



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:36 pm BST

PDB ID : 6NH1
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-fluoro-5-(3-(methylamino)prop-1-yn-1-yl)phenethyl)-4-methylpyridine-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2018-12-21
Resolution : 2.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

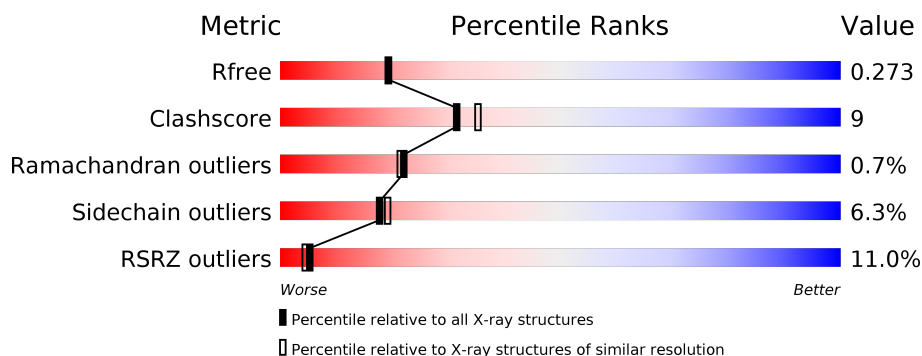
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>17%</div> <div> <div>66%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	440	<div> <div>7%</div> <div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
1	C	440	<div> <div>12%</div> <div> <div>68%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	440	<div> <div>5%</div> <div> <div>72%</div> <div>20%</div> <div>•</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTB	A	510	-	-	X	-
9	H4B	B	501	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13616 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	404	Total	C	N	O	S	0	3	0
			3241	2063	572	589	17			
1	C	402	Total	C	N	O	S	0	2	0
			3218	2050	565	587	16			
1	D	404	Total	C	N	O	S	0	3	0
			3241	2063	572	589	17			

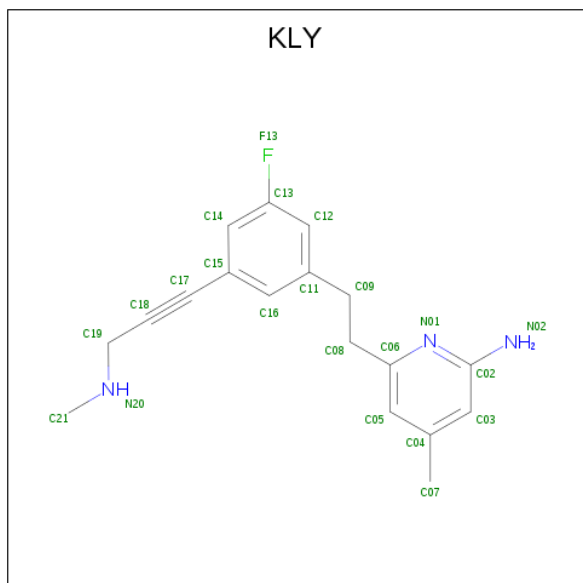
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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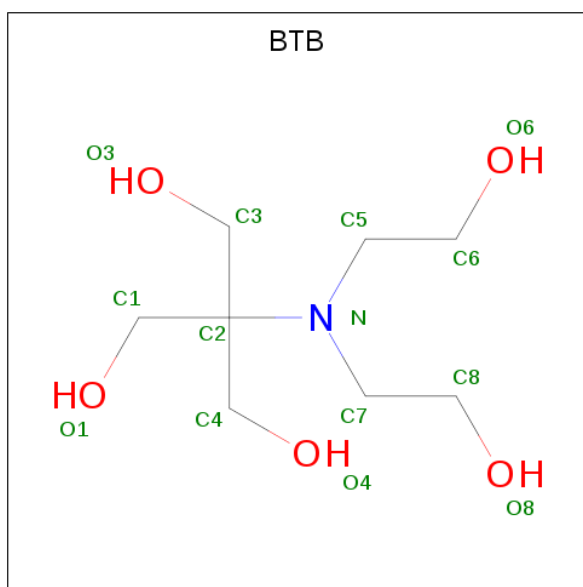
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-(2-{3-fluoro-5-[3-(methylamino)prop-1-yn-1-yl]phenyl}ethyl)-4-methylpyridine-2-amine (three-letter code: KLY) (formula: C₁₈H₂₀FN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			22	18	1	3		
3	B	1	Total	C	F	N	0	0
			22	18	1	3		
3	C	1	Total	C	F	N	0	0
			22	18	1	3		
3	D	1	Total	C	F	N	0	0
			22	18	1	3		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

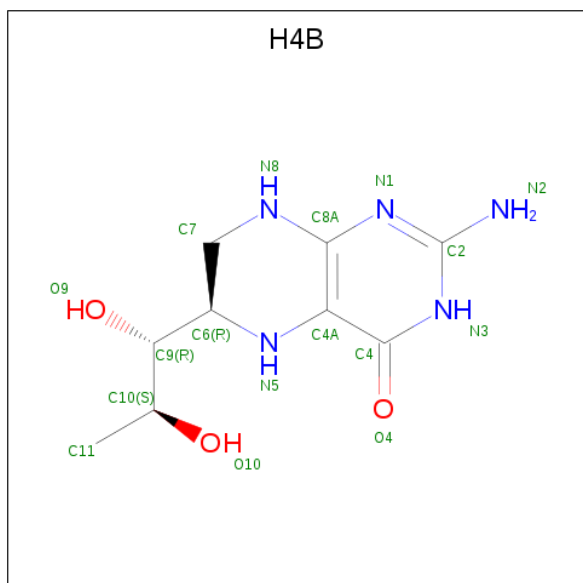
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 9 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



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

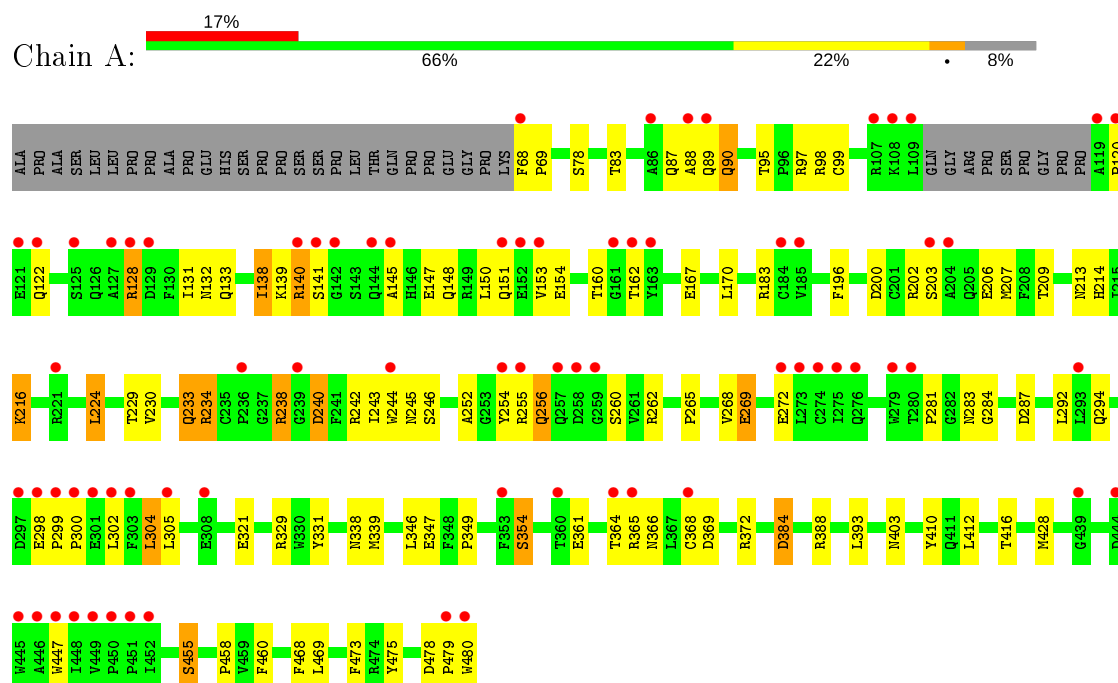
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	28	Total 28	O 28	0	0
10	B	56	Total 56	O 56	0	0
10	C	29	Total 29	O 29	0	0
10	D	60	Total 60	O 60	0	0

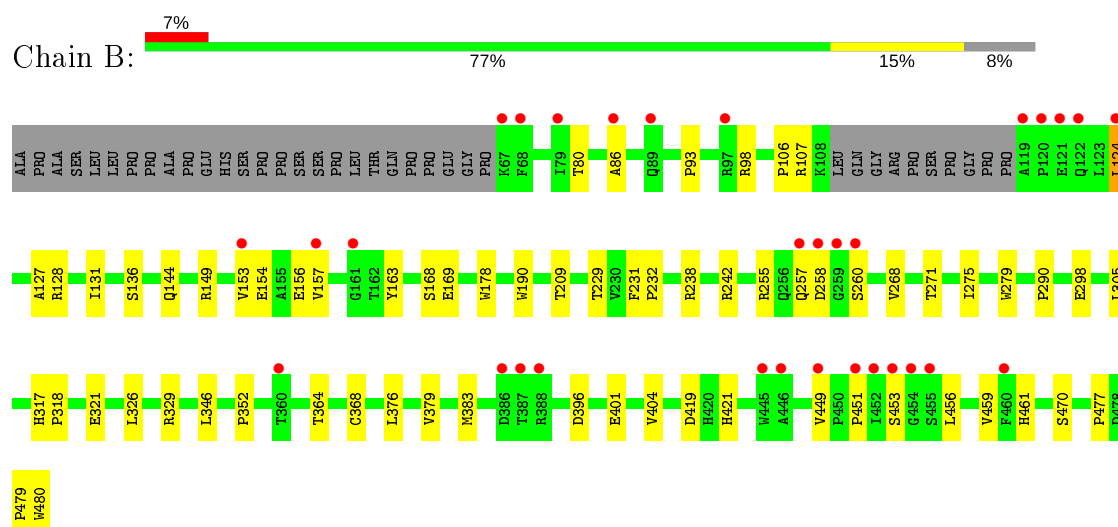
3 Residue-property plots [i](#)

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

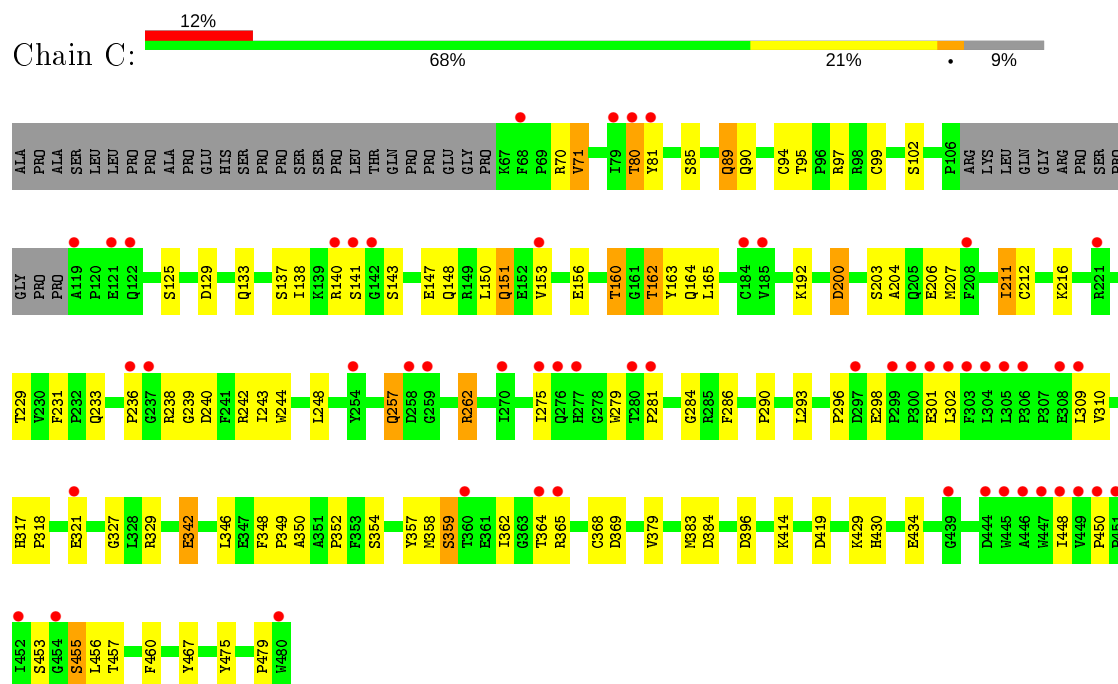
- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A



