	0.46
4:C:505:BTB:HO6	4:C:505:BTB:HO8	1.56	0.46
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.97	0.46
1:D:364:THR:HG21	1:D:452:ILE:HG23	1.97	0.46
1:A:231:PHE:HB3	1:A:232:PRO:CD	2.45	0.46
1:A:361:GLU:HG2	1:A:365:ARG:HH12	1.81	0.45
1:C:429:LYS:HD2	1:C:429:LYS:HA	1.82	0.45
4:B:505:BTB:O3	4:B:505:BTB:H51	2.15	0.45
1:A:109:LEU:H	1:A:109:LEU:HG	1.25	0.45
1:A:229:THR:O	1:A:352:PRO:HD2	2.16	0.45
4:D:505:BTB:H81	4:D:505:BTB:H52	1.52	0.45
1:A:308:GLU:H	1:A:308:GLU:CD	2.23	0.45
1:A:103:LEU:HD12	1:B:463:GLU:HB3	1.99	0.45
1:A:119:ALA:N	10:A:612:HOH:O	2.49	0.45
1:A:144:GLN:CG	1:A:145:ALA:H	2.30	0.45
1:A:364:THR:O	1:A:368:CYS:HB2	2.16	0.45
1:D:308:GLU:H	1:D:308:GLU:CD	2.25	0.45
1:A:140:ARG:HD3	1:A:144:GLN:NE2	2.31	0.45
1:C:156:GLU:O	1:C:160:THR:HG22	2.18	0.44
1:D:128:ARG:HH21	1:D:154:GLU:CD	2.25	0.44
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.52	0.44
1:B:135:TYR:HA	1:B:138:ILE:HG12	1.98	0.44
1:C:147:GLU:O	1:C:151:GLN:HG2	2.16	0.44
1:C:216:LYS:HG2	1:C:217:TYR:N	2.30	0.44
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.53	0.44
1:D:160:THR:OG1	1:D:162:THR:O	2.36	0.44
1:D:454:GLY:O	1:D:460:PHE:HB2	2.17	0.44
1:B:321:GLU:HB2	1:C:378:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:THR:HG21	10:C:703:HOH:O	2.18	0.43
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.54	0.43
1:A:358:MET:HE3	1:A:360:THR:OG1	2.18	0.43
1:B:214:HIS:CD2	1:B:214:HIS:C	2.96	0.43
1:B:135:TYR:CD1	1:B:138:ILE:HD11	2.54	0.43
1:C:97:ARG:CZ	1:C:97:ARG:HB3	2.48	0.43
1:A:162:THR:OG1	1:A:163:TYR:N	2.51	0.43
1:B:170:LEU:HD11	1:B:230:VAL:HG21	2.01	0.43
4:B:508:BTB:H41	4:B:508:BTB:O8	2.19	0.43
1:A:308:GLU:OE1	1:A:308:GLU:N	2.43	0.43
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.43
1:C:340:LEU:HD11	1:C:347:GLU:HB3	2.00	0.43
1:C:404:VAL:HG23	1:D:393:LEU:HD12	2.01	0.43
1:D:107:ARG:H	1:D:107:ARG:HG3	1.63	0.43
4:A:503:BTB:H41	4:A:503:BTB:H72	1.78	0.43
1:B:89:GLN:OE1	1:B:470:SER:N	2.34	0.43
1:A:143:SER:OG	1:A:144:GLN:N	2.52	0.43
1:C:213:ASN:HA	1:C:216:LYS:HD3	2.00	0.43
1:B:261:VAL:HG11	1:B:265:PRO:HA	2.01	0.42
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.54	0.42
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.54	0.42
1:C:358:MET:HE3	1:C:360:THR:OG1	2.19	0.42
4:B:508:BTB:H52	4:B:508:BTB:H82	1.53	0.42
1:D:364:THR:O	1:D:368:CYS:HB2	2.20	0.42
1:A:68:PHE:N	10:A:620:HOH:O	2.53	0.42
4:A:504:BTB:H72	4:A:504:BTB:H11	1.59	0.42
1:B:70:ARG:HE	1:B:79:ILE:HD13	1.85	0.42
1:B:124:LEU:HD21	1:B:154:GLU:HA	2.02	0.42
1:A:125:SER:HA	1:A:128:ARG:HE	1.85	0.42
1:A:257:GLN:HA	10:A:686:HOH:O	2.18	0.42
1:C:178:TRP:HZ3	1:C:193:LEU:HB2	1.85	0.42
1:D:319:THR:HB	4:D:504:BTB:O3	2.19	0.42
1:A:224:LEU:HB2	1:A:416:THR:HB	2.02	0.41
1:D:275:ILE:HG12	1:D:275:ILE:H	1.72	0.41
1:D:361:GLU:HG2	2:D:501:HEM:O2A	2.19	0.41
1:D:470:SER:HA	1:D:471:PRO:C	2.45	0.41
1:D:124:LEU:HD13	1:D:128:ARG:NH2	2.36	0.41
4:B:508:BTB:O3	4:B:508:BTB:H71	2.19	0.41
1:C:130:PHE:O	1:C:133:GLN:HB2	2.21	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.89	0.41
1:B:71:VAL:N	1:B:80:THR:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ILE:HG23	1:D:189:GLN:HG2	2.02	0.41
4:D:505:BTB:H11	4:D:505:BTB:H71	1.32	0.41
1:A:334:PRO:HB3	1:A:357:TYR:CZ	2.55	0.41
1:D:247:GLN:HA	1:D:335:ALA:O	2.21	0.41
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.02	0.41
1:B:306:PRO:HA	1:B:307:PRO:HD3	1.95	0.41
1:D:85:SER:HB3	1:D:467:TYR:CE1	2.56	0.41
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.56	0.41
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.03	0.40
1:A:265:PRO:HA	1:A:268:VAL:HG23	2.04	0.40
1:D:285:ARG:HH21	1:D:373:TYR:HD2	1.70	0.40
1:A:232:PRO:HG2	1:A:241:PHE:CE1	2.57	0.40
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.61	0.40
1:D:308:GLU:OE1	1:D:308:GLU:N	2.49	0.40

All (1) 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:A:152:GLU:OE2	4:D:505:BTB:O4[2_851]	2.12	0.08

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%)	374 (93%)	25 (6%)	3 (1%)	18	21
1	B	401/440 (91%)	391 (98%)	10 (2%)	0	100	100
1	C	399/440 (91%)	388 (97%)	10 (2%)	1 (0%)	36	44
1	D	403/440 (92%)	397 (98%)	6 (2%)	0	100	100
All	All	1605/1760 (91%)	1550 (97%)	51 (3%)	4 (0%)	36	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	108	LYS
1	A	283	ASN
1	C	89	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/373 (92%)	325 (94%)	20 (6%)	18	24
1	B	344/373 (92%)	329 (96%)	15 (4%)	25	35
1	C	342/373 (92%)	327 (96%)	15 (4%)	25	35
1	D	346/373 (93%)	341 (99%)	5 (1%)	59	74
All	All	1377/1492 (92%)	1322 (96%)	55 (4%)	28	40

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	97	ARG
1	A	103	LEU
1	A	109	LEU
1	A	121	GLU
1	A	122	GLN
1	A	133	GLN
1	A	139	LYS
1	A	140	ARG
1	A	141	SER
1	A	151	GLN
1	A	201	CYS
1	A	224	LEU
1	A	256	GLN
1	A	258	ASP
1	A	272	GLU

