



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2025 – 02:22 PM EST

PDB ID : 9MZ3 / pdb\_00009mz3  
Title : Structure of human endothelial nitric oxide synthase heme domain bound 2-(2-amino-6-fluoro-4-methylquinolin-7-yl)-5-(2-aminoethyl)phenol  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-01-22  
Resolution : 1.95 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

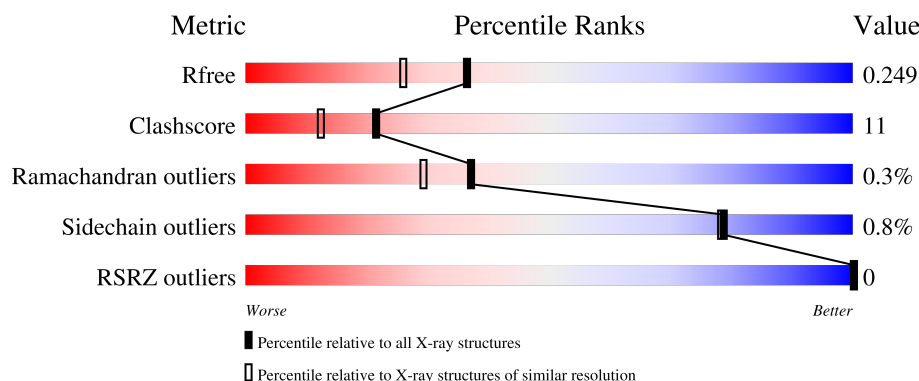
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	440	
1	C	440	
1	D	440	

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
5	BTB	D	507	-	-	X	-
6	ACT	C	505	-	-	X	-
6	ACT	D	505	-	-	X	-
7	GOL	A	514	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	402	Total	C	N	O	S	0	2	0
			3217	2048	567	586	16			
1	C	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	D	402	Total	C	N	O	S	0	2	0
			3217	2049	566	586	16			

There are 4 discrepancies between the modelled and reference sequences:

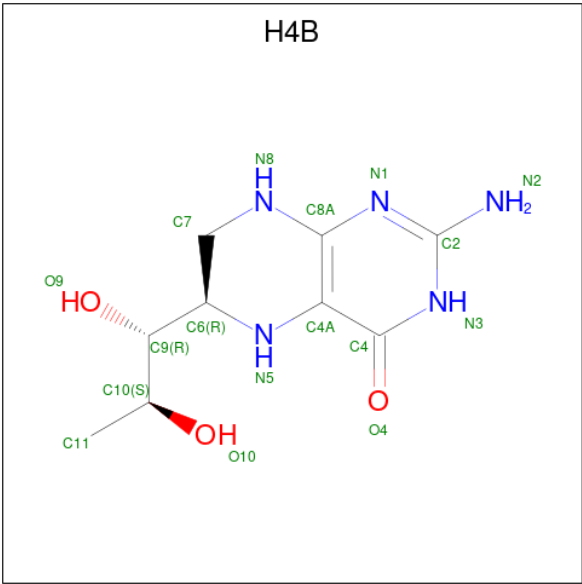
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



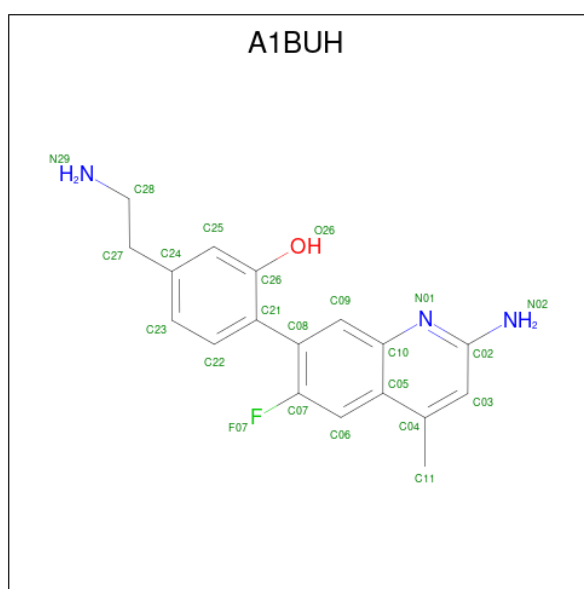
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