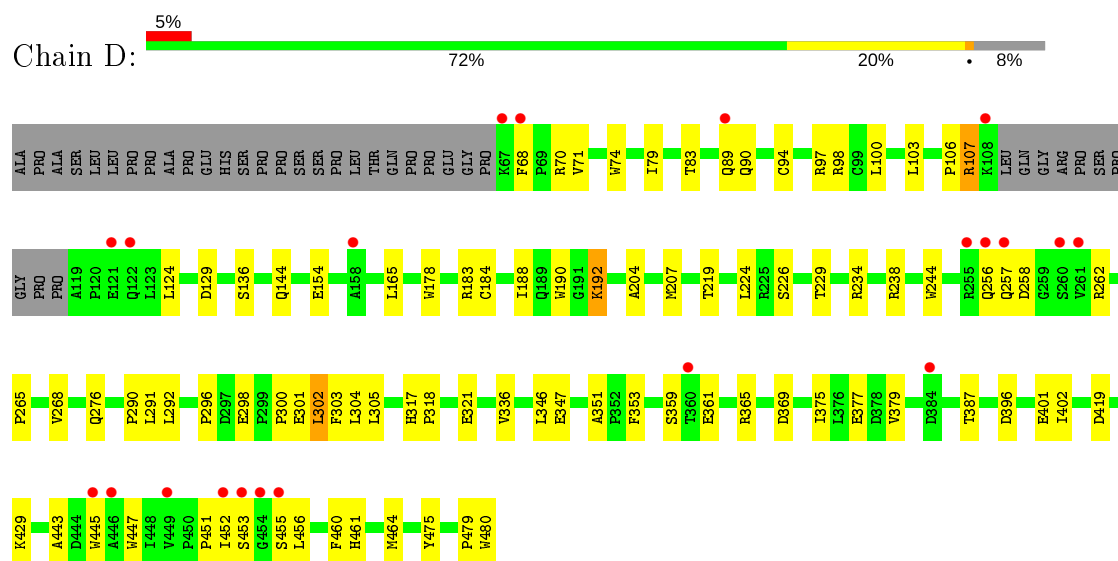
- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A



• 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	59.26 Å 152.46 Å 108.82 Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	38.99 – 2.22 38.99 – 2.22	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.99-2.22) 96.5 (38.99-2.22)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.22 Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.212 , 0.280 0.205 , 0.273	Depositor DCC
R_{free} test set	4608 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13616	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CL, GD, BTB, HEM, KLY

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	0.39	0/3335	0.57	0/4543
1	B	0.42	0/3339	0.57	0/4548
1	C	0.40	0/3316	0.55	0/4518
1	D	0.44	0/3339	0.60	1/4548 (0.0%)
All	All	0.41	0/13329	0.57	1/18157 (0.0%)

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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLN	Peptide
1	D	257	GLN	Peptide

5.2 Too-close contacts ⓘ

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	66	0
1	B	3241	0	3152	40	0
1	C	3218	0	3122	60	0
1	D	3241	0	3152	50	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	6	0
3	A	22	0	0	1	0
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	2	0
4	A	56	0	76	12	0
4	B	56	0	71	7	0
4	C	14	0	19	5	0
4	D	28	0	36	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	8	1	0
6	C	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	34	0	30	0	0
9	C	17	0	13	0	0
9	D	17	0	15	0	0
10	A	28	0	0	1	0
10	B	56	0	0	3	0
10	C	29	0	0	1	0
10	D	60	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13616	0	12968	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (237) 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	2.10	0.85
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.14	0.80
1:B:298:GLU:HG3	4:B:506:BTB:H31	1.66	0.77
4:A:510:BTB:O1	4:A:510:BTB:O4	1.94	0.76
1:D:100:LEU:HB3	1:D:103:LEU:HD12	1.68	0.75
1:D:321:GLU:OE2	4:D:504:BTB:O8	2.05	0.74
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.70	0.73
1:B:383:MET:HE1	1:B:401:GLU:HB2	1.70	0.72
4:A:510:BTB:O4	1:C:257:GLN:O	2.06	0.70
1:D:192:LYS:NZ	10:D:602:HOH:O	2.24	0.69
3:D:503:KLY:N20	10:D:603:HOH:O	2.25	0.69
1:A:361:GLU:OE2	3:A:502:KLY:N02	2.25	0.69
1:B:321:GLU:OE1	4:B:505:BTB:O4	2.12	0.68
1:D:321:GLU:OE1	4:D:504:BTB:H41	1.94	0.68
1:D:144:GLN:NE2	10:D:604:HOH:O	2.26	0.67
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.30	0.67
1:B:154:GLU:HA	1:B:157:VAL:HG12	1.77	0.67
1:A:365:ARG:NH1	1:A:369:ASP:OD2	2.28	0.67
4:A:510:BTB:O1	4:A:510:BTB:O3	2.13	0.66
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.78	0.66
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.78	0.65
1:B:238:ARG:NH2	10:B:602:HOH:O	2.27	0.65
1:D:443:ALA:HB1	1:D:464:MET:HE3	1.80	0.64
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.79	0.63
1:A:196:PHE:HB2	1:A:229:THR:HG22	1.79	0.63
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.81	0.63
1:C:453:SER:HA	1:D:452:ILE:HG22	1.81	0.62
1:A:88:ALA:HB3	1:A:469:LEU:HD23	1.81	0.62
1:B:480:TRP:OXT	10:B:601:HOH:O	2.16	0.62
1:A:167:GLU:OE2	6:A:507:GOL:O3	2.17	0.61
1:C:239:GLY:HA2	1:C:296:PRO:HB3	1.81	0.61
2:A:501:HEM:HMA2	2:A:501:HEM:HBA2	1.81	0.61
1:C:455:SER:HB3	1:D:451:PRO:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:TRP:CZ2	1:D:300:PRO:HG3	2.36	0.61
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.81	0.61
1:A:214:HIS:ND1	1:A:229:THR:HG23	2.16	0.60
1:D:361:GLU:HB3	1:D:365:ARG:NH2	2.17	0.60
1:C:200:ASP:OD1	1:C:200:ASP:N	2.35	0.60
1:C:147:GLU:O	1:C:151:GLN:NE2	2.34	0.60
1:A:97:ARG:NH2	1:B:86:ALA:O	2.35	0.59
4:C:504:BTB:O8	4:C:504:BTB:O6	2.18	0.59
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.84	0.59
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.82	0.59
2:B:502:HEM:HBB2	2:B:502:HEM:HHC	1.84	0.59
1:A:252:ALA:HB2	1:A:287:ASP:HB2	1.84	0.58
1:C:71:VAL:HG12	1:C:80:THR:HG23	1.86	0.58
1:C:359:SER:OG	1:C:419:ASP:HA	2.04	0.57
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.86	0.57
1:B:379:VAL:HG12	1:B:383:MET:HE3	1.86	0.57
1:A:242:ARG:HH22	1:A:478:ASP:HA	1.70	0.57
1:C:212:CYS:O	1:C:216:LYS:HG2	2.05	0.57
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.33	0.56
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.44	0.56
1:A:269:GLU:O	1:A:272:GLU:HB3	2.05	0.56
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.87	0.56
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.41	0.55
1:C:327:GLY:O	1:C:329:ARG:NH1	2.39	0.55
1:C:156:GLU:OE2	1:C:164:GLN:N	2.38	0.54
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.42	0.54
1:A:213:ASN:O	1:A:216:LYS:HG3	2.08	0.54
1:D:298:GLU:OE2	4:D:505:BTB:N	2.40	0.54
1:C:231:PHE:HB2	1:C:350:ALA:HB3	1.90	0.54
1:D:443:ALA:CB	1:D:464:MET:HE3	2.37	0.54
1:A:214:HIS:HD1	1:A:229:THR:HG23	1.74	0.53
1:C:138:ILE:HG13	1:C:140:ARG:HG2	1.90	0.53
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.17	0.53
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.91	0.53
1:C:160:THR:HG22	1:C:162:THR:H	1.73	0.53
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.91	0.52
1:A:255:ARG:HG3	1:A:256:GLN:H	1.74	0.52
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.92	0.52
1:C:206:GLU:OE1	1:C:206:GLU:N	2.38	0.52
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.91	0.51
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.45	0.51
1:B:124:LEU:HD23	1:B:157:VAL:HG11	1.92	0.51
1:D:68:PHE:CD2	1:D:83:THR:HG22	2.45	0.51
4:B:511:BTB:H41	4:B:511:BTB:O8	2.11	0.51
1:C:203:SER:OG	1:C:204:ALA:N	2.44	0.51
1:A:384:ASP:OD2	4:A:510:BTB:O1	2.27	0.50
1:A:364:THR:O	1:A:368:CYS:HB2	2.11	0.50
1:D:184:CYS:HB2	2:D:501:HEM:ND	2.25	0.50
1:D:379:VAL:HG21	1:D:402:ILE:HD11	1.93	0.50
1:A:238:ARG:HD2	1:A:238:ARG:N	2.27	0.49
1:D:154:GLU:OE2	10:D:601:HOH:O	2.18	0.49
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.47	0.49
1:D:377:GLU:H	1:D:377:GLU:CD	2.16	0.49
1:D:445:TRP:HA	1:D:464:MET:CE	2.42	0.49
1:D:455:SER:HA	1:D:460:PHE:CG	2.47	0.49
4:C:504:BTB:O1	4:C:504:BTB:O4	2.21	0.49
1:A:128:ARG:O	1:A:132:ASN:ND2	2.46	0.49
1:B:242:ARG:HH21	1:B:479:PRO:HD3	1.77	0.49
1:D:204:ALA:O	1:D:207:MET:HB2	2.13	0.49
1:B:449:VAL:HG22	1:B:459:VAL:HG23	1.94	0.49
1:D:336:VAL:HG22	1:D:353:PHE:CZ	2.48	0.49
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.48	0.49
4:C:504:BTB:HO8	4:C:504:BTB:HO6	1.59	0.48
1:A:479:PRO:HD2	1:A:480:TRP:CZ3	2.48	0.48
1:B:242:ARG:NH2	1:B:477:PRO:O	2.34	0.48
1:C:216:LYS:HD3	1:C:309:LEU:HD11	1.96	0.48
1:B:257:GLN:HG2	1:B:258:ASP:N	2.29	0.48
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.95	0.48
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.28	0.48
1:A:331:TYR:O	1:A:410:TYR:OH	2.29	0.48
4:A:510:BTB:H41	1:C:257:GLN:OE1	2.14	0.48
1:A:214:HIS:NE2	1:A:354:SER:HB3	2.29	0.47
1:A:298:GLU:HG2	4:A:505:BTB:H12	1.94	0.47
1:D:188:ILE:HD13	1:D:429:LYS:HG3	1.96	0.47
1:A:366:ASN:OD1	1:A:372:ARG:NH2	2.48	0.47
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.50	0.47
1:A:196:PHE:CD2	1:A:229:THR:HG22	2.48	0.47
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.25	0.47
1:A:455:SER:HB3	1:B:451:PRO:HB2	1.97	0.47
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.96	0.47
1:A:224:LEU:HB2	1:A:416:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HG	1:A:302:LEU:HD23	1.97	0.47
1:C:244:TRP:CD1	1:C:479:PRO:HG3	2.50	0.47
1:C:129:ASP:O	1:C:133:GLN:HG3	2.14	0.46
1:C:262:ARG:HH11	1:C:284:GLY:HA2	1.81	0.46
1:D:361:GLU:HB3	1:D:365:ARG:HH22	1.78	0.46
1:A:388:ARG:HG3	4:A:510:BTB:H82	1.98	0.46
1:A:145:ALA:HA	1:A:148:GLN:HB3	1.97	0.46
1:A:160:THR:HG22	1:A:162:THR:H	1.80	0.46
4:C:504:BTB:H72	4:C:504:BTB:H32	1.34	0.46
1:D:219:THR:HA	1:D:224:LEU:HD13	1.97	0.46
1:D:375:ILE:O	1:D:379:VAL:HG23	2.15	0.46
1:D:89:GLN:HG3	1:D:90:GLN:N	2.31	0.46
1:C:141:SER:C	1:C:143:SER:H	2.19	0.46
1:C:165:LEU:HG	1:C:346:LEU:HD12	1.99	0.45
1:C:379:VAL:O	1:C:383:MET:HG3	2.16	0.45
1:A:90:GLN:HB3	1:A:468:PHE:CD1	2.50	0.45
1:B:231:PHE:HB3	1:B:232:PRO:CD	2.46	0.45
1:B:379:VAL:CG1	1:B:383:MET:HE3	2.46	0.45
1:A:240:ASP:HB3	1:A:349:PRO:HG2	1.98	0.45
1:D:291:LEU:HD11	1:D:305:LEU:HD21	1.99	0.45
1:B:419:ASP:OD1	1:B:421:HIS:N	2.50	0.45
1:C:192:LYS:HD3	1:C:192:LYS:N	2.32	0.45
4:D:504:BTB:H42	4:D:504:BTB:H72	1.71	0.45
1:B:124:LEU:HA	1:B:124:LEU:HD22	1.73	0.45
1:D:238:ARG:HD2	1:D:238:ARG:HA	1.63	0.45
1:B:364:THR:O	1:B:368:CYS:HB2	2.17	0.45
1:D:165:LEU:HG	1:D:346:LEU:HD12	1.98	0.45
1:D:445:TRP:HA	1:D:464:MET:HE2	1.99	0.45
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.97	0.45
1:A:233:GLN:O	1:A:233:GLN:HG2	2.16	0.45
1:A:338:ASN:N	10:A:604:HOH:O	2.50	0.45
1:A:183:ARG:HD3	1:A:447:TRP:CE2	2.51	0.45
4:D:505:BTB:H81	4:D:505:BTB:H52	1.32	0.45
1:A:393:LEU:HD12	1:B:404:VAL:HG23	2.00	0.44
1:B:127:ALA:O	1:B:131:ILE:HG12	2.17	0.44
1:B:163:TYR:CZ	1:B:346:LEU:HD11	2.53	0.44
1:C:293:LEU:HD13	1:C:293:LEU:HA	1.69	0.44
1:A:339:MET:HE2	1:A:473:PHE:HB3	2.00	0.44
1:C:97:ARG:NH2	10:C:604:HOH:O	2.44	0.44
4:A:503:BTB:H11	4:A:503:BTB:H51	1.72	0.44
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:HD12	1:D:124:LEU:HA	1.86	0.44
1:A:131:ILE:CD1	1:A:153:VAL:HG21	2.47	0.43
1:A:299:PRO:HB2	1:A:300:PRO:HD2	2.00	0.43
4:B:506:BTB:H72	4:B:506:BTB:H42	1.42	0.43
1:C:207:MET:SD	1:C:293:LEU:HD12	2.58	0.43
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.52	0.43
4:A:510:BTB:H11	4:A:510:BTB:H52	1.56	0.43
2:A:501:HEM:CMA	2:A:501:HEM:HBA2	2.48	0.43
4:A:510:BTB:H72	4:A:510:BTB:H42	1.89	0.43
1:B:255:ARG:HB3	10:B:605:HOH:O	2.18	0.43
1:C:153:VAL:HG13	1:C:163:TYR:CG	2.54	0.43
1:A:151:GLN:HA	1:A:154:GLU:HG2	2.01	0.43
1:B:128:ARG:NH1	1:B:154:GLU:OE1	2.52	0.43
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.53	0.43
1:D:359:SER:OG	1:D:419:ASP:HA	2.19	0.43
4:B:506:BTB:H52	4:B:506:BTB:H11	1.72	0.43
1:C:430:HIS:CE1	1:C:434:GLU:HG3	2.53	0.43
1:A:242:ARG:HB2	1:A:294:GLN:HE21	1.83	0.42
1:A:244:TRP:CE2	1:A:479:PRO:HG2	2.53	0.42
1:C:229:THR:O	1:C:352:PRO:HD2	2.19	0.42
1:A:246:SER:HA	1:A:338:ASN:ND2	2.35	0.42
1:C:342:GLU:HA	1:C:346:LEU:O	2.18	0.42
1:D:229:THR:O	1:D:351:ALA:HA	2.20	0.42
1:D:74:TRP:HB2	1:D:461:HIS:HB3	2.01	0.42
1:A:203:SER:HB3	1:A:206:GLU:HB2	2.00	0.42
1:B:229:THR:O	1:B:352:PRO:HD2	2.18	0.42
1:C:448:ILE:HD13	1:C:448:ILE:HA	1.89	0.42
1:C:242:ARG:HA	1:C:242:ARG:HD2	1.81	0.42
1:B:149:ARG:O	1:B:153:VAL:HG23	2.19	0.42
1:C:233:GLN:OE1	1:C:346:LEU:HD13	2.20	0.42
1:A:455:SER:HA	1:A:460:PHE:CG	2.55	0.42
4:A:510:BTB:HO3	4:A:510:BTB:HO1	1.63	0.42
2:B:502:HEM:HBA2	2:B:502:HEM:CMA	2.50	0.42
1:C:262:ARG:NH1	1:C:284:GLY:HA2	2.34	0.42
1:D:265:PRO:HA	1:D:268:VAL:HG23	2.02	0.42
1:A:321:GLU:CD	1:A:321:GLU:H	2.23	0.42
1:B:124:LEU:HD21	1:B:154:GLU:HB3	2.02	0.42
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.92	0.42
1:C:211:ILE:HD13	1:C:248:LEU:HD22	2.01	0.42
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.75	0.41
1:A:252:ALA:HB1	1:A:254:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HH11	1:B:461:HIS:CE1	2.38	0.41
1:C:150:LEU:HB2	1:C:151:GLN:NE2	2.36	0.41
1:C:358:MET:HE2	2:C:501:HEM:CMA	2.50	0.41
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.55	0.41
1:A:243:ILE:HG22	1:A:245:ASN:H	1.84	0.41
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.56	0.41
1:D:234:ARG:NH1	1:D:347:GLU:OE2	2.54	0.41
1:A:339:MET:HE2	1:A:339:MET:HB3	1.95	0.41
1:B:156:GLU:OE2	1:B:163:TYR:HA	2.20	0.41
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.56	0.41
1:C:286:PHE:CD2	1:C:329:ARG:HD2	2.56	0.41
1:D:301:GLU:HB3	1:D:303:PHE:HE1	1.85	0.41
1:A:412:LEU:HA	1:A:412:LEU:HD12	1.79	0.41
1:A:428:MET:HG3	1:A:458:PRO:HB2	2.03	0.41
1:A:244:TRP:NE1	1:A:479:PRO:HG2	2.35	0.41
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.56	0.41
1:C:364:THR:O	1:C:368:CYS:HB2	2.20	0.41
1:C:85:SER:HB3	1:C:467:TYR:CE1	2.56	0.41
1:A:138:ILE:O	1:A:140:ARG:HG2	2.21	0.41
1:A:139:LYS:O	1:A:141:SER:N	2.53	0.41
1:C:243:ILE:HG12	1:C:293:LEU:HD11	2.02	0.41
1:A:262:ARG:HE	1:A:284:GLY:HA3	1.86	0.41
1:A:298:GLU:CD	4:A:505:BTB:H12	2.42	0.41
1:B:326:LEU:HD23	4:B:510:BTB:H52	2.03	0.41
1:C:70:ARG:HB2	1:C:81:TYR:CE2	2.55	0.41
4:D:505:BTB:H32	4:D:505:BTB:H51	1.66	0.41
1:A:68:PHE:CD2	1:A:83:THR:HG22	2.56	0.41
1:D:238:ARG:HG3	1:D:296:PRO:HB3	2.02	0.41
1:D:292:LEU:HD23	1:D:302:LEU:HD13	2.02	0.41
2:D:501:HEM:HBA1	3:D:503:KLY:C09	2.51	0.41
1:C:240:ASP:OD1	1:C:349:PRO:HG2	2.22	0.40
1:C:455:SER:HA	1:C:460:PHE:CG	2.56	0.40
1:A:244:TRP:HE1	1:A:294:GLN:NE2	2.19	0.40
4:B:510:BTB:H32	4:B:510:BTB:H51	1.66	0.40
1:C:279:TRP:HB2	1:C:302:LEU:HD21	2.03	0.40
1:B:271:THR:O	1:B:275:ILE:HG13	2.21	0.40
1:C:298:GLU:OE2	4:C:504:BTB:N	2.54	0.40
1:A:304:LEU:HD23	1:A:305:LEU:H	1.87	0.40
1:B:149:ARG:NE	1:B:169:GLU:OE2	2.52	0.40
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/440 (91%)	364 (90%)	33 (8%)	5 (1%)	13	9
1	B	403/440 (92%)	383 (95%)	18 (4%)	2 (0%)	29	30
1	C	400/440 (91%)	382 (96%)	16 (4%)	2 (0%)	29	30
1	D	403/440 (92%)	389 (96%)	12 (3%)	2 (0%)	29	30
All	All	1608/1760 (91%)	1518 (94%)	79 (5%)	11 (1%)	22	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PRO
1	A	283	ASN
1	A	90	GLN
1	D	107	ARG
1	B	107	ARG
1	C	89	GLN
1	A	140	ARG
1	A	281	PRO
1	C	236	PRO
1	D	106	PRO
1	B	260	SER