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	301	GLU
1	A	309	LEU
1	A	329	ARG
1	B	67	LYS
1	B	70	ARG
1	B	78	SER
1	B	122	GLN
1	B	144	GLN
1	B	148	GLN
1	B	154	GLU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	213	ASN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	268	VAL
1	B	389	THR
1	B	396	ASP
1	C	90	GLN
1	C	103	LEU
1	C	125	SER
1	C	137	SER
1	C	140	ARG
1	C	141	SER
1	C	154	GLU
1	C	160	THR
1	C	192	LYS
1	C	202	ARG
1	C	216	LYS
1	C	257	GLN
1	C	308	GLU
1	C	342	GLU
1	C	417	ILE
1	D	71	VAL
1	D	89	GLN
1	D	107	ARG
1	D	108	LYS
1	D	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	B	87	GLN
1	B	122	GLN
1	B	151	GLN
1	C	122	GLN
1	C	164	GLN
1	C	220	ASN
1	C	233	GLN
1	D	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 17 are monoatomic - leaving 22 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	$\# Z > 2$
3	KLA	D	502	-	27,27,27	0.52	0	33,37,37	1.47	5 (15%)
4	BTB	B	505	-	13,13,13	0.50	0	7,16,16	1.09	1 (14%)
4	BTB	A	504	-	13,13,13	0.40	0	7,16,16	0.74	0
2	HEM	C	502	1	50,50,50	1.86	9 (18%)	67,82,82	1.49	13 (19%)
4	BTB	C	505	-	13,13,13	0.40	0	7,16,16	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	502	1	50,50,50	1.48	9 (18%)	67,82,82	1.26	9 (13%)
3	KLA	A	509	-	27,27,27	0.57	0	33,37,37	1.30	6 (18%)
4	BTB	D	505	-	13,13,13	0.53	0	7,16,16	0.88	0
3	KLA	C	504	-	27,27,27	0.45	0	33,37,37	1.53	7 (21%)
4	BTB	A	503	9	13,13,13	0.46	0	7,16,16	1.21	2 (28%)
2	HEM	D	501	1	50,50,50	1.57	5 (10%)	67,82,82	1.31	9 (13%)
3	KLA	A	502	-	27,27,27	0.51	0	33,37,37	1.84	5 (15%)
8	H4B	B	501	-	17,18,18	0.85	0	14,26,26	1.75	5 (35%)
3	KLA	B	503	-	27,27,27	0.69	0	33,37,37	1.56	6 (18%)
8	H4B	C	503	-	17,18,18	0.88	0	14,26,26	1.80	5 (35%)
3	KLA	D	503	-	27,27,27	0.54	0	33,37,37	1.53	5 (15%)
4	BTB	D	504	9	13,13,13	0.62	0	7,16,16	0.96	1 (14%)
4	BTB	B	508	-	13,13,13	0.71	0	7,16,16	0.70	0
6	GOL	A	507	-	5,5,5	0.40	0	5,5,5	0.44	0
4	BTB	B	504	9	13,13,13	0.50	0	7,16,16	0.76	0
6	GOL	C	508	-	5,5,5	0.37	0	5,5,5	0.48	0
2	HEM	A	501	1	50,50,50	1.78	7 (14%)	67,82,82	1.35	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KLA	D	502	-	-	4/10/19/19	0/3/3/3
4	BTB	B	505	-	-	5/21/21/21	-
4	BTB	A	504	-	-	6/21/21/21	-
2	HEM	C	502	1	-	2/14/54/54	-
4	BTB	C	505	-	-	6/21/21/21	-
2	HEM	B	502	1	-	4/14/54/54	-
3	KLA	A	509	-	-	3/10/19/19	0/3/3/3
4	BTB	D	505	-	-	11/21/21/21	-
3	KLA	C	504	-	-	4/10/19/19	0/3/3/3
4	BTB	A	503	9	-	4/21/21/21	-
2	HEM	D	501	1	-	2/14/54/54	-
3	KLA	A	502	-	-	4/10/19/19	0/3/3/3
8	H4B	B	501	-	-	4/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KLA	B	503	-	-	3/10/19/19	0/3/3/3
8	H4B	C	503	-	-	3/8/17/17	0/2/2/2
3	KLA	D	503	-	-	2/10/19/19	0/3/3/3
4	BTB	D	504	9	-	6/21/21/21	-
4	BTB	B	508	-	-	4/21/21/21	-
6	GOL	A	507	-	-	3/4/4/4	-
4	BTB	B	504	9	-	3/21/21/21	-
6	GOL	C	508	-	-	2/4/4/4	-
2	HEM	A	501	1	-	1/14/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	HEM	FE-NB	7.42	2.17	1.94
2	A	501	HEM	FE-NB	7.09	2.16	1.94
2	C	502	HEM	FE-NA	5.41	2.13	1.95
2	A	501	HEM	FE-NA	5.38	2.12	1.95
2	D	501	HEM	FE-NB	5.35	2.11	1.94
2	B	502	HEM	FE-NC	4.89	2.11	1.95
2	D	501	HEM	FE-NC	4.77	2.10	1.95
2	C	502	HEM	FE-NC	4.65	2.10	1.95
2	A	501	HEM	FE-NC	4.18	2.09	1.95
2	D	501	HEM	FE-NA	3.35	2.06	1.95
2	B	502	HEM	FE-NB	3.15	2.04	1.94
2	C	502	HEM	CAC-C3C	3.12	1.55	1.47
2	D	501	HEM	CAB-C3B	3.07	1.55	1.47
2	C	502	HEM	CAB-C3B	3.04	1.55	1.47
2	B	502	HEM	FE-ND	3.02	2.04	1.94
2	A	501	HEM	CAC-C3C	3.01	1.55	1.47
2	B	502	HEM	CAC-C3C	2.96	1.55	1.47
2	B	502	HEM	CAB-C3B	2.92	1.55	1.47
2	C	502	HEM	FE-ND	2.91	2.03	1.94
2	D	501	HEM	CAC-C3C	2.90	1.55	1.47
2	A	501	HEM	CAB-C3B	2.81	1.54	1.47
2	C	502	HEM	CMB-C2B	2.22	1.55	1.50
2	A	501	HEM	CMA-C3A	2.20	1.55	1.50
2	B	502	HEM	CMA-C3A	2.16	1.55	1.50
2	B	502	HEM	CMC-C2C	2.10	1.55	1.50
2	B	502	HEM	C3B-C2B	-2.09	1.32	1.37
2	B	502	HEM	CMB-C2B	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	HEM	C2A-C3A	-2.05	1.33	1.38
2	A	501	HEM	CMD-C2D	2.02	1.54	1.50
2	C	502	HEM	CMD-C2D	2.00	1.54	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	KLA	C02-N01-C06	5.74	122.36	118.07
3	C	504	KLA	C02-N01-C06	4.55	121.47	118.07
3	D	503	KLA	C02-N01-C06	4.13	121.16	118.07
8	C	503	H4B	C2-N1-C8A	3.94	120.31	113.36
3	B	503	KLA	C14-C13-C12	-3.74	118.95	123.50
8	B	501	H4B	C2-N1-C8A	3.70	119.89	113.36
2	C	502	HEM	C3B-C4B-NB	-3.63	106.86	109.47
3	D	502	KLA	C11-C12-C13	3.52	121.82	118.75
3	A	502	KLA	C05-C06-N01	-3.51	118.73	122.73
3	D	503	KLA	C09-C08-C06	-3.31	105.65	113.01
3	D	502	KLA	C14-C13-C12	-3.26	119.53	123.50
2	C	502	HEM	CBD-CAD-C3D	-3.23	103.59	112.53
3	A	502	KLA	C08-C06-N01	3.14	120.82	116.06
2	C	502	HEM	C3D-C4D-ND	-3.13	106.73	110.17
3	A	502	KLA	C14-C13-C12	-3.13	119.70	123.50
3	C	504	KLA	C14-C13-C12	-3.09	119.75	123.50
2	D	501	HEM	CBD-CAD-C3D	-3.04	104.14	112.53
2	C	502	HEM	C2A-C1A-NA	-3.02	106.81	110.15
2	A	501	HEM	C3B-C4B-NB	-2.95	107.35	109.47
2	A	501	HEM	C3B-C2B-C1B	2.94	108.62	106.41
3	D	503	KLA	C14-C13-C12	-2.90	119.97	123.50
3	B	503	KLA	C08-C06-N01	2.87	120.41	116.06
2	D	501	HEM	C3B-C2B-C1B	2.86	108.56	106.41
2	C	502	HEM	C4D-ND-C1D	2.85	108.58	105.21
3	B	503	KLA	C11-C12-C13	2.79	121.19	118.75
8	C	503	H4B	C2-N3-C4	-2.78	120.06	125.11
2	C	502	HEM	C1B-NB-C4B	2.78	108.50	105.21
2	A	501	HEM	CBD-CAD-C3D	-2.77	104.88	112.53
8	C	503	H4B	C4A-C4-N3	2.72	119.60	112.13
3	A	509	KLA	C14-C13-C12	-2.69	120.23	123.50
2	B	502	HEM	CAB-C3B-C2B	-2.68	119.72	128.43
2	B	502	HEM	C3B-C4B-NB	-2.66	107.56	109.47
8	B	501	H4B	C4A-C4-N3	2.66	119.43	112.13
3	B	503	KLA	C02-N01-C06	2.65	120.05	118.07
2	A	501	HEM	CAA-CBA-CGA	-2.63	106.68	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	KLA	C11-C12-C13	2.63	121.04	118.75
8	B	501	H4B	C2-N3-C4	-2.62	120.36	125.11
2	D	501	HEM	C1B-NB-C4B	2.59	108.28	105.21
2	D	501	HEM	C3D-C4D-ND	-2.59	107.34	110.17
2	D	501	HEM	C4D-ND-C1D	2.58	108.27	105.21
8	B	501	H4B	O4-C4-C4A	-2.58	121.05	127.26
2	B	502	HEM	CHA-C4D-ND	2.52	127.49	124.37
2	A	501	HEM	C1B-NB-C4B	2.50	108.17	105.21
3	D	503	KLA	C18-C22-C23	-2.49	109.26	113.50
3	A	509	KLA	C02-N01-C06	2.48	119.92	118.07
3	D	502	KLA	C02-N01-C06	2.46	119.91	118.07
2	A	501	HEM	C3D-C4D-ND	-2.45	107.49	110.17
2	C	502	HEM	C3B-C2B-C1B	2.41	108.22	106.41
2	A	501	HEM	CHA-C4D-ND	2.41	127.35	124.37
2	C	502	HEM	C3C-C2C-C1C	2.40	109.32	107.05
2	B	502	HEM	C3B-C2B-C1B	2.40	108.21	106.41
3	B	503	KLA	F13-C13-C12	2.39	121.67	118.28
4	A	503	BTB	O3-C3-C2	-2.38	105.80	111.40
2	B	502	HEM	CBD-CAD-C3D	-2.37	105.98	112.53
8	C	503	H4B	O4-C4-C4A	-2.37	121.55	127.26
2	C	502	HEM	CHD-C1D-ND	2.34	126.94	124.42
2	B	502	HEM	CMA-C3A-C2A	2.33	130.56	125.62
2	D	501	HEM	C3B-C4B-NB	-2.32	107.80	109.47
4	B	505	BTB	O4-C4-C2	-2.32	105.95	111.40
3	D	502	KLA	C08-C09-C11	-2.31	105.38	113.23
2	D	501	HEM	CAB-C3B-C2B	-2.28	121.03	128.43
3	A	509	KLA	C18-C22-C23	-2.25	109.67	113.50
2	C	502	HEM	CBA-CAA-C2A	-2.24	106.35	112.53
3	C	504	KLA	C23-C24-C25	2.23	107.24	104.52
2	C	502	HEM	CHA-C4D-ND	2.22	127.11	124.37
3	D	503	KLA	C08-C06-N01	2.21	119.40	116.06
3	C	504	KLA	C11-C12-C13	2.20	120.67	118.75
2	A	501	HEM	C4D-ND-C1D	2.19	107.80	105.21
3	A	509	KLA	C08-C06-N01	2.18	119.37	116.06
2	B	502	HEM	CAA-CBA-CGA	-2.18	107.88	113.67
4	D	504	BTB	O4-C4-C2	-2.17	106.29	111.40
2	C	502	HEM	CHC-C4B-C3B	2.17	129.41	125.07
3	C	504	KLA	C05-C06-N01	-2.17	120.26	122.73
2	A	501	HEM	C3C-C2C-C1C	2.16	109.08	107.05
2	D	501	HEM	CHA-C4D-ND	2.14	127.02	124.37
8	C	503	H4B	C4-C4A-N5	2.14	122.09	116.27
3	C	504	KLA	C08-C06-N01	2.13	119.29	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	KLA	C09-C08-C06	-2.12	108.29	113.01
2	D	501	HEM	C2B-C1B-NB	-2.10	107.43	109.84
2	A	501	HEM	CHC-C1C-NC	2.09	126.73	124.45
4	A	503	BTB	O4-C4-C2	-2.09	106.49	111.40
2	B	502	HEM	C4D-ND-C1D	2.08	107.67	105.21
8	B	501	H4B	C4-C4A-N5	2.08	121.93	116.27
2	B	502	HEM	C2D-C1D-ND	-2.07	107.51	109.90
3	A	509	KLA	F13-C13-C12	2.07	121.22	118.28
3	D	502	KLA	C16-C15-C14	2.06	121.81	119.01
2	C	502	HEM	C2D-C1D-ND	-2.04	107.55	109.90
3	B	503	KLA	C18-C22-C23	-2.03	110.04	113.50
3	C	504	KLA	F13-C13-C12	2.02	121.16	118.28