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

- Molecule 4 is (2M)-5-(2-aminoethyl)-2-(2-amino-6-fluoro-4-methylquinolin-7-yl)phenol (CCD ID: A1BUH) (formula: C<sub>18</sub>H<sub>18</sub>FN<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	B	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	C	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	D	1	Total 23	C 18	F 1	N 3	O 1	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

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

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

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Ca 1 1	0	0
11	B	1	Total Ca 1 1	0	0

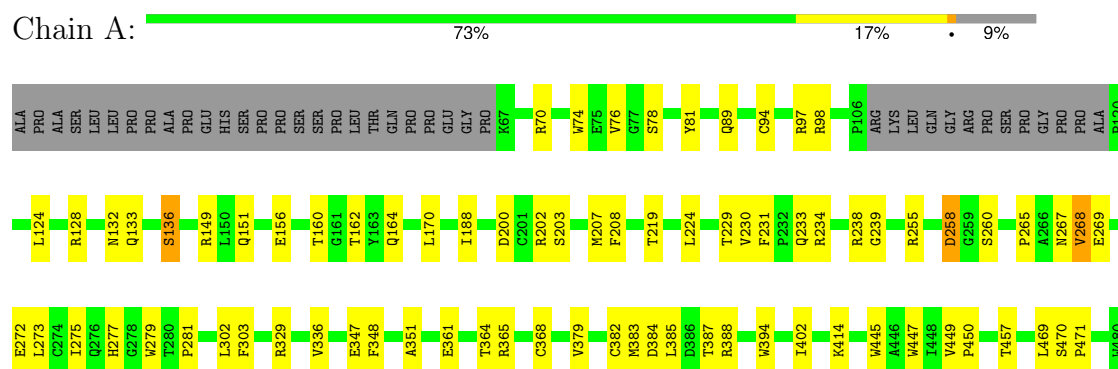
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	151	Total O 151 151	0	0
12	B	225	Total O 225 225	0	0
12	C	131	Total O 131 131	0	0
12	D	228	Total O 228 228	0	0

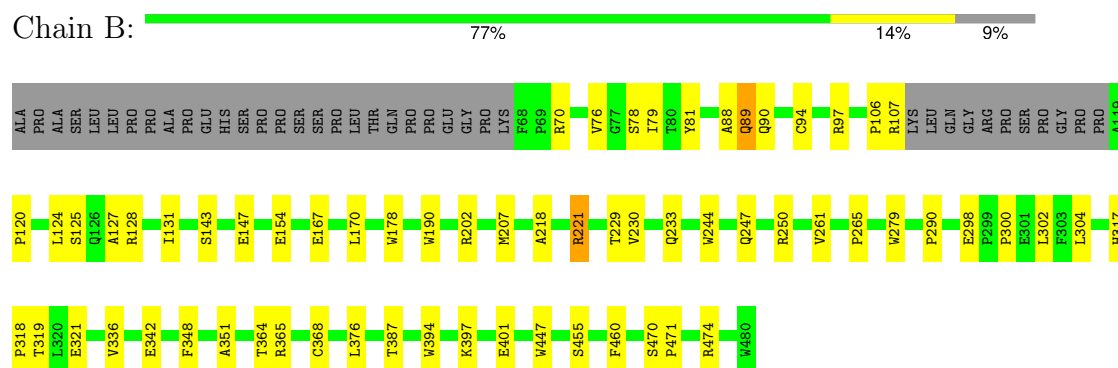
### 3 Residue-property plots [i](#)