5.3.2 Protein sidechains [i](#)

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%)	316 (92%)	29 (8%)	11	10
1	B	346/373 (93%)	334 (96%)	12 (4%)	36	44
1	C	343/373 (92%)	314 (92%)	29 (8%)	10	9
1	D	346/373 (93%)	329 (95%)	17 (5%)	25	29
All	All	1380/1492 (92%)	1293 (94%)	87 (6%)	18	19

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	87	GLN
1	A	89	GLN
1	A	95	THR
1	A	98	ARG
1	A	99	CYS
1	A	128	ARG
1	A	133	GLN
1	A	138	ILE
1	A	200	ASP
1	A	202	ARG
1	A	207	MET
1	A	209	THR
1	A	216	LYS
1	A	224	LEU
1	A	233	GLN
1	A	234	ARG
1	A	238	ARG
1	A	240	ASP
1	A	256	GLN
1	A	260	SER
1	A	269	GLU
1	A	304	LEU
1	A	329	ARG
1	A	346	LEU
1	A	354	SER
1	A	384	ASP
1	A	403	ASN
1	A	455	SER
1	B	80	THR
1	B	98	ARG
1	B	124	LEU
1	B	136	SER

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Mol	Chain	Res	Type
1	B	144	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	209	THR
1	B	268	VAL
1	B	329	ARG
1	B	396	ASP
1	B	470	SER
1	C	71	VAL
1	C	80	THR
1	C	89	GLN
1	C	90	GLN
1	C	95	THR
1	C	99	CYS
1	C	102	SER
1	C	125	SER
1	C	137	SER
1	C	148	GLN
1	C	151	GLN
1	C	160	THR
1	C	162	THR
1	C	200	ASP
1	C	211	ILE
1	C	238	ARG
1	C	257	GLN
1	C	262	ARG
1	C	301	GLU
1	C	310	VAL
1	C	321	GLU
1	C	342	GLU
1	C	354	SER
1	C	359	SER
1	C	384	ASP
1	C	396	ASP
1	C	414	LYS
1	C	429	LYS
1	C	455	SER
1	D	70	ARG
1	D	71	VAL
1	D	79	ILE
1	D	97	ARG
1	D	98	ARG

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Mol	Chain	Res	Type
1	D	107	ARG
1	D	129	ASP
1	D	136	SER
1	D	192	LYS
1	D	226	SER
1	D	256	GLN
1	D	258	ASP
1	D	262	ARG
1	D	276	GLN
1	D	302	LEU
1	D	387	THR
1	D	396	ASP