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	KLA	C17-C18-C22-C23
3	A	502	KLA	C17-C18-C22-N21
3	A	509	KLA	C15-C17-C18-C22
3	A	509	KLA	C17-C18-C22-C23
3	A	509	KLA	C17-C18-C22-N21
3	B	503	KLA	C15-C17-C18-C22
3	C	504	KLA	C15-C17-C18-C22
3	D	502	KLA	C15-C17-C18-C22
3	D	503	KLA	C15-C17-C18-C22
4	A	503	BTB	O1-C1-C2-C3
4	A	503	BTB	O1-C1-C2-C4
4	A	503	BTB	O1-C1-C2-N
4	A	504	BTB	C1-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	A	504	BTB	N-C2-C3-O3
4	B	504	BTB	O1-C1-C2-C3
4	B	504	BTB	O1-C1-C2-C4
4	B	504	BTB	O1-C1-C2-N
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C3-C2-C4-O4
4	B	505	BTB	N-C2-C4-O4
4	B	508	BTB	C1-C2-C3-O3
4	B	508	BTB	N-C2-C3-O3
4	B	508	BTB	C8-C7-N-C5
4	C	505	BTB	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	505	BTB	C4-C2-C3-O3
4	C	505	BTB	N-C2-C3-O3
4	C	505	BTB	C1-C2-C4-O4
4	C	505	BTB	C3-C2-C4-O4
4	C	505	BTB	N-C2-C4-O4
4	D	504	BTB	O1-C1-C2-C3
4	D	505	BTB	O1-C1-C2-C4
4	D	505	BTB	O1-C1-C2-N
4	D	505	BTB	C1-C2-N-C7
4	D	505	BTB	C8-C7-N-C5
6	A	507	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-C3
8	B	501	H4B	N5-C6-C9-O9
8	B	501	H4B	C7-C6-C9-O9
8	B	501	H4B	C7-C6-C9-C10
8	C	503	H4B	C7-C6-C9-O9
8	C	503	H4B	C7-C6-C9-C10
4	A	504	BTB	N-C7-C8-O8
2	C	502	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C2A-CAA-CBA-CGA
2	B	502	HEM	C2A-CAA-CBA-CGA
4	D	504	BTB	N-C5-C6-O6
4	D	504	BTB	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
2	D	501	HEM	C2A-CAA-CBA-CGA
2	B	502	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	A	504	BTB	C3-C2-C4-O4
4	D	505	BTB	N-C7-C8-O8
2	C	502	HEM	C4B-C3B-CAB-CBB
2	B	502	HEM	C3A-C2A-CAA-CBA
8	B	501	H4B	N5-C6-C9-C10
8	C	503	H4B	N5-C6-C9-O9
3	C	504	KLA	C17-C18-C22-C23
3	D	502	KLA	C17-C18-C22-C23
3	D	503	KLA	C17-C18-C22-C23
4	D	504	BTB	O1-C1-C2-N
4	D	505	BTB	N-C2-C3-O3
4	D	505	BTB	C3-C2-N-C5
4	D	505	BTB	C3-C2-N-C7
4	D	505	BTB	C4-C2-N-C5

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Mol	Chain	Res	Type	Atoms
4	D	505	BTB	C4-C2-N-C7
2	B	502	HEM	C1A-C2A-CAA-CBA
4	B	508	BTB	C4-C2-C3-O3
3	A	502	KLA	C14-C15-C17-C18
4	B	505	BTB	N-C5-C6-O6
3	A	502	KLA	C16-C15-C17-C18
3	B	503	KLA	C14-C15-C17-C18
3	B	503	KLA	C16-C15-C17-C18
3	D	502	KLA	C14-C15-C17-C18
3	D	502	KLA	C16-C15-C17-C18
6	A	507	GOL	O2-C2-C3-O3
3	C	504	KLA	C14-C15-C17-C18
3	C	504	KLA	C16-C15-C17-C18
4	D	504	BTB	O1-C1-C2-C4
4	A	503	BTB	N-C7-C8-O8
4	A	504	BTB	N-C2-C4-O4
4	B	505	BTB	N-C2-C3-O3
4	D	504	BTB	N-C2-C3-O3
4	D	505	BTB	C1-C2-N-C5

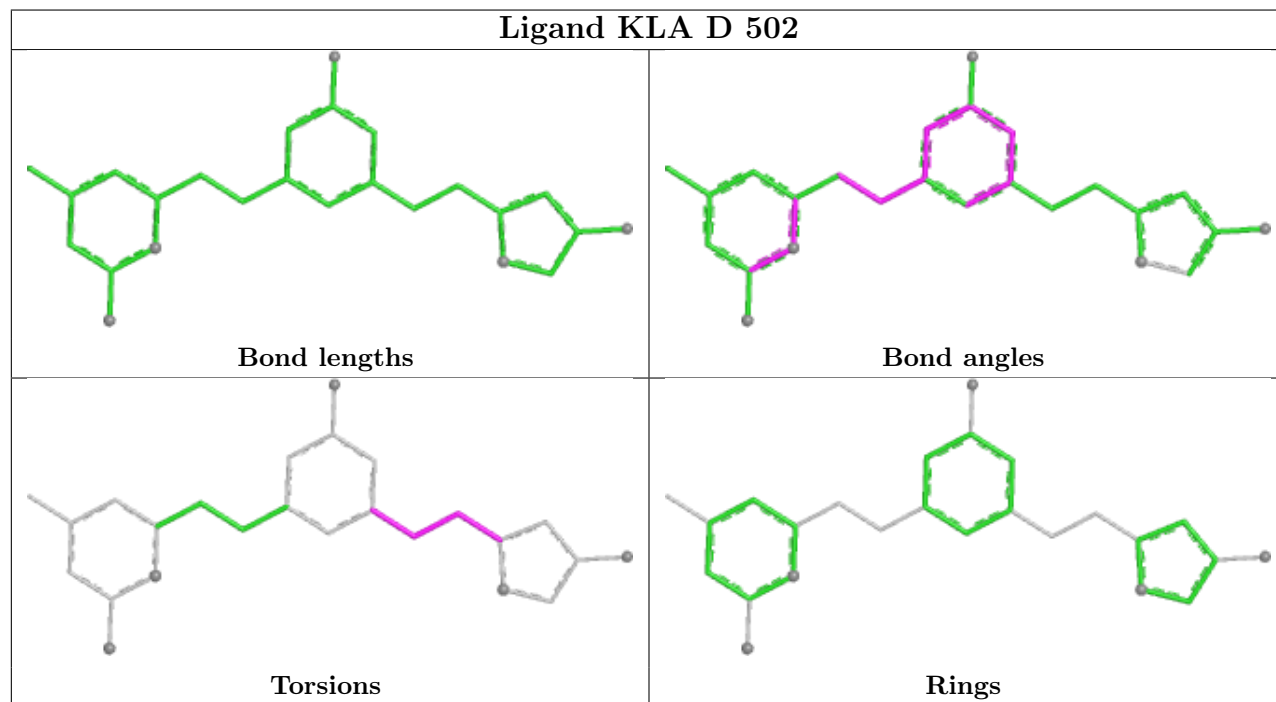
There are no ring outliers.

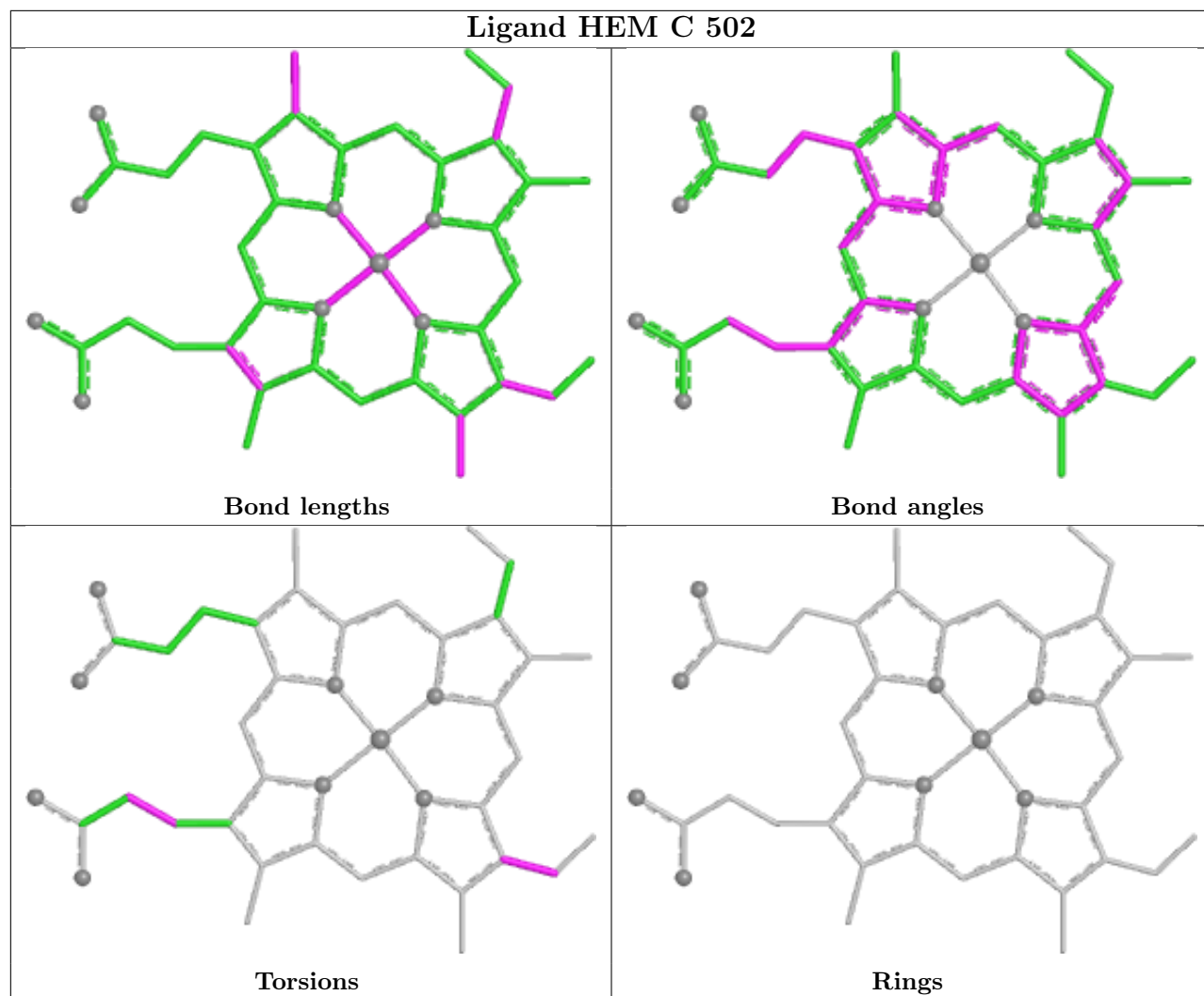
15 monomers are involved in 36 short contacts:

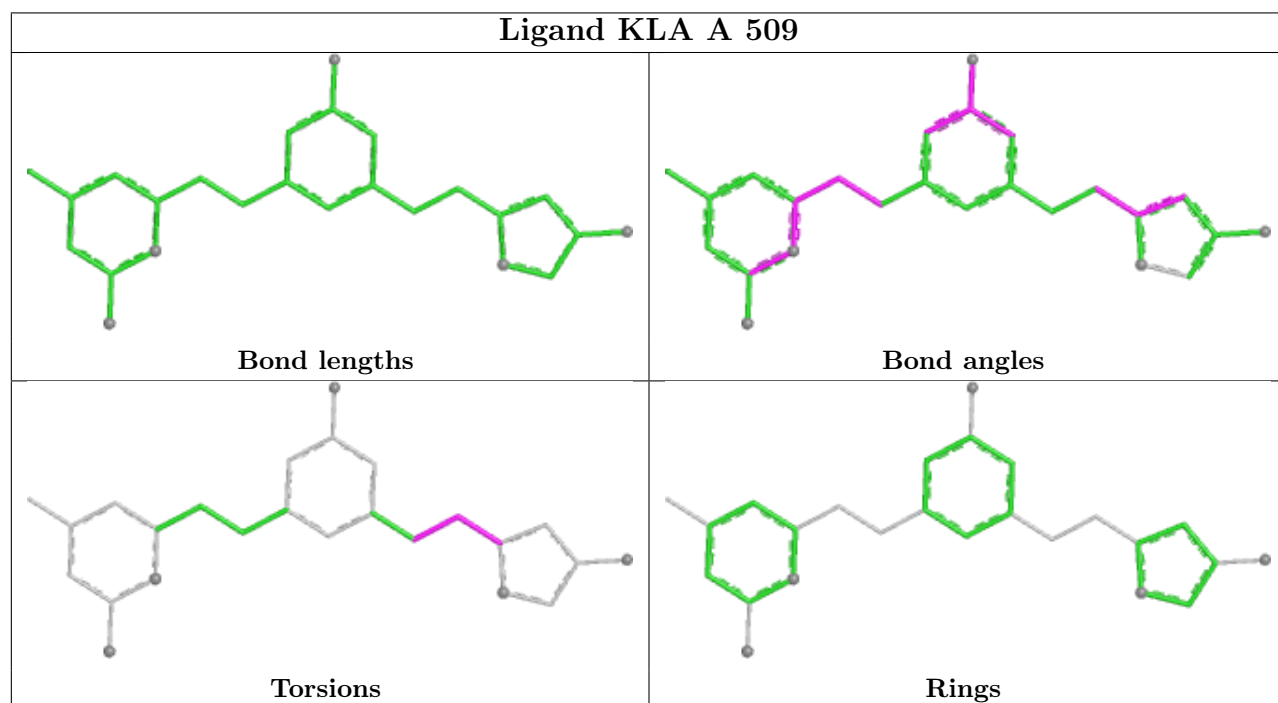
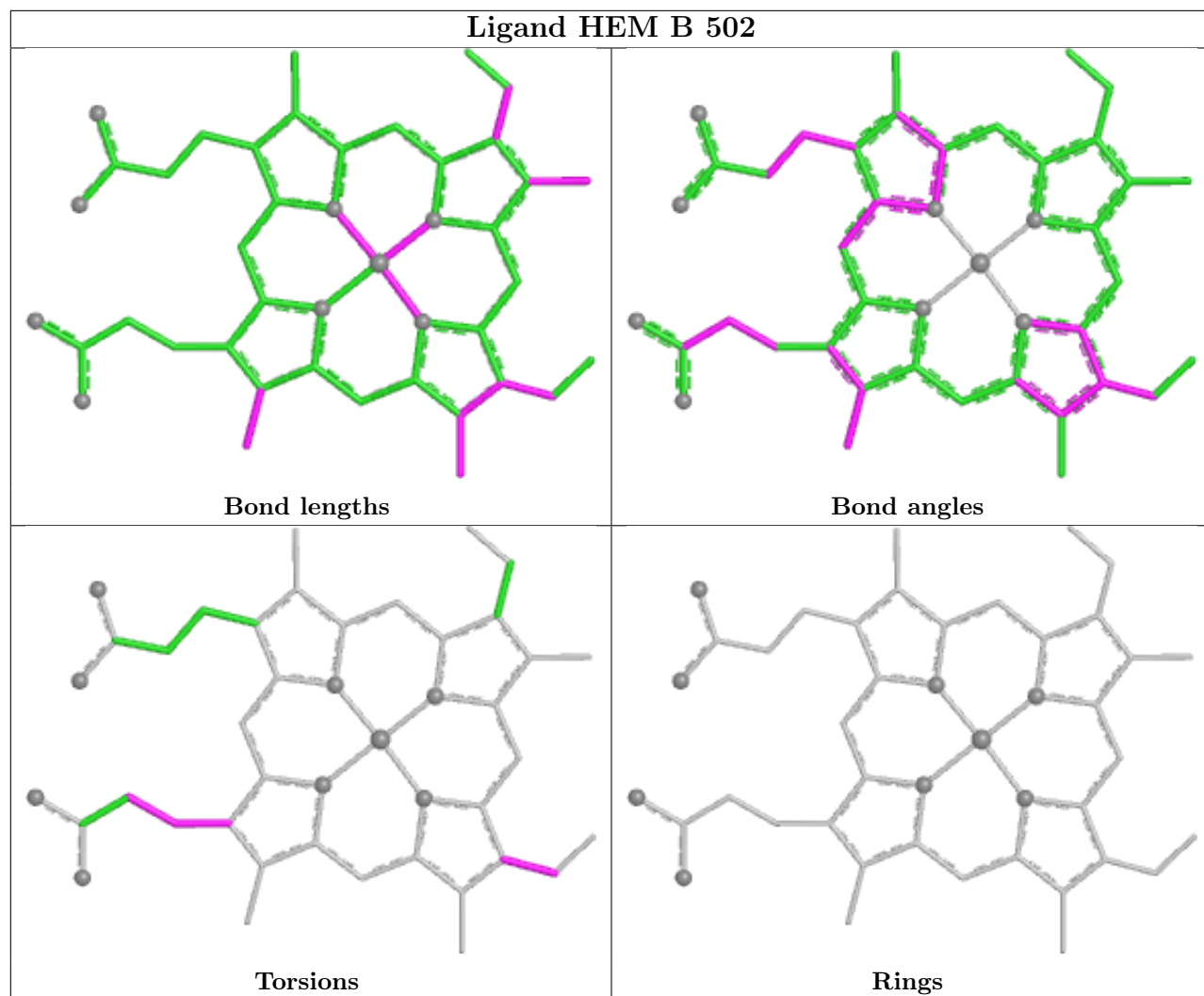
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	BTB	4	0
4	A	504	BTB	2	0
2	C	502	HEM	4	0
4	C	505	BTB	1	0
2	B	502	HEM	2	0
4	D	505	BTB	3	1
4	A	503	BTB	4	0
2	D	501	HEM	4	0
3	A	502	KLA	1	0
8	B	501	H4B	1	0
8	C	503	H4B	1	0
4	D	504	BTB	3	0
4	B	508	BTB	3	0
4	B	504	BTB	1	0
2	A	501	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