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

Mol	Chain	Res	Type
1	A	294	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 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	B	502	1	27,50,50	1.89	5 (18%)	17,82,82	2.37	7 (41%)
9	H4B	B	503	-	16,18,18	0.85	0	11,26,26	2.60	6 (54%)
2	HEM	D	501	1	27,50,50	1.79	4 (14%)	17,82,82	2.09	9 (52%)
4	BTB	B	505	8	13,13,13	0.53	0	7,16,16	0.72	0
4	BTB	A	505	-	13,13,13	0.43	0	7,16,16	0.66	0
4	BTB	A	510	-	13,13,13	1.64	2 (15%)	7,16,16	2.65	2 (28%)
4	BTB	A	504	-	13,13,13	0.53	0	7,16,16	1.13	0
9	H4B	D	502	-	16,18,18	0.85	0	11,26,26	2.88	6 (54%)
4	BTB	B	511	-	13,13,13	0.82	1 (7%)	7,16,16	1.54	2 (28%)
2	HEM	A	501	1	27,50,50	1.89	5 (18%)	17,82,82	2.12	4 (23%)
9	H4B	C	502	2	16,18,18	1.24	1 (6%)	11,26,26	2.70	4 (36%)
4	BTB	B	510	8	13,13,13	0.38	0	7,16,16	0.82	0
3	KLY	A	502	-	22,23,23	1.55	1 (4%)	28,30,30	2.07	8 (28%)
6	GOL	A	507	-	5,5,5	0.41	0	5,5,5	0.61	0
3	KLY	C	503	-	22,23,23	1.56	1 (4%)	28,30,30	1.97	9 (32%)
9	H4B	B	501	-	16,18,18	0.92	0	11,26,26	2.47	6 (54%)
2	HEM	C	501	1,9	27,50,50	1.90	4 (14%)	17,82,82	1.88	3 (17%)
4	BTB	A	503	8	13,13,13	0.35	0	7,16,16	0.55	0
4	BTB	C	504	-	13,13,13	0.48	0	7,16,16	0.31	0
4	BTB	D	505	-	13,13,13	0.63	0	7,16,16	1.06	0
3	KLY	B	504	-	22,23,23	1.42	1 (4%)	28,30,30	1.99	11 (39%)
4	BTB	B	506	-	13,13,13	0.38	0	7,16,16	0.79	0
3	KLY	D	503	-	22,23,23	1.53	1 (4%)	28,30,30	2.67	13 (46%)
4	BTB	D	504	8	13,13,13	0.73	0	7,16,16	1.36	1 (14%)
6	GOL	C	506	-	5,5,5	0.46	0	5,5,5	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	502	1	-	3/6/54/54	-
9	H4B	B	503	-	-	4/8/17/17	0/2/2/2
2	HEM	D	501	1	-	1/6/54/54	-
4	BTB	B	505	8	-	4/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	A	505	-	-	11/21/21/21	-
4	BTB	A	510	-	-	8/21/21/21	-
4	BTB	A	504	-	-	5/21/21/21	-
9	H4B	D	502	-	-	4/8/17/17	0/2/2/2
4	BTB	B	511	-	-	5/21/21/21	-
2	HEM	A	501	1	-	3/6/54/54	-
9	H4B	C	502	2	-	0/8/17/17	0/2/2/2
4	BTB	B	510	8	-	4/21/21/21	-
3	KLY	A	502	-	-	3/8/10/10	0/2/2/2
6	GOL	A	507	-	-	4/4/4/4	-
3	KLY	C	503	-	-	0/8/10/10	0/2/2/2
9	H4B	B	501	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1,9	-	1/6/54/54	-
4	BTB	A	503	8	-	1/21/21/21	-
4	BTB	C	504	-	-	7/21/21/21	-
4	BTB	D	505	-	-	9/21/21/21	-
3	KLY	B	504	-	-	1/8/10/10	0/2/2/2
4	BTB	B	506	-	-	3/21/21/21	-
3	KLY	D	503	-	-	1/8/10/10	0/2/2/2
4	BTB	D	504	8	-	7/21/21/21	-
6	GOL	C	506	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	KLY	C15-C17	-6.98	1.27	1.44
3	D	503	KLY	C15-C17	-6.54	1.28	1.44
3	A	502	KLY	C15-C17	-6.36	1.29	1.44
3	B	504	KLY	C15-C17	-6.11	1.29	1.44
2	B	502	HEM	C3B-C2B	-5.35	1.32	1.40
2	C	501	HEM	C3B-C2B	-4.73	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.40	1.34	1.40
4	A	510	BTB	C4-C2	-4.34	1.47	1.53
2	D	501	HEM	C3B-C2B	-4.24	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.03	1.34	1.40
2	D	501	HEM	C3C-C2C	-3.87	1.35	1.40
2	C	501	HEM	C3B-CAB	3.85	1.55	1.47
2	A	501	HEM	C3C-CAC	3.77	1.55	1.47
2	D	501	HEM	C3C-CAC	3.71	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	C3C-C2C	-3.68	1.35	1.40
2	C	501	HEM	C3C-CAC	3.65	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.61	1.35	1.40
2	B	502	HEM	C3B-CAB	3.60	1.55	1.47
2	B	502	HEM	C3C-CAC	3.60	1.55	1.47
2	A	501	HEM	C3B-CAB	3.54	1.55	1.47
2	D	501	HEM	C3B-CAB	3.50	1.55	1.47
4	A	510	BTB	C1-C2	-3.27	1.49	1.53
9	C	502	H4B	C4-C4A	-3.01	1.37	1.41
2	A	501	HEM	CAA-C2A	2.65	1.55	1.52
4	B	511	BTB	C1-C2	-2.10	1.50	1.53
2	B	502	HEM	CAA-C2A	2.03	1.55	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	502	H4B	C4-C4A-C8A	7.04	120.82	114.57
9	D	502	H4B	C4-C4A-C8A	6.04	119.93	114.57
4	A	510	BTB	O4-C4-C2	-5.72	95.78	111.44
3	D	503	KLY	C14-C15-C17	-5.62	109.88	120.19
3	D	503	KLY	C02-N01-C06	5.47	122.25	118.10
3	A	502	KLY	C08-C06-N01	5.42	124.02	115.95
3	D	503	KLY	C16-C15-C17	5.36	130.03	120.19
9	B	501	H4B	C4-C4A-C8A	5.18	119.17	114.57
3	D	503	KLY	C15-C17-C18	-4.75	163.82	176.52
2	A	501	HEM	CMA-C3A-C4A	-4.67	121.29	128.46
2	B	502	HEM	CAD-CBD-CGD	-4.34	105.39	112.67
2	B	502	HEM	CMA-C3A-C4A	-4.33	121.81	128.46
3	C	503	KLY	C02-N01-C06	4.27	121.34	118.10
9	B	503	H4B	C4-C4A-C8A	4.23	118.33	114.57
2	D	501	HEM	CMA-C3A-C4A	-4.12	122.13	128.46
3	C	503	KLY	C15-C17-C18	-4.01	165.79	176.52
3	B	504	KLY	C16-C15-C17	3.96	127.46	120.19
3	C	503	KLY	C12-C13-C14	-3.92	118.57	123.52
9	B	503	H4B	C4-C4A-N5	3.81	122.32	119.12
2	C	501	HEM	CAA-CBA-CGA	-3.79	106.31	112.67
3	D	503	KLY	C05-C06-N01	-3.79	118.88	122.90
3	B	504	KLY	C14-C15-C17	-3.70	113.40	120.19
3	A	502	KLY	C02-N01-C06	3.69	120.90	118.10
9	D	502	H4B	C4A-N5-C6	-3.64	111.25	121.16
3	D	503	KLY	C12-C13-C14	-3.53	119.06	123.52
3	A	502	KLY	C08-C06-C05	-3.51	116.58	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	H4B	N3-C2-N1	-3.51	119.92	125.42
2	A	501	HEM	CAA-CBA-CGA	-3.49	106.81	112.67
3	B	504	KLY	C08-C06-N01	3.44	121.07	115.95
3	A	502	KLY	N02-C02-N01	3.42	121.90	116.49
3	A	502	KLY	C12-C13-C14	-3.40	119.23	123.52
2	D	501	HEM	CBD-CAD-C3D	-3.38	106.25	112.48
2	C	501	HEM	CMA-C3A-C4A	-3.34	123.33	128.46
2	A	501	HEM	CBA-CAA-C2A	3.32	118.61	112.49
3	A	502	KLY	C05-C06-N01	-3.30	119.40	122.90
3	D	503	KLY	C09-C11-C12	-3.29	115.14	120.54
4	D	504	BTB	O3-C3-C2	3.21	120.24	111.44
9	B	501	H4B	N3-C2-N1	-3.20	120.40	125.42
3	D	503	KLY	C08-C06-N01	3.18	120.68	115.95
2	B	502	HEM	CBA-CAA-C2A	3.17	118.33	112.49
9	D	502	H4B	C4-C4A-N5	3.17	121.78	119.12
3	B	504	KLY	C12-C13-C14	-3.17	119.52	123.52
3	A	502	KLY	F13-C13-C12	3.15	122.75	118.25
3	B	504	KLY	C15-C17-C18	-3.14	168.13	176.52
9	B	501	H4B	C4-N3-C2	3.10	120.86	115.93
2	A	501	HEM	CMA-C3A-C2A	3.08	130.74	124.94
2	B	502	HEM	CAA-CBA-CGA	-3.05	107.55	112.67
9	B	503	H4B	C4-N3-C2	3.05	120.77	115.93
2	D	501	HEM	C4A-C3A-C2A	2.97	109.06	107.00
9	D	502	H4B	C4-N3-C2	2.97	120.64	115.93
4	B	511	BTB	O1-C1-C2	-2.95	103.37	111.44
9	B	503	H4B	C2-N1-C8A	2.94	121.13	114.54
4	A	510	BTB	O1-C1-C2	-2.90	103.51	111.44
3	C	503	KLY	C08-C09-C11	-2.89	103.12	113.28
9	D	502	H4B	N3-C2-N1	-2.82	120.99	125.42
9	C	502	H4B	N3-C2-N1	-2.78	121.06	125.42
2	B	502	HEM	CMA-C3A-C2A	2.71	130.06	124.94
9	C	502	H4B	C2-N1-C8A	2.70	120.59	114.54
9	B	501	H4B	C2-N1-C8A	2.69	120.57	114.54
3	B	504	KLY	C05-C06-N01	-2.67	120.07	122.90
3	A	502	KLY	C11-C12-C13	2.65	121.22	118.81
9	D	502	H4B	C2-N1-C8A	2.61	120.39	114.54
2	C	501	HEM	CBA-CAA-C2A	-2.61	107.67	112.49
2	D	501	HEM	CMC-C2C-C3C	2.56	129.47	124.68
2	B	502	HEM	C1D-C2D-C3D	2.56	108.78	107.00
3	C	503	KLY	C08-C06-N01	2.51	119.69	115.95
2	B	502	HEM	CBD-CAD-C3D	-2.45	107.96	112.48
3	D	503	KLY	C09-C11-C16	2.44	124.55	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	KLY	F13-C13-C12	2.38	121.66	118.25
3	B	504	KLY	N02-C02-N01	2.38	120.25	116.49
3	B	504	KLY	F13-C13-C12	2.34	121.60	118.25
3	C	503	KLY	C11-C12-C13	2.34	120.94	118.81
3	B	504	KLY	C09-C11-C12	-2.33	116.71	120.54
3	D	503	KLY	N02-C02-N01	2.32	120.15	116.49
3	C	503	KLY	C04-C05-C06	-2.30	118.81	120.32
2	D	501	HEM	CAD-CBD-CGD	-2.30	108.81	112.67
9	B	503	H4B	N2-C2-N3	2.30	120.83	117.25
3	B	504	KLY	C08-C09-C11	-2.26	105.34	113.28
2	D	501	HEM	C3C-C4C-NC	-2.25	106.70	110.94
3	B	504	KLY	C02-N01-C06	2.24	119.80	118.10
4	B	511	BTB	O4-C4-C2	-2.20	105.41	111.44
9	C	502	H4B	C4-N3-C2	2.17	119.37	115.93
2	D	501	HEM	CMD-C2D-C1D	-2.15	125.17	128.46
3	D	503	KLY	C15-C16-C11	-2.14	118.11	120.29
3	C	503	KLY	C14-C15-C17	-2.09	116.36	120.19
9	B	501	H4B	C4-C4A-N5	2.09	120.87	119.12
2	D	501	HEM	C1D-C2D-C3D	2.09	108.45	107.00
3	C	503	KLY	F13-C13-C12	2.07	121.20	118.25
2	D	501	HEM	CMA-C3A-C2A	2.05	128.81	124.94
9	B	501	H4B	N2-C2-N3	2.02	120.39	117.25
3	D	503	KLY	C11-C12-C13	2.00	120.63	118.81

There are no chirality outliers.