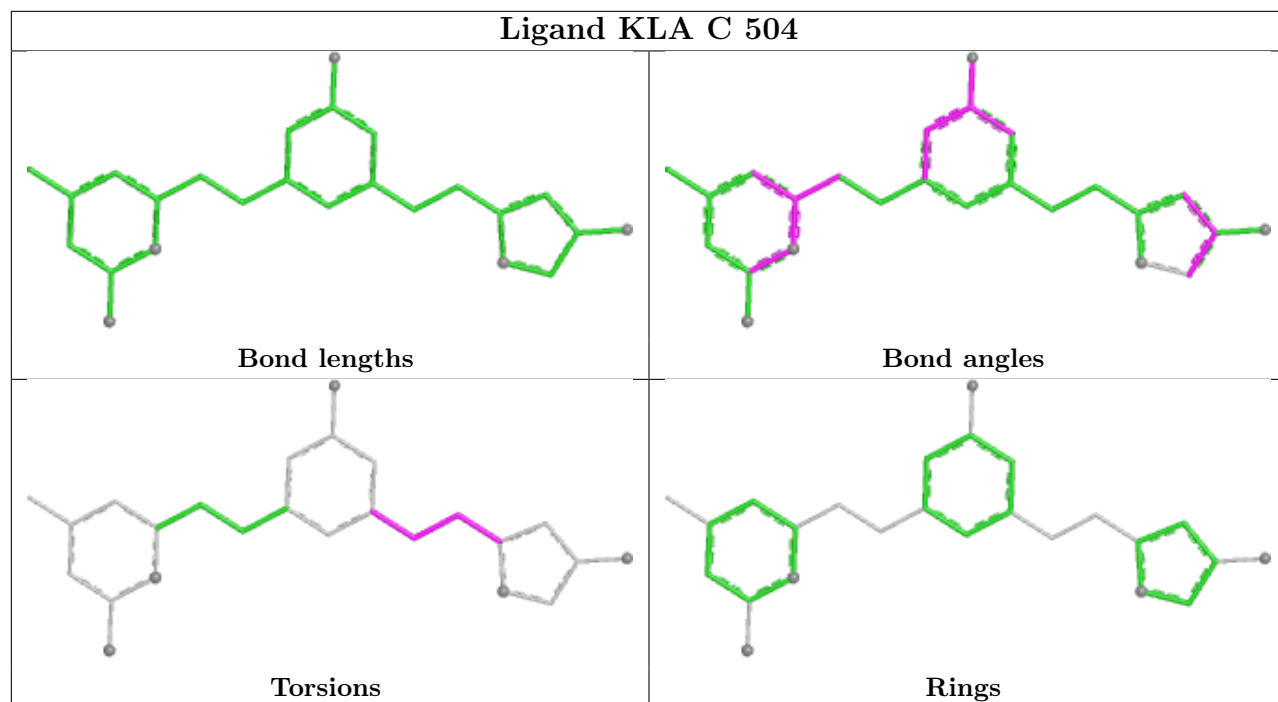
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



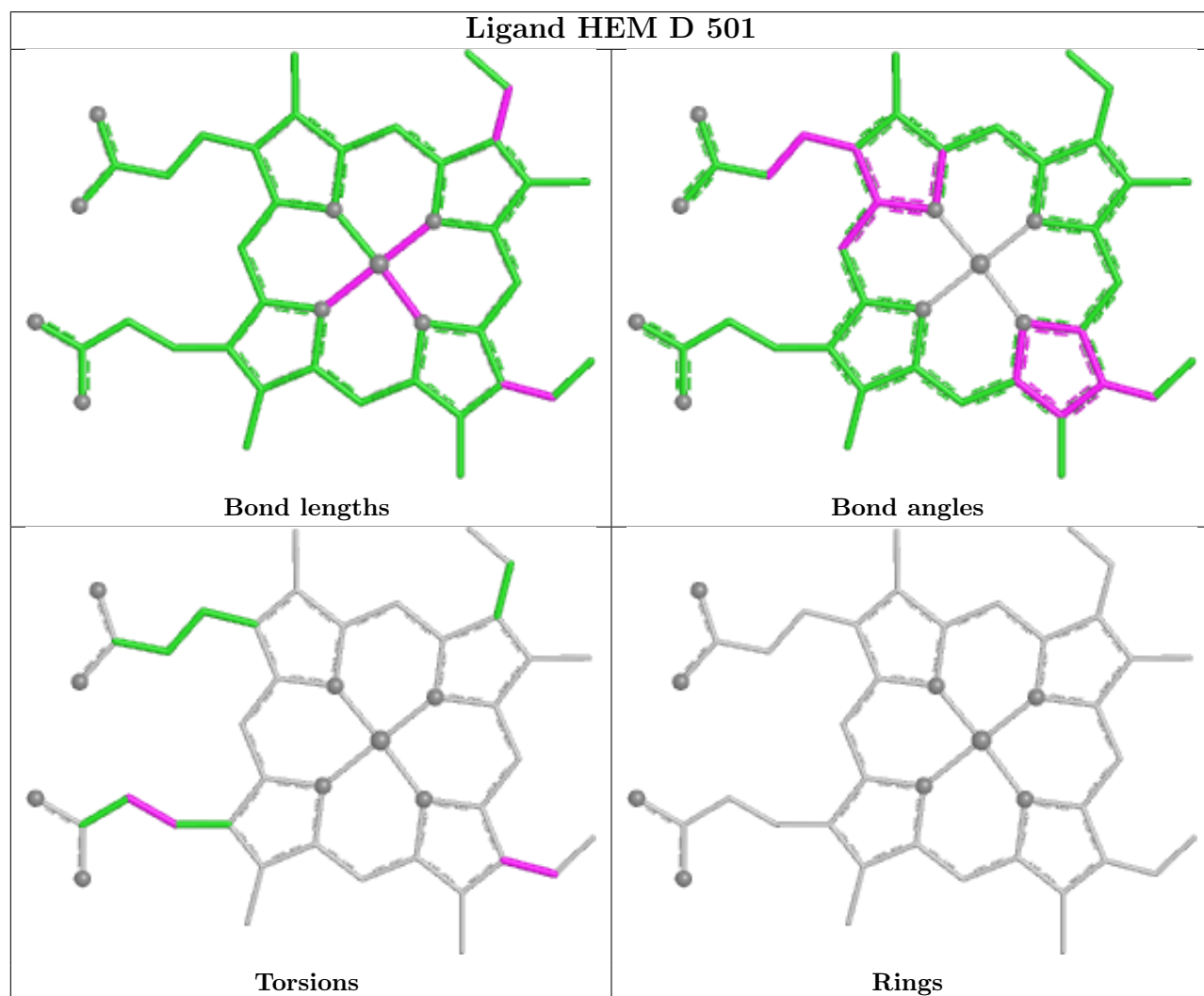


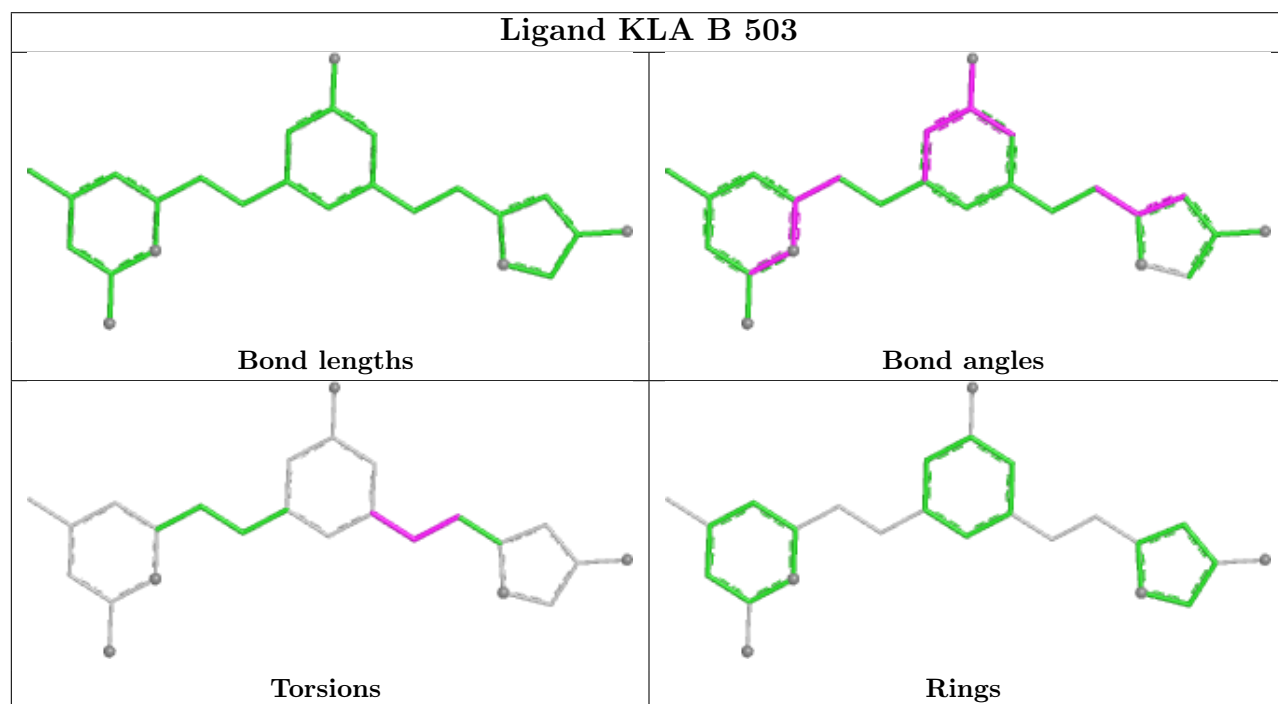
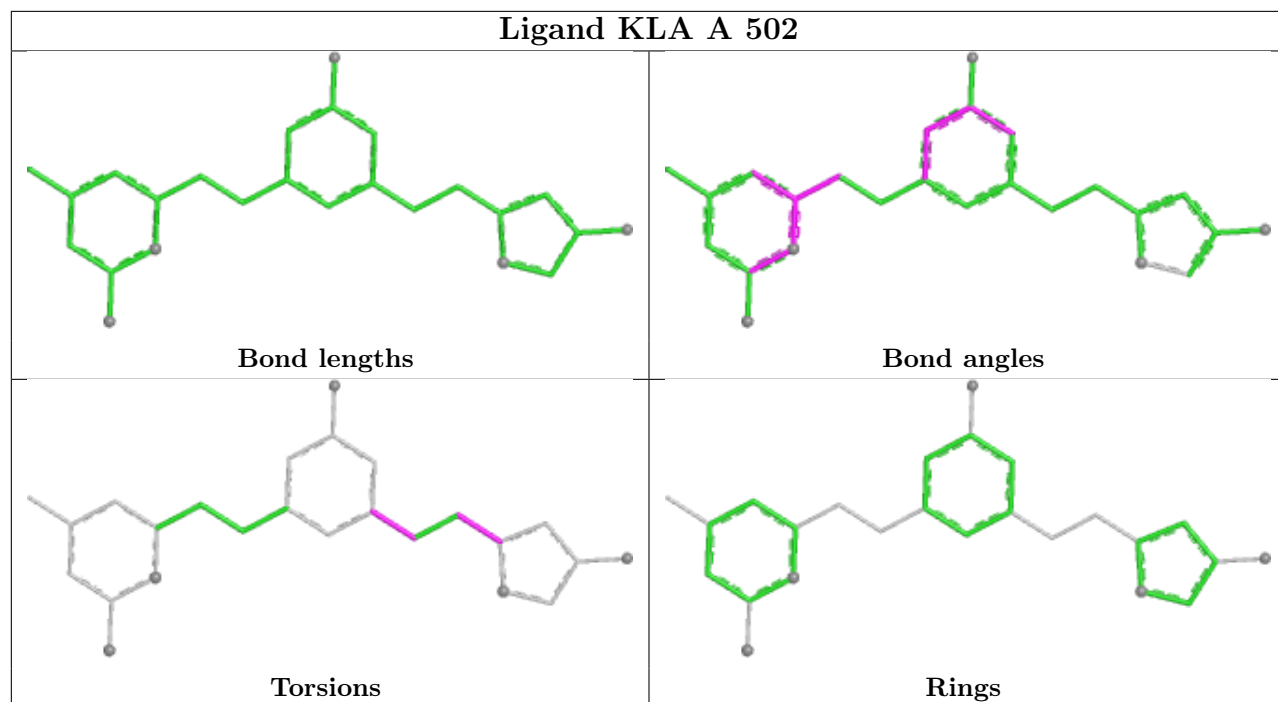


Ligand KLA C 504

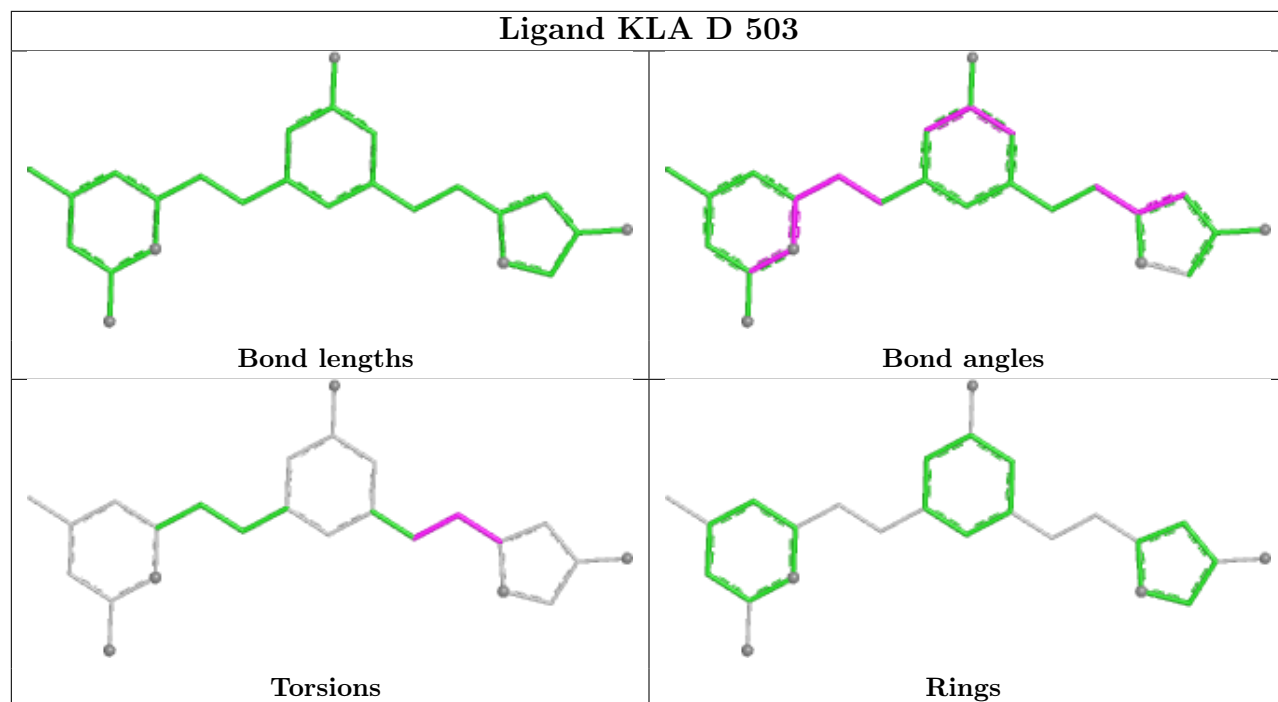


Ligand HEM D 501

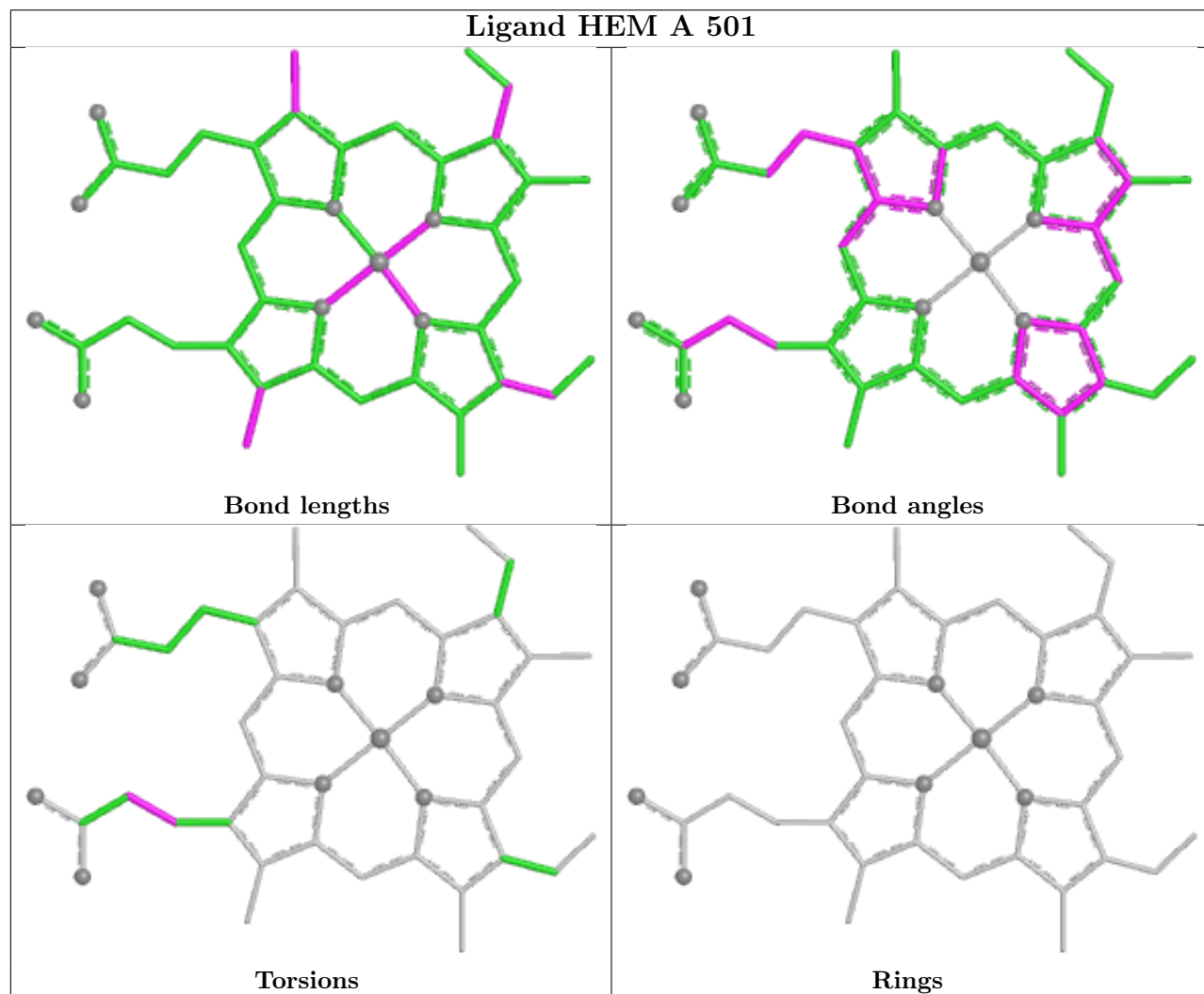




Ligand KLA D 503



Ligand HEM A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	-1.33	0 100 100	16, 40, 88, 121	2 (0%)
1	B	402/440 (91%)	-1.50	0 100 100	14, 28, 63, 103	3 (0%)
1	C	401/440 (91%)	-1.41	0 100 100	16, 36, 72, 111	2 (0%)
1	D	404/440 (91%)	-1.53	0 100 100	12, 27, 53, 107	3 (0%)
All	All	1611/1760 (91%)	-1.44	0 100 100	12, 32, 72, 121	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CL	C	511	1/1	0.96	0.09	244,244,244,244	0
7	CL	B	509	1/1	0.97	0.09	178,178,178,178	0
7	CL	C	510	1/1	0.97	0.11	210,210,210,210	0
4	BTB	C	505	14/14	0.97	0.04	53,69,82,82	0