All (94) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	A	505	BTB	C1-C2-N-C5
4	A	505	BTB	C1-C2-N-C7
4	A	505	BTB	C3-C2-N-C5
4	A	505	BTB	C3-C2-N-C7
4	A	505	BTB	C4-C2-N-C5
4	A	505	BTB	C4-C2-N-C7
4	A	510	BTB	C1-C2-C3-O3
4	A	510	BTB	C4-C2-N-C7
4	A	510	BTB	C6-C5-N-C7
4	A	504	BTB	O1-C1-C2-C3
4	A	504	BTB	O1-C1-C2-C4
4	A	504	BTB	O1-C1-C2-N
3	B	504	KLY	C18-C19-N20-C21
9	D	502	H4B	N5-C6-C9-O9
9	D	502	H4B	N5-C6-C9-C10
9	D	502	H4B	C7-C6-C9-O9
9	D	502	H4B	C7-C6-C9-C10
4	B	511	BTB	C1-C2-C3-O3
4	B	511	BTB	C4-C2-C3-O3
4	B	511	BTB	N-C2-C3-O3
4	B	511	BTB	C8-C7-N-C5
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
4	B	510	BTB	O1-C1-C2-C3
4	B	510	BTB	O1-C1-C2-C4
4	B	510	BTB	O1-C1-C2-N
3	A	502	KLY	C18-C19-N20-C21
6	A	507	GOL	O1-C1-C2-C3
9	B	501	H4B	C7-C6-C9-O9
9	B	501	H4B	C7-C6-C9-C10
4	D	505	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-C4-O4
4	D	505	BTB	C3-C2-C4-O4
4	D	505	BTB	N-C2-C4-O4
4	D	505	BTB	C8-C7-N-C5
2	C	501	HEM	C2A-CAA-CBA-CGA
4	A	503	BTB	C8-C7-N-C5
4	C	504	BTB	C1-C2-C3-O3
4	C	504	BTB	C3-C2-C4-O4
4	B	506	BTB	O1-C1-C2-C3

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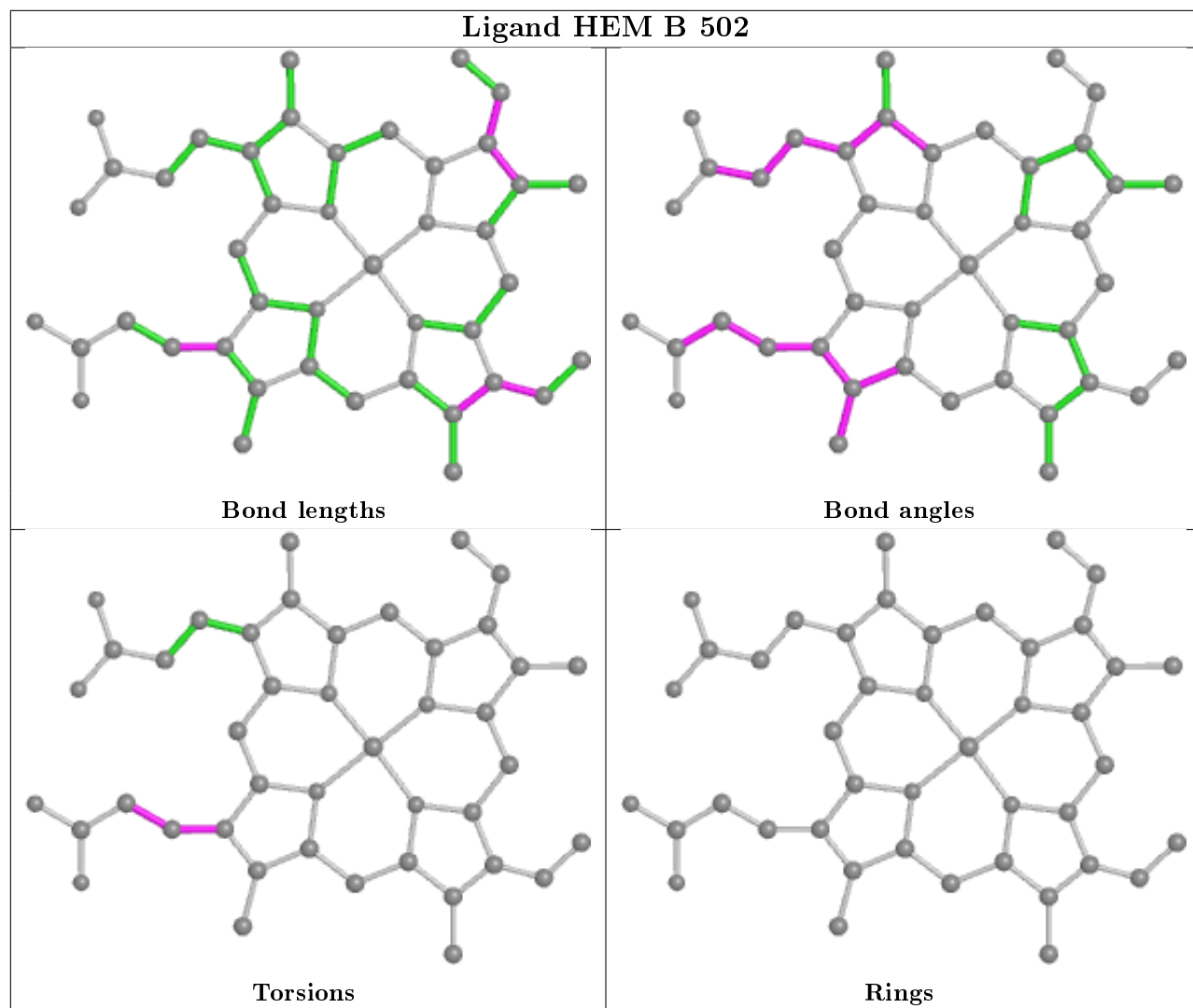
Mol	Chain	Res	Type	Atoms
4	B	506	BTB	O1-C1-C2-C4
3	D	503	KLY	C18-C19-N20-C21
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	C3-C2-C4-O4
6	C	506	GOL	O1-C1-C2-C3
4	B	510	BTB	N-C5-C6-O6
4	D	504	BTB	N-C7-C8-O8
4	D	505	BTB	N-C7-C8-O8
6	A	507	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
6	C	506	GOL	O1-C1-C2-O2
4	B	511	BTB	N-C5-C6-O6
6	A	507	GOL	O2-C2-C3-O3
4	A	504	BTB	N-C5-C6-O6
4	A	510	BTB	N-C7-C8-O8
3	A	502	KLY	N01-C06-C08-C09
9	B	501	H4B	N5-C6-C9-O9
4	C	504	BTB	C1-C2-C4-O4
4	A	505	BTB	N-C2-C3-O3
4	A	510	BTB	N-C2-C3-O3
4	A	510	BTB	C1-C2-N-C7
4	A	510	BTB	C3-C2-N-C7
4	D	505	BTB	C1-C2-N-C7
4	C	504	BTB	O1-C1-C2-N
4	C	504	BTB	N-C2-C3-O3
4	C	504	BTB	N-C2-C4-O4
4	B	506	BTB	O1-C1-C2-N
4	D	504	BTB	N-C2-C4-O4
4	D	504	BTB	N-C5-C6-O6
3	A	502	KLY	C05-C06-C08-C09
4	B	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
4	A	505	BTB	C1-C2-C4-O4
4	A	510	BTB	C4-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	C	504	BTB	C4-C2-C3-O3
4	D	504	BTB	C1-C2-C4-O4

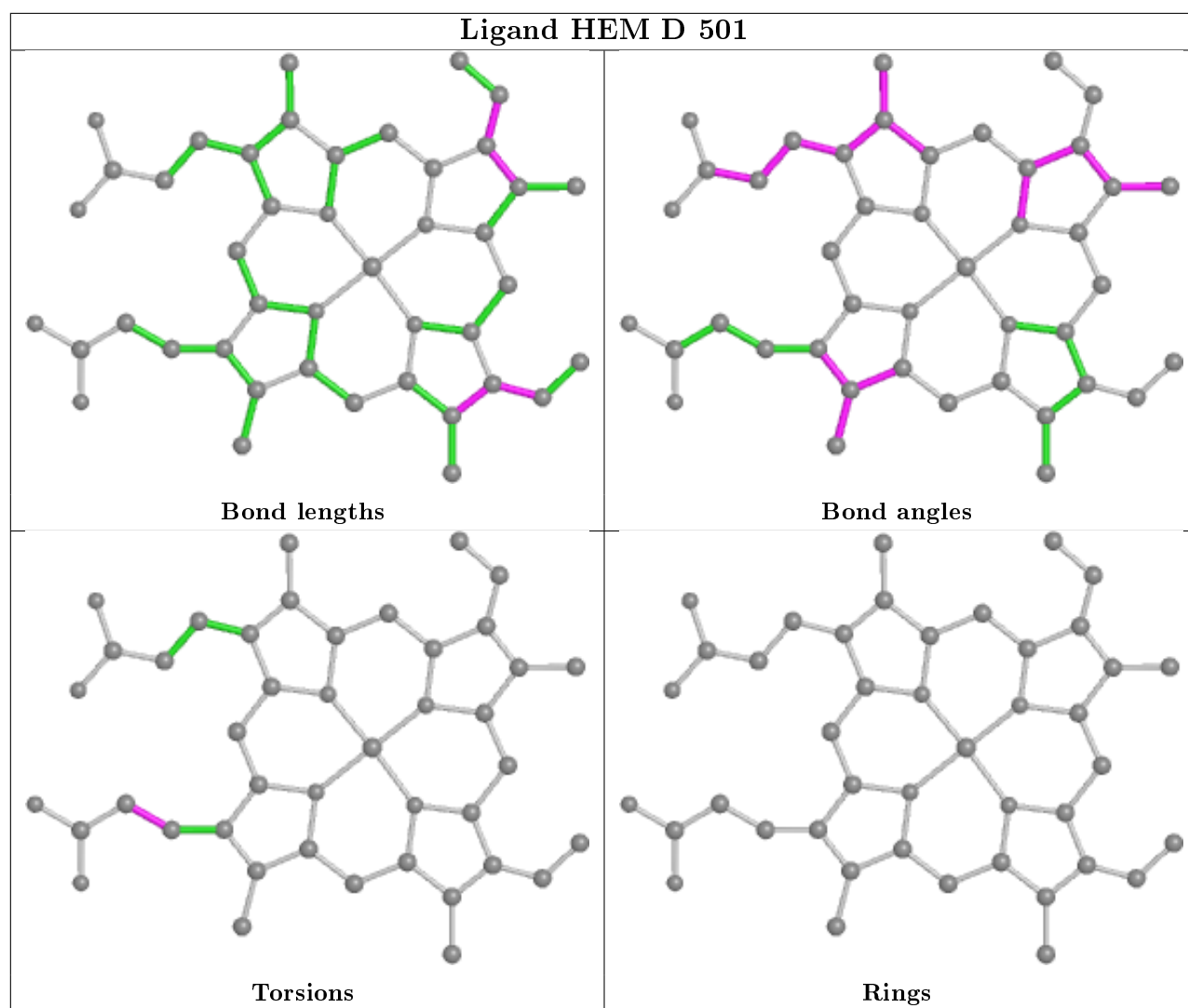
There are no ring outliers.

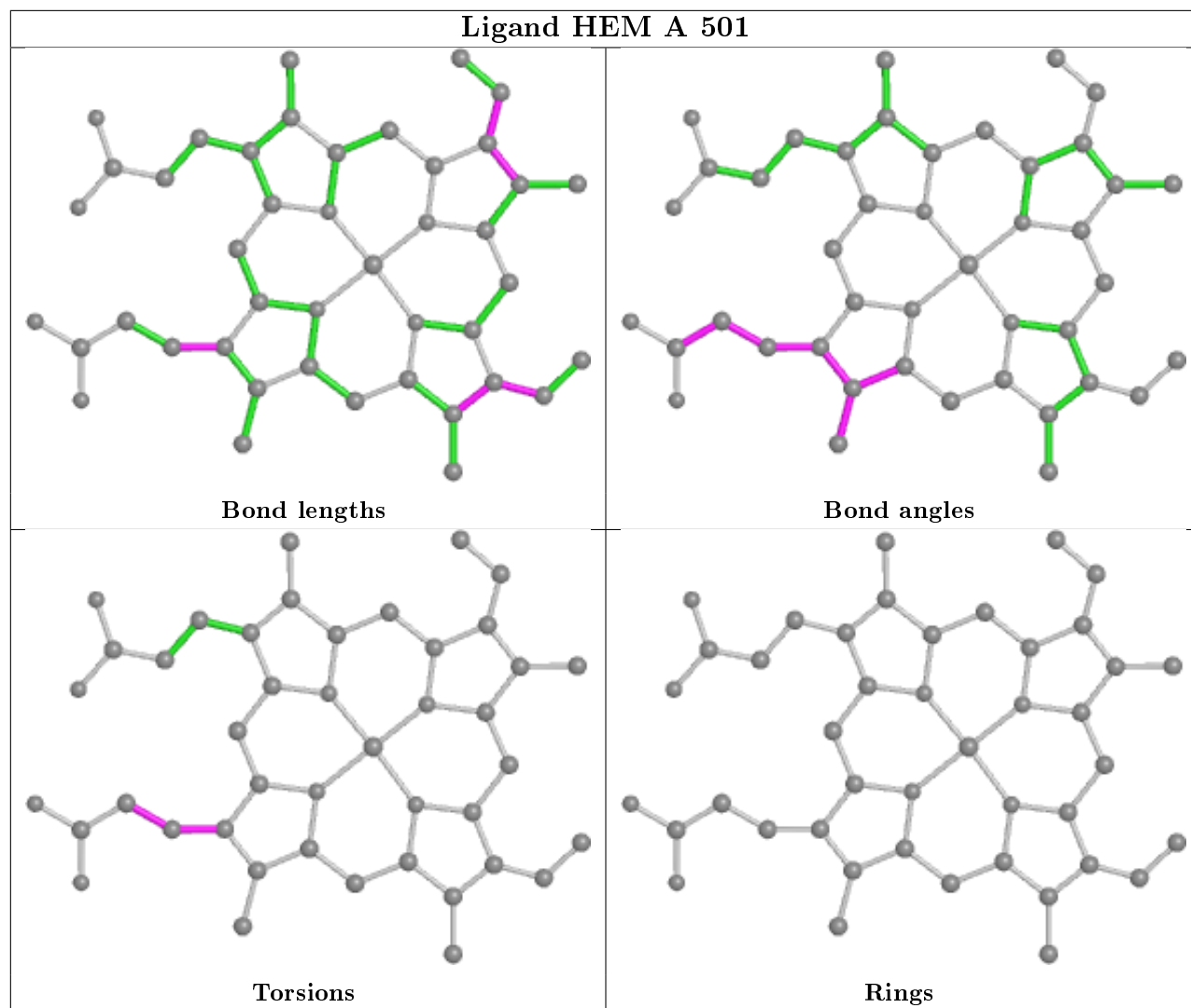
17 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	HEM	2	0
2	D	501	HEM	6	0
4	B	505	BTB	1	0
4	A	505	BTB	2	0
4	A	510	BTB	9	0
4	B	511	BTB	1	0
2	A	501	HEM	5	0
4	B	510	BTB	2	0
3	A	502	KLY	1	0
6	A	507	GOL	1	0
2	C	501	HEM	3	0
4	A	503	BTB	1	0
4	C	504	BTB	5	0
4	D	505	BTB	3	0
4	B	506	BTB	3	0
3	D	503	KLY	2	0
4	D	504	BTB	3	0

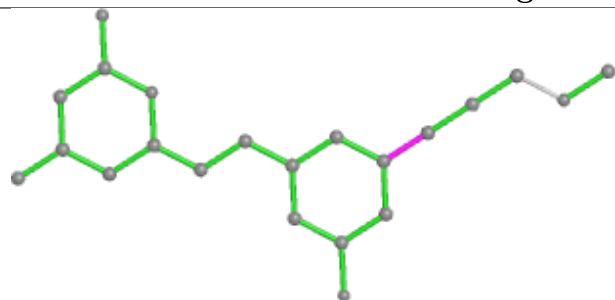
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



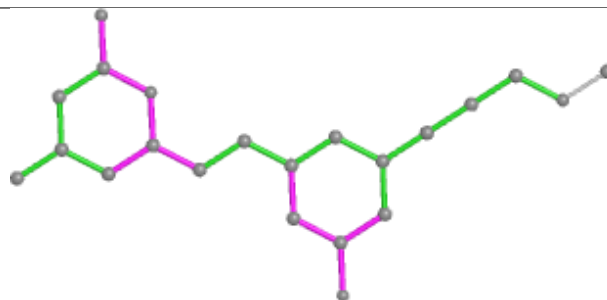




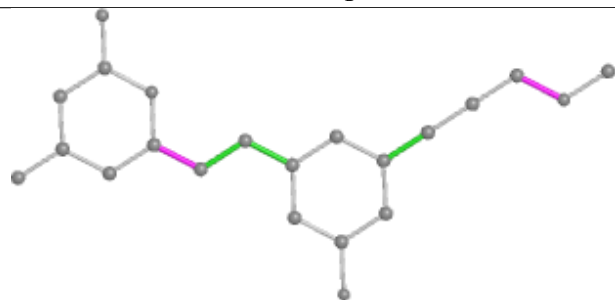
Ligand KLY A 502



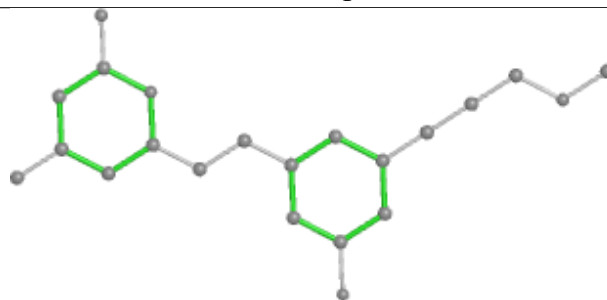
Bond lengths



Bond angles

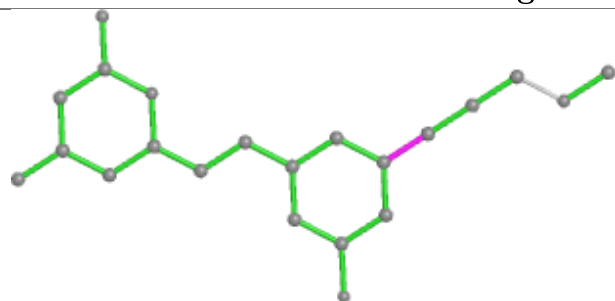


Torsions

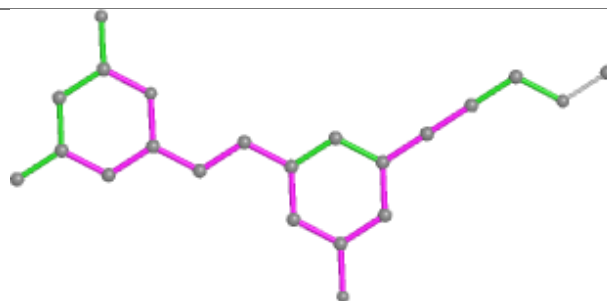


Rings

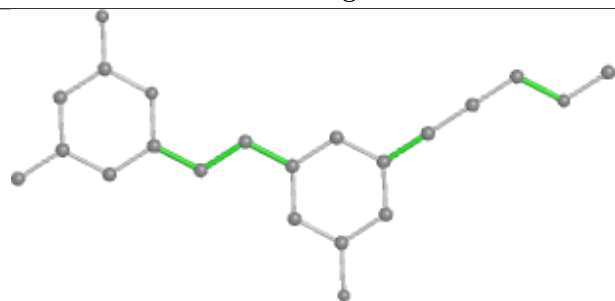
Ligand KLY C 503



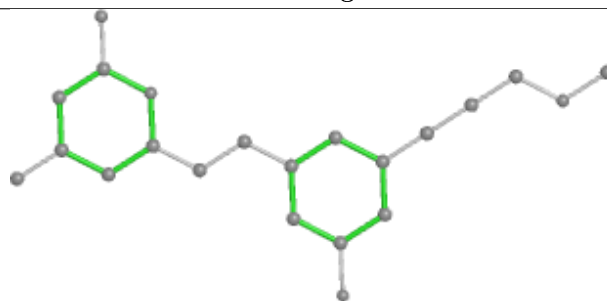
Bond lengths



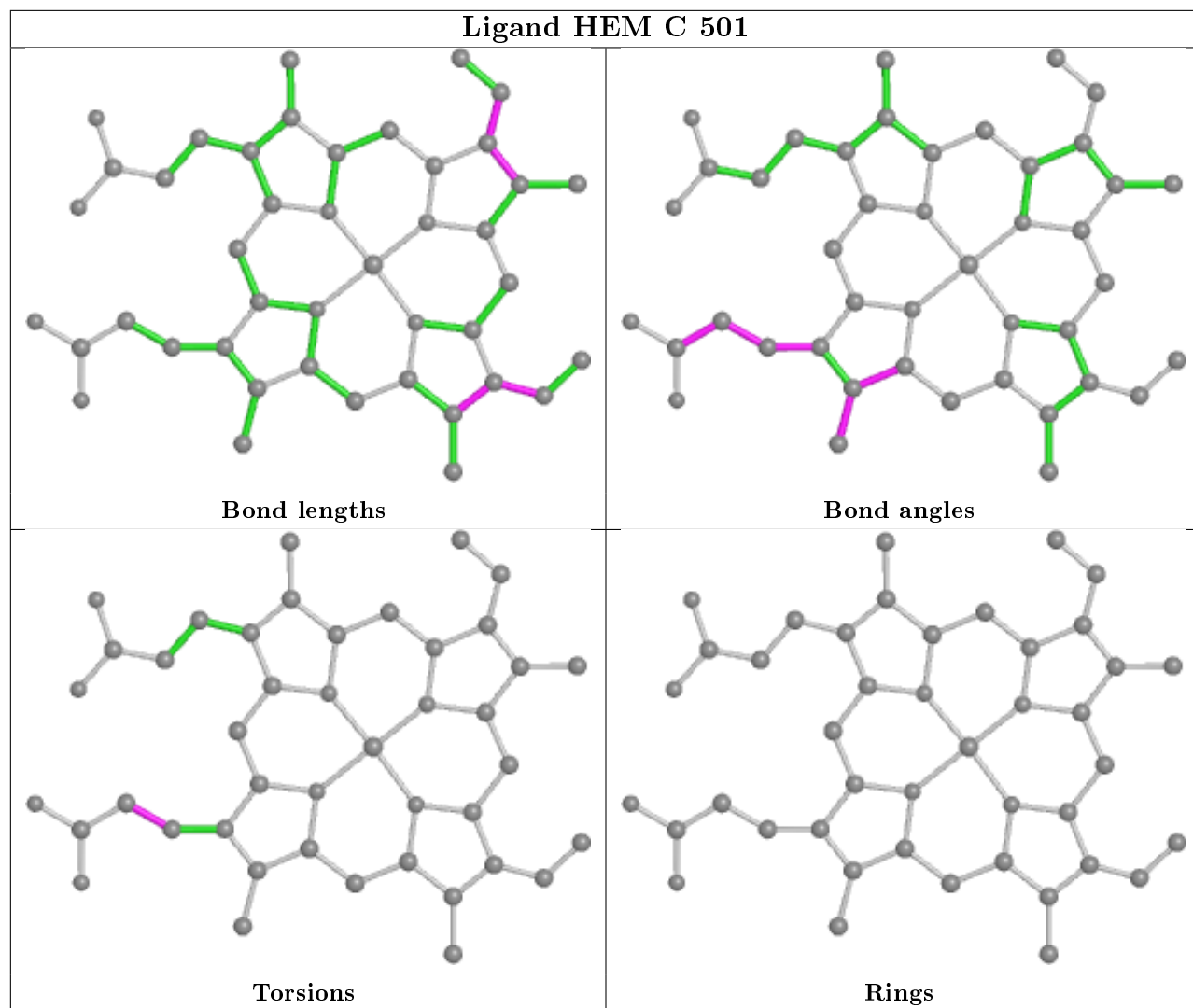
Bond angles

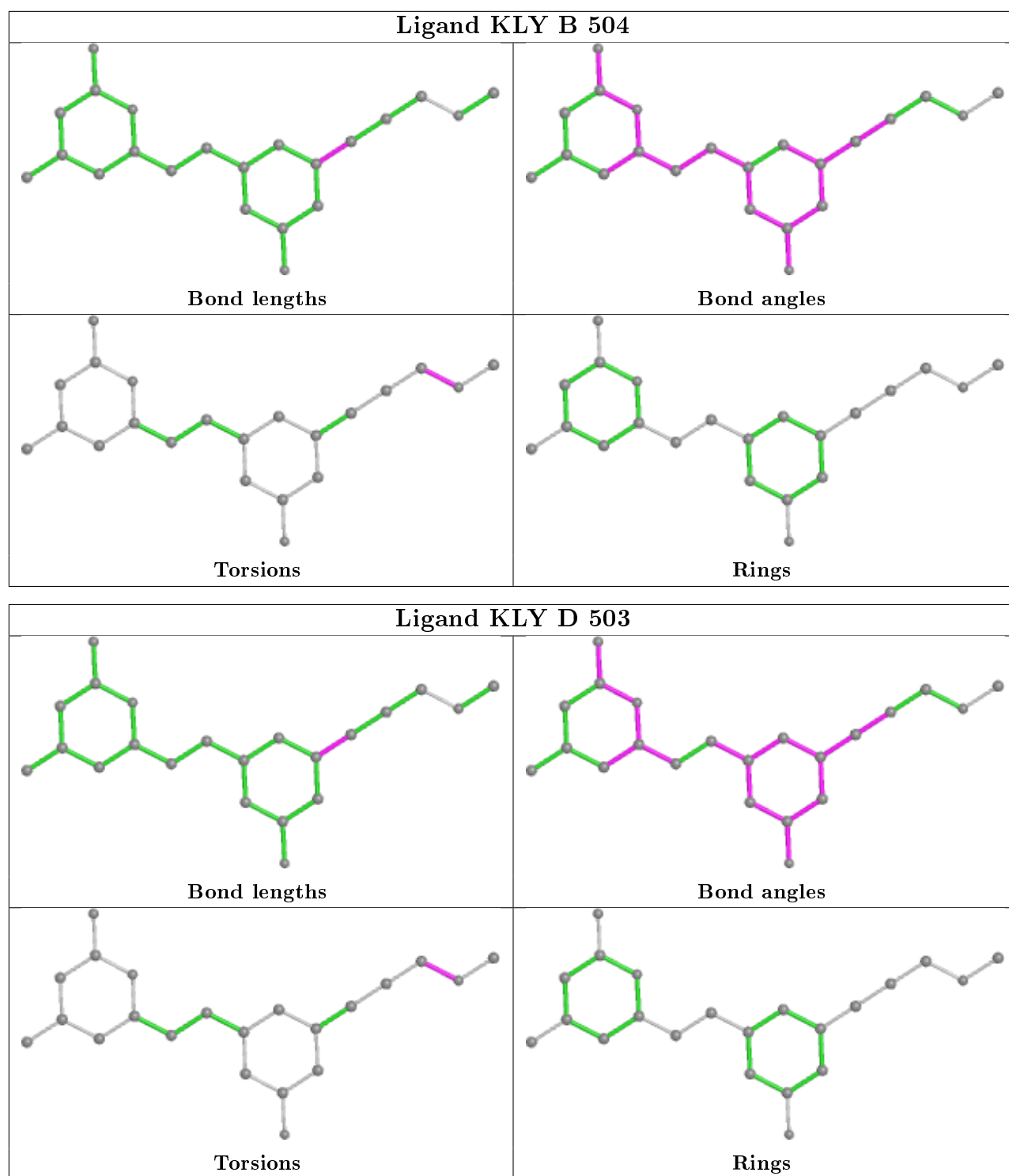


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.94	73 (18%) 1 1	47, 84, 141, 177	0
1	B	404/440 (91%)	0.17	31 (7%) 13 12	38, 63, 106, 155	0
1	C	402/440 (91%)	0.64	53 (13%) 3 2	45, 79, 124, 171	0
1	D	404/440 (91%)	0.09	21 (5%) 27 25	38, 62, 100, 152	0
All	All	1614/1760 (91%)	0.46	178 (11%) 5 4	38, 70, 127, 177	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	9.0
1	A	204	ALA	5.6
1	B	388	ARG	5.5
1	A	259	GLY	5.4
1	A	153	VAL	5.1
1	A	107	ARG	5.0
1	A	274	CYS	4.8
1	A	447	TRP	4.7
1	A	89	GLN	4.4
1	D	257	GLN	4.3
1	C	451	PRO	4.2
1	A	108	LYS	4.2
1	A	300	PRO	4.1
1	C	259	GLY	4.1
1	C	439	GLY	4.1
1	C	452	ILE	4.0
1	C	142	GLY	4.0
1	C	119	ALA	4.0
1	A	279	TRP	4.0
1	A	119	ALA	4.0
1	C	280	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.9
1	A	293	LEU	3.9
1	A	480	TRP	3.8
1	D	67	LYS	3.8
1	A	451	PRO	3.8
1	B	452	ILE	3.7
1	B	259	GLY	3.7
1	A	301	GLU	3.6
1	A	448	ILE	3.6
1	C	450	PRO	3.6
1	C	306	PRO	3.6
1	B	257	GLN	3.6
1	A	162	THR	3.6
1	C	300	PRO	3.5
1	A	275	ILE	3.5
1	D	89	GLN	3.5
1	A	452	ILE	3.5
1	C	447	TRP	3.5
1	A	280	THR	3.5
1	C	302	LEU	3.4
1	C	448	ILE	3.4
1	A	449	VAL	3.4
1	C	445	TRP	3.4
1	C	449	VAL	3.4
1	A	273	LEU	3.4
1	A	244	TRP	3.4
1	A	450	PRO	3.4
1	C	304	LEU	3.3
1	A	128	ARG	3.3
1	A	127	ALA	3.3
1	A	142	GLY	3.3
1	B	89	GLN	3.2
1	C	236	PRO	3.2
1	A	122	GLN	3.2
1	B	79	ILE	3.2
1	A	152	GLU	3.2
1	A	302	LEU	3.2
1	A	255	ARG	3.2
1	C	308	GLU	3.1
1	A	144	GLN	3.1
1	C	480	TRP	3.1
1	D	68	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	256	GLN	3.0
1	A	446	ALA	3.0
1	A	236	PRO	3.0
1	A	445	TRP	3.0