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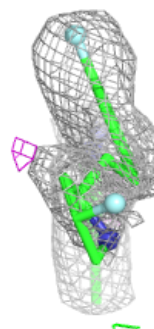
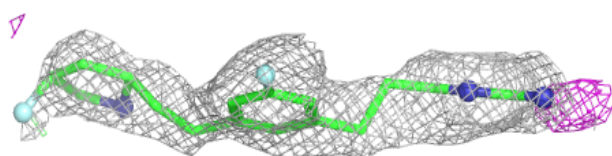
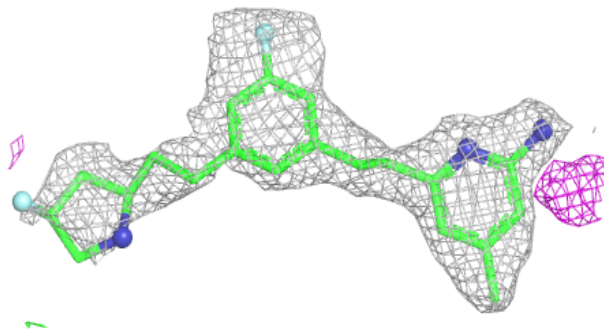
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	C	508	6/6	0.98	0.09	49,51,59,60	0
4	BTB	B	505	14/14	0.98	0.04	45,60,70,73	0
4	BTB	D	505	14/14	0.98	0.03	49,59,74,75	0
6	GOL	A	507	6/6	0.98	0.03	48,59,64,65	0
9	GD	C	501	1/1	0.98	0.09	222,222,222,222	0
4	BTB	D	504	14/14	0.99	0.04	31,57,71,74	0
3	KLA	C	504	25/25	0.99	0.04	22,52,61,69	0
3	KLA	D	503	25/25	0.99	0.04	17,38,57,61	0
4	BTB	A	503	14/14	0.99	0.07	69,78,88,92	0
4	BTB	A	504	14/14	0.99	0.03	58,62,68,71	0
3	KLA	A	502	25/25	0.99	0.06	28,58,74,87	0
4	BTB	B	508	14/14	0.99	0.04	35,54,71,74	0
8	H4B	B	501	17/17	0.99	0.04	32,59,74,80	0
8	H4B	C	503	17/17	0.99	0.04	26,51,77,79	0
3	KLA	A	509	25/25	0.99	0.04	23,44,62,69	0
5	ZN	A	506	1/1	1.00	0.03	39,39,39,39	0
5	ZN	A	510	1/1	1.00	0.01	33,33,33,33	0
5	ZN	C	506	1/1	1.00	0.01	26,26,26,26	0
5	ZN	C	507	1/1	1.00	0.02	35,35,35,35	0
5	ZN	C	513	1/1	1.00	0.01	27,27,27,27	0
2	HEM	B	502	43/43	1.00	0.02	3,12,42,73	0
4	BTB	B	504	14/14	1.00	0.03	32,47,59,62	0
7	CL	A	508	1/1	1.00	0.05	54,54,54,54	0
7	CL	B	506	1/1	1.00	0.02	24,24,24,24	0
3	KLA	B	503	25/25	1.00	0.03	3,38,58,65	0
7	CL	C	509	1/1	1.00	0.07	49,49,49,49	0
2	HEM	C	502	43/43	1.00	0.03	19,31,42,58	0
3	KLA	D	502	25/25	1.00	0.03	2,34,48,49	0
7	CL	D	507	1/1	1.00	0.04	29,29,29,29	0
2	HEM	D	501	43/43	1.00	0.02	3,12,45,63	0
2	HEM	A	501	43/43	1.00	0.03	13,34,44,62	0
9	GD	B	507	1/1	1.00	0.01	34,34,34,34	0
5	ZN	A	505	1/1	1.00	0.01	28,28,28,28	0
9	GD	C	512	1/1	1.00	0.04	174,174,174,174	0
9	GD	D	506	1/1	1.00	0.01	43,43,43,43	0

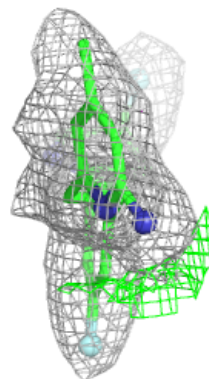
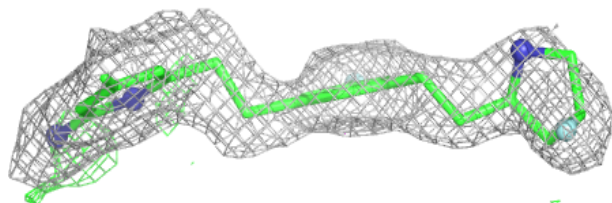
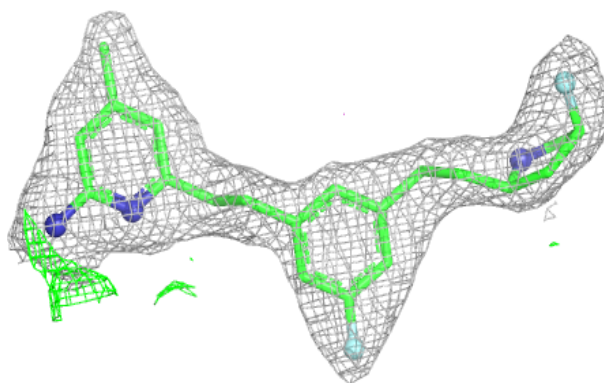
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KLA C 504:

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

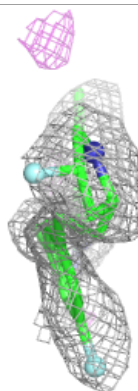
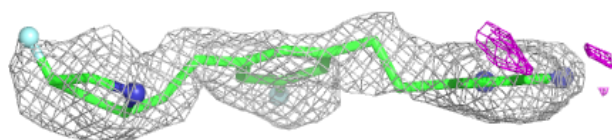
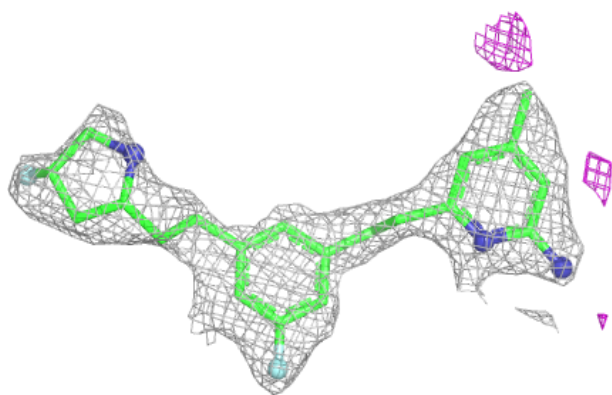
**Electron density around KLA D 503:**

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

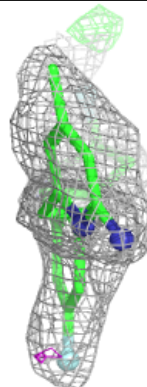
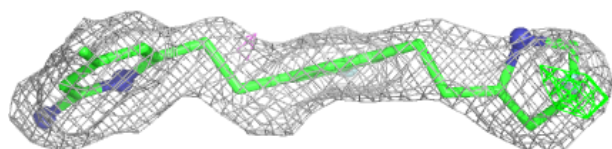
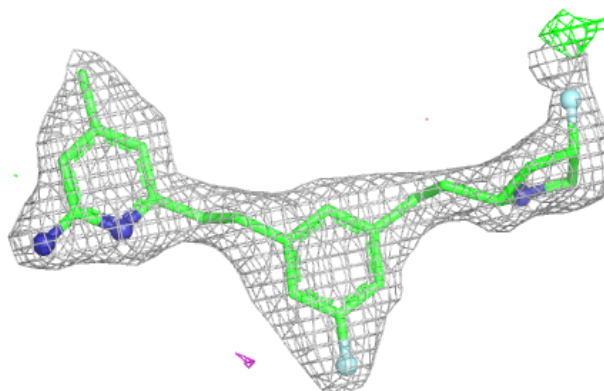


Electron density around KLA A 502:

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

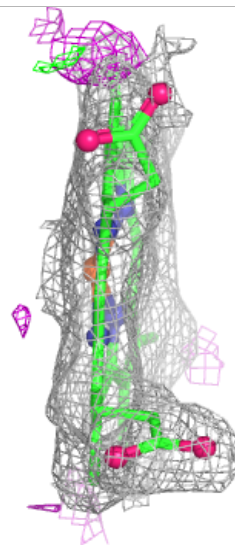
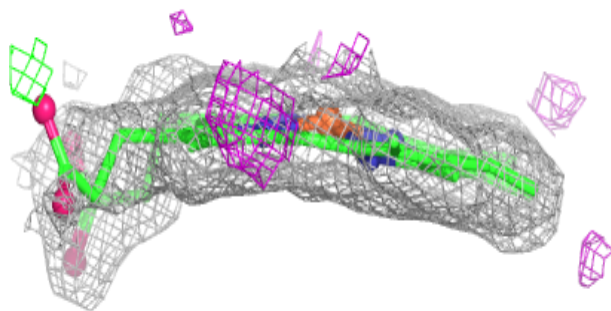
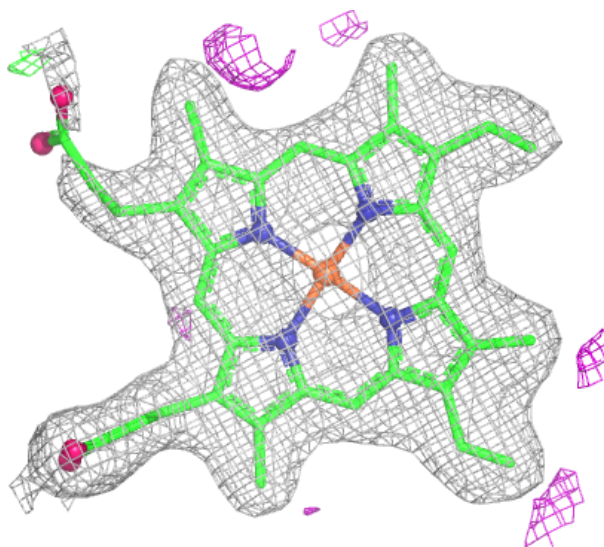
**Electron density around KLA A 509:**

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



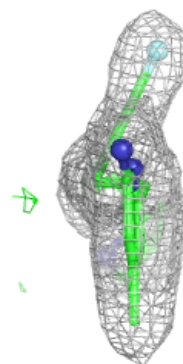
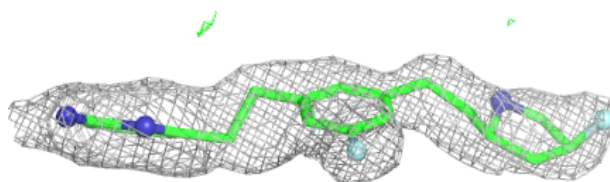
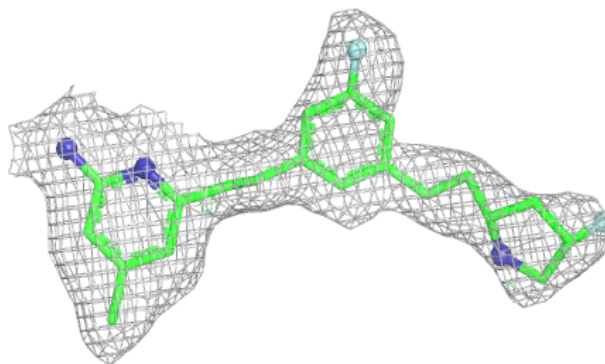
Electron density around HEM B 502:

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



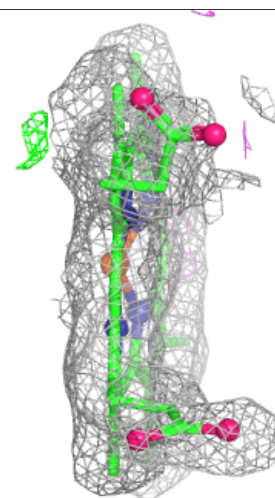
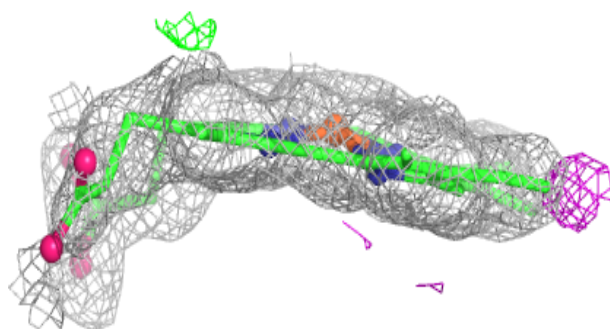
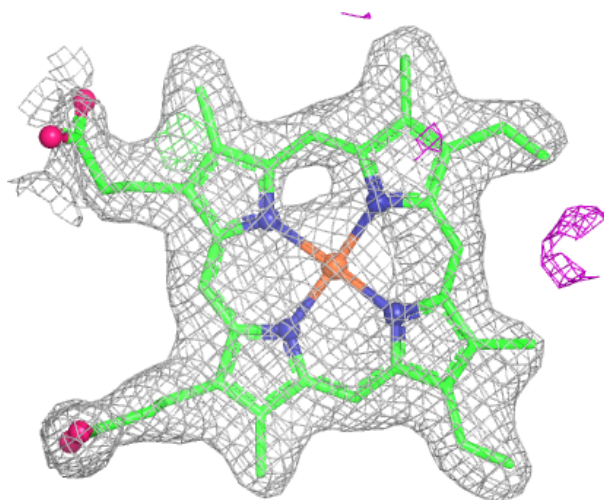
Electron density around KLA B 503:

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



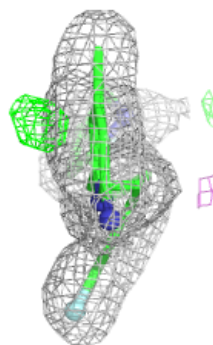
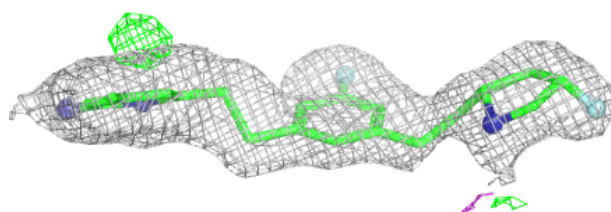
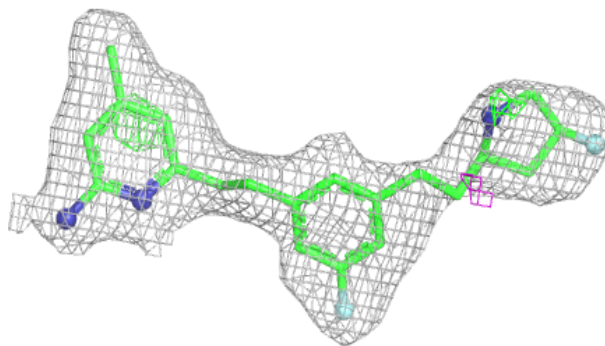
Electron density around HEM C 502:

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



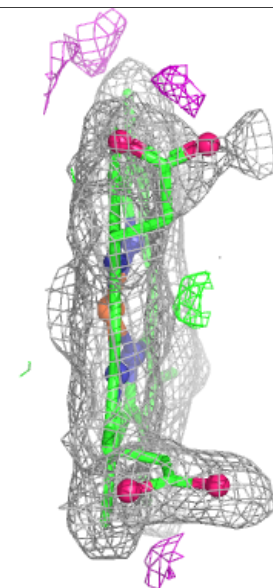
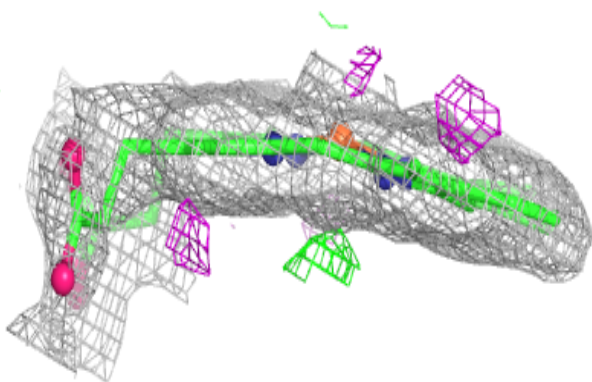
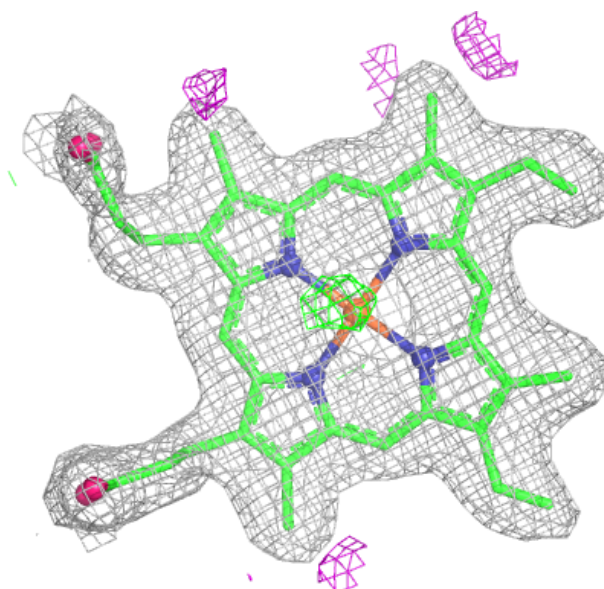
Electron density around KLA D 502:

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



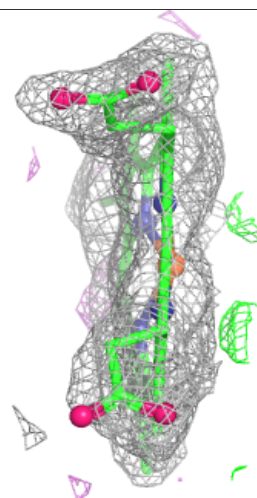
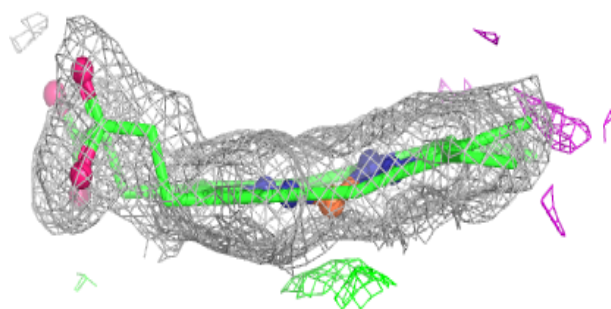
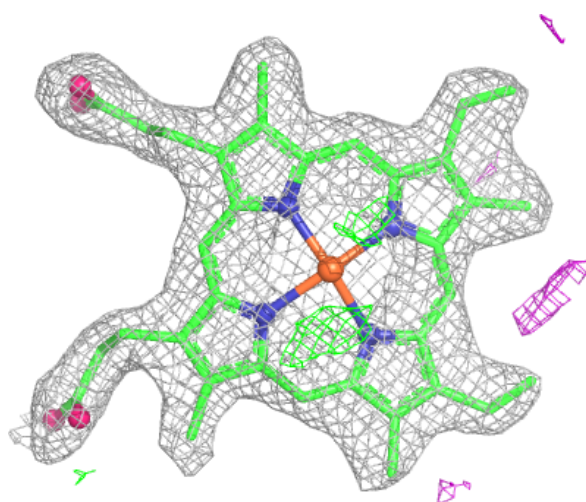
Electron density around HEM D 501:

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



Electron density around HEM 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.