1	C	79	ILE	2.9
1	C	303	PHE	2.9
1	B	258	ASP	2.9
1	B	449	VAL	2.9
1	A	305	LEU	2.9
1	A	163	TYR	2.9
1	C	297	ASP	2.9
1	C	68	PHE	2.8
1	C	275	ILE	2.8
1	D	454	GLY	2.8
1	D	260	SER	2.8
1	A	297	ASP	2.8
1	A	184	CYS	2.8
1	C	301	GLU	2.8
1	D	452	ILE	2.8
1	D	446	ALA	2.7
1	A	140	ARG	2.7
1	A	254	TYR	2.7
1	C	122	GLN	2.7
1	B	460	PHE	2.7
1	A	258	ASP	2.7
1	B	454	GLY	2.7
1	C	299	PRO	2.7
1	C	81	TYR	2.7
1	C	153	VAL	2.7
1	B	386	ASP	2.7
1	A	303	PHE	2.7
1	A	439	GLY	2.7
1	A	151	GLN	2.6
1	C	305	LEU	2.6
1	B	86	ALA	2.6
1	A	444	ASP	2.6
1	B	260	SER	2.6
1	A	299	PRO	2.6
1	A	479	PRO	2.6
1	C	237	GLY	2.6
1	D	122	GLN	2.6
1	D	445	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	365	ARG	2.5
1	B	97	ARG	2.5
1	A	364	THR	2.5
1	B	120	PRO	2.5
1	D	449	VAL	2.5
1	C	446	ALA	2.5
1	A	360	THR	2.5
1	C	321	GLU	2.5
1	A	308	GLU	2.5
1	D	255	ARG	2.5
1	B	68	PHE	2.4
1	D	121	GLU	2.4
1	A	239	GLY	2.4
1	C	258	ASP	2.4
1	B	161	GLY	2.4
1	D	360	THR	2.4
1	A	141	SER	2.4
1	C	185	VAL	2.4
1	C	208	PHE	2.4
1	A	257	GLN	2.4
1	A	86	ALA	2.4
1	A	185	VAL	2.4
1	B	446	ALA	2.4
1	A	125	SER	2.4
1	C	221	ARG	2.3
1	A	221	ARG	2.3
1	C	444	ASP	2.3
1	A	161	GLY	2.3
1	B	451	PRO	2.3
1	A	129	ASP	2.3
1	A	298	GLU	2.3
1	B	153	VAL	2.3
1	C	80	THR	2.2
1	B	455	SER	2.2
1	A	120	PRO	2.2
1	C	140	ARG	2.2
1	B	67	LYS	2.2
1	C	364	THR	2.2
1	B	121	GLU	2.2
1	A	68	PHE	2.2
1	A	368	CYS	2.2
1	B	122	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	277	HIS	2.2
1	D	158	ALA	2.2
1	B	453	SER	2.2
1	C	141	SER	2.2
1	B	124	LEU	2.1
1	C	254	TYR	2.1
1	A	88	ALA	2.1
1	A	353	PHE	2.1
1	D	108	LYS	2.1
1	C	365	ARG	2.1
1	A	121	GLU	2.1
1	B	119	ALA	2.1
1	B	360	THR	2.1
1	C	360	THR	2.1
1	C	270	ILE	2.1
1	B	445	TRP	2.1
1	A	276	GLN	2.1
1	A	145	ALA	2.1
1	B	157	VAL	2.1
1	B	387	THR	2.1
1	C	309	LEU	2.1
1	C	454	GLY	2.1
1	D	261	VAL	2.1
1	D	384	ASP	2.0
1	D	453	SER	2.0
1	D	455	SER	2.0
1	C	276	GLN	2.0
1	C	281	PRO	2.0
1	C	184	CYS	2.0
1	C	121	GLU	2.0
1	A	203	SER	2.0

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

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

6.3 Carbohydrates [i](#)

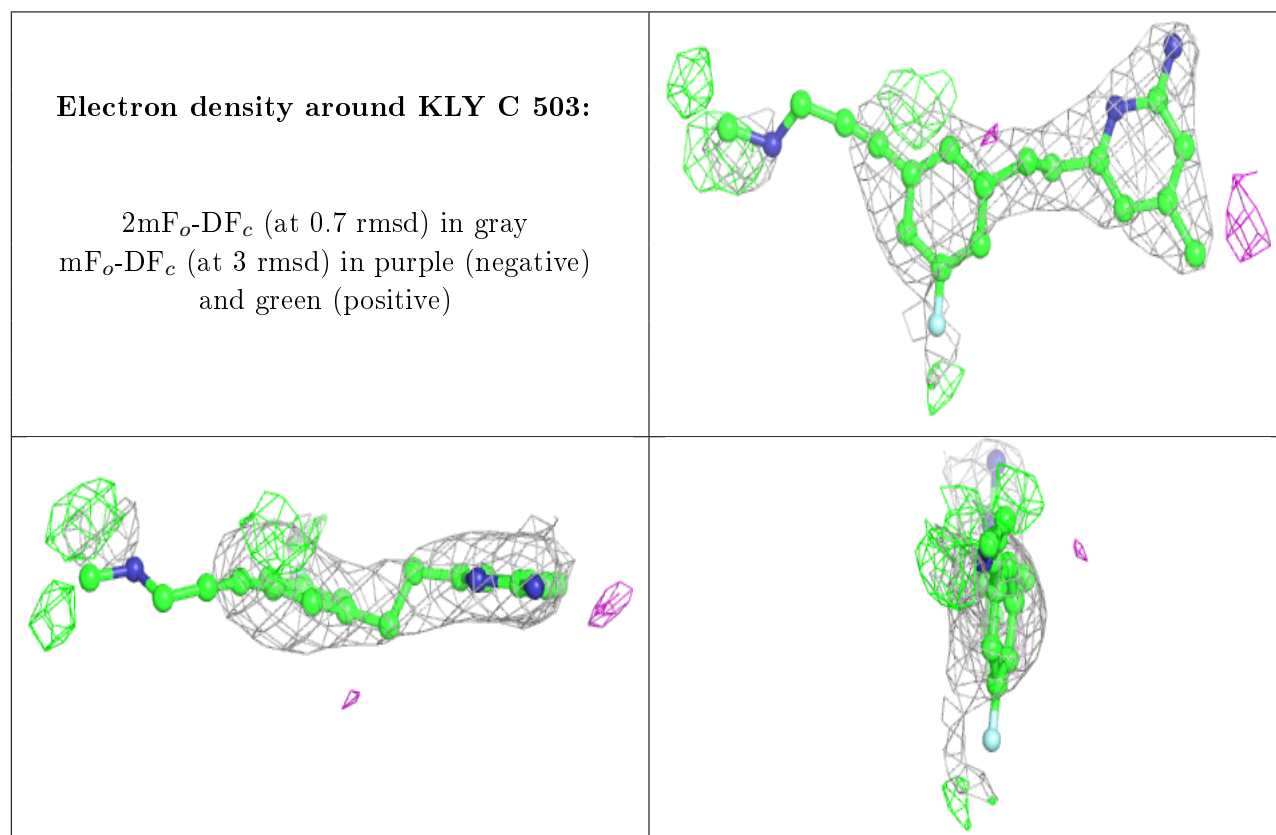
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

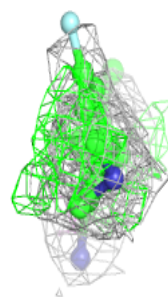
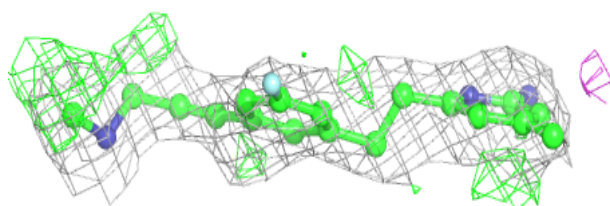
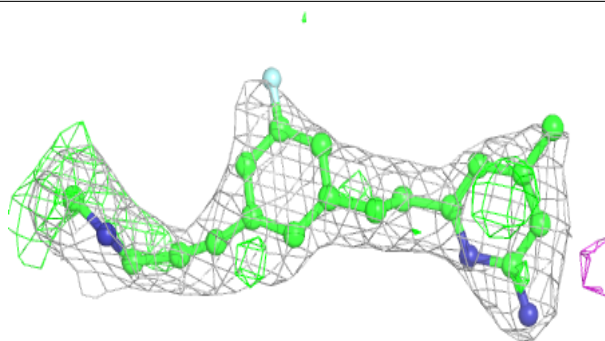
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	H4B	B	501	17/17	0.70	0.52	99,130,139,139	0
9	H4B	B	503	17/17	0.73	0.37	72,118,142,142	0
4	BTB	C	504	14/14	0.76	0.18	108,126,139,143	0
9	H4B	C	502	17/17	0.80	0.40	102,116,139,140	0
4	BTB	A	505	14/14	0.81	0.17	109,129,143,147	0
3	KLY	C	503	22/22	0.81	0.46	64,97,124,130	0
4	BTB	B	510	14/14	0.84	0.23	100,126,159,161	0
9	H4B	D	502	17/17	0.84	0.34	78,99,117,118	0
3	KLY	D	503	22/22	0.84	0.26	39,79,91,110	0
8	GD	C	508	1/1	0.85	0.13	286,286,286,286	0
3	KLY	A	502	22/22	0.86	0.49	58,99,135,136	0
7	CL	C	507	1/1	0.87	0.25	69,69,69,69	0
7	CL	A	508	1/1	0.88	0.29	85,85,85,85	0
8	GD	A	509	1/1	0.88	0.08	262,262,262,262	0
4	BTB	B	506	14/14	0.89	0.27	73,87,103,108	0
3	KLY	B	504	22/22	0.89	0.26	44,83,107,113	0
6	GOL	C	506	6/6	0.89	0.28	74,89,95,96	0
4	BTB	D	504	14/14	0.90	0.18	51,88,97,97	0
4	BTB	B	505	14/14	0.91	0.15	54,76,101,106	0
4	BTB	A	503	14/14	0.91	0.19	107,119,134,139	0
6	GOL	A	507	6/6	0.91	0.27	68,92,106,108	0
4	BTB	B	511	14/14	0.91	0.18	52,74,110,115	0
4	BTB	D	505	14/14	0.92	0.25	86,95,115,118	0
4	BTB	A	504	14/14	0.92	0.12	67,98,105,107	0
7	CL	D	507	1/1	0.93	0.13	60,60,60,60	0
4	BTB	A	510	14/14	0.94	0.19	33,78,123,134	0
7	CL	B	507	1/1	0.95	0.14	59,59,59,59	0
5	ZN	B	509	1/1	0.95	0.17	60,60,60,60	1
2	HEM	D	501	43/43	0.96	0.13	42,60,76,90	0
2	HEM	A	501	43/43	0.96	0.25	62,74,91,119	0
2	HEM	B	502	43/43	0.96	0.16	37,63,91,126	0
2	HEM	C	501	43/43	0.96	0.23	47,73,94,132	0
5	ZN	D	508	1/1	0.97	0.15	56,56,56,56	1
5	ZN	A	506	1/1	0.97	0.08	73,73,73,73	0
8	GD	B	508	1/1	0.98	0.12	67,67,67,67	0
8	GD	D	506	1/1	0.98	0.13	67,67,67,67	0
5	ZN	C	505	1/1	0.99	0.10	61,61,61,61	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.

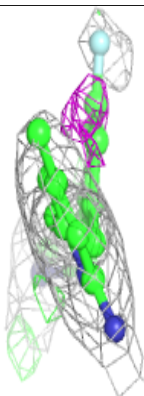
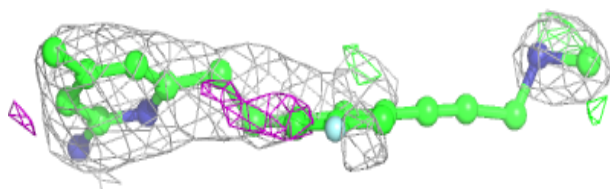
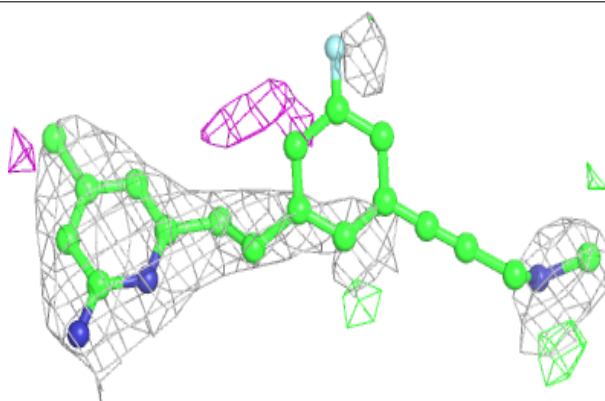


Electron density around KLY D 503:

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

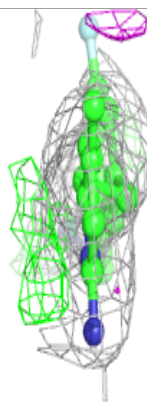
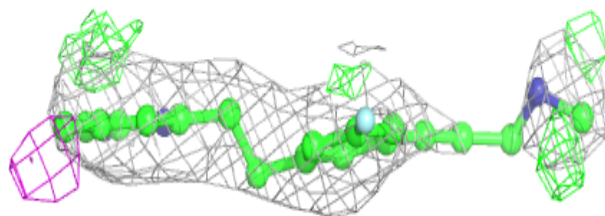
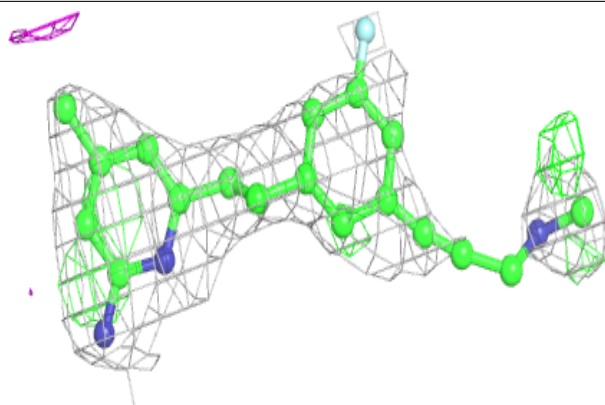
**Electron density around KLY A 502:**

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



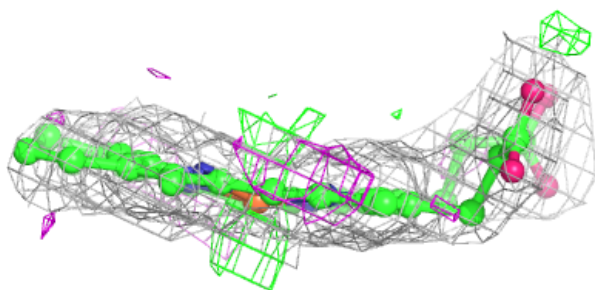
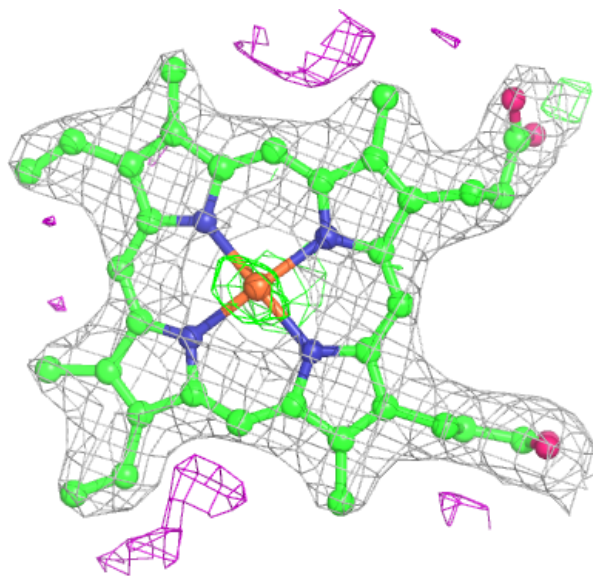
Electron density around KLY B 504:

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



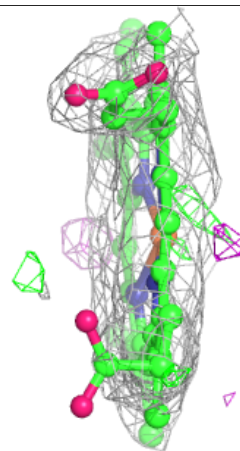
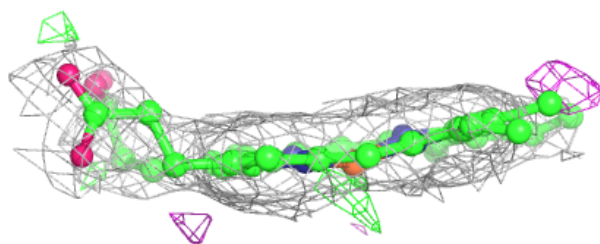
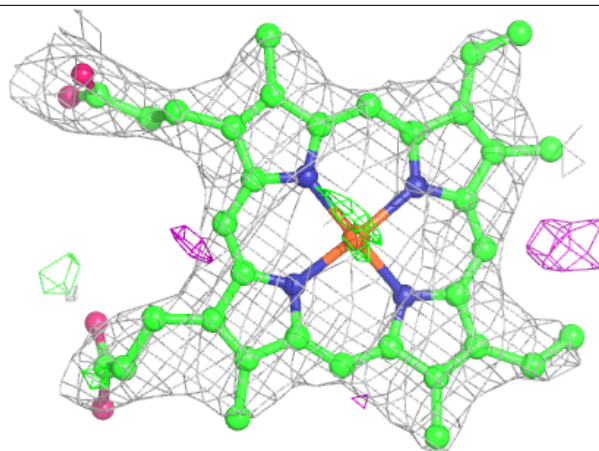
Electron density around HEM D 501:

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



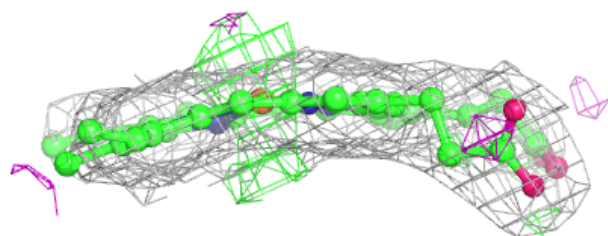
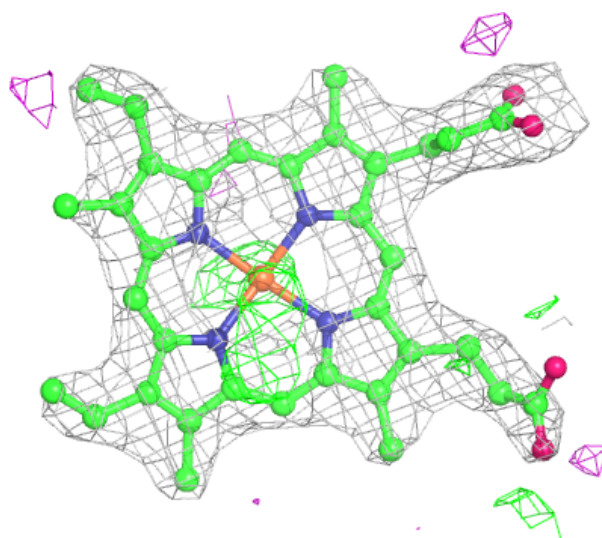
Electron density around HEM A 501:

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



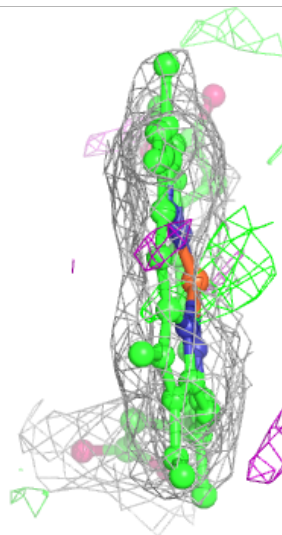
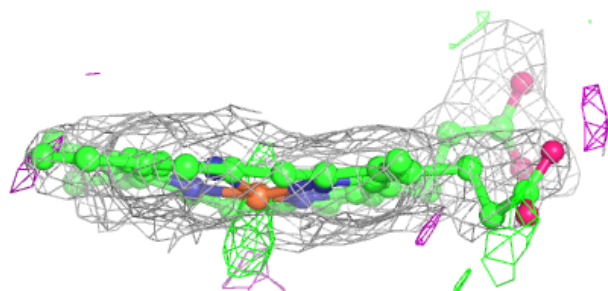
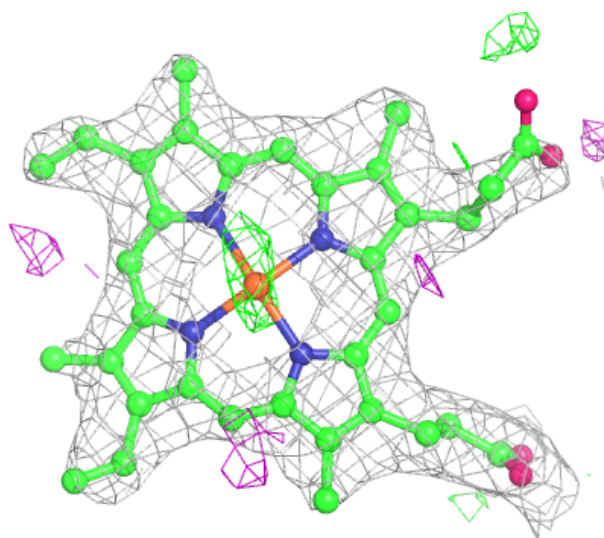
Electron density around HEM B 502:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.