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

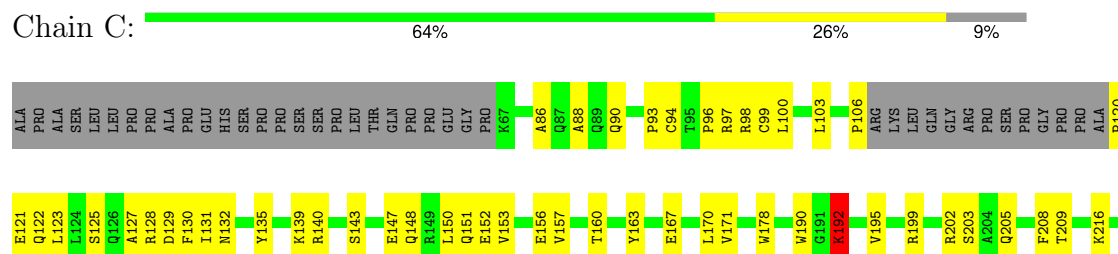
- Molecule 1: Nitric oxide synthase, endothelial

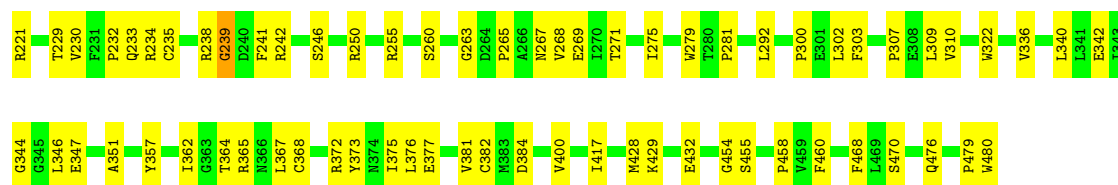


- Molecule 1: Nitric oxide synthase, endothelial

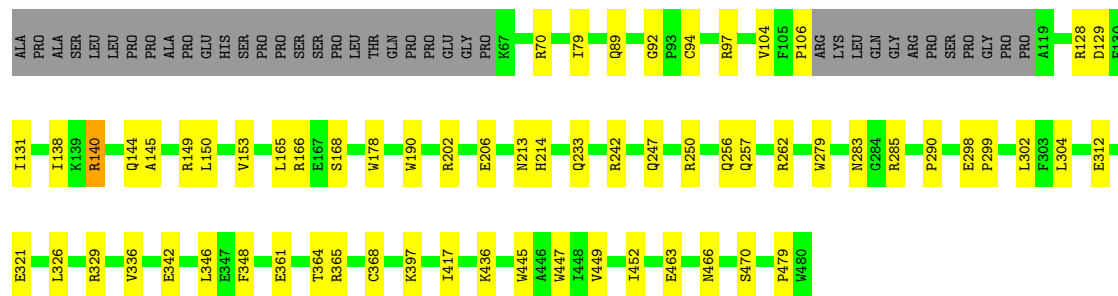


- Molecule 1: Nitric oxide synthase, endothelial





- Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.08Å 151.26Å 107.98Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	46.56 – 1.95 46.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.56-1.95) 100.0 (46.56-1.95)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.206 , 0.250 0.207 , 0.249	Depositor DCC
$R_{free}$ test set	6950 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, A1BUH, BTB, HEM, GOL, GD, CA, H4B, ACT, ZN

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	0.42	1/3302 (0.0%)	0.60	0/4498
1	B	0.43	1/3315 (0.0%)	0.61	1/4517 (0.0%)
1	C	0.37	0/3302	0.62	1/4498 (0.0%)
1	D	0.38	0/3315	0.58	1/4517 (0.0%)
All	All	0.40	2/13234 (0.0%)	0.60	3/18030 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ARG	NE-CZ	7.87	1.41	1.33
1	A	268	VAL	CB-CG1	-6.04	1.32	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	CG-CD-NE	-7.50	95.51	112.00
1	C	192	LYS	CD-CE-NZ	-5.56	94.10	111.90
1	D	140	ARG	CG-CD-NE	5.36	123.78	112.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3207	0	3112	58	0
1	B	3217	0	3121	50	1
1	C	3207	0	3112	98	0
1	D	3217	0	3122	56	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	3	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	23	0	0	3	0
4	B	23	0	0	2	0
4	C	23	0	0	3	0
4	D	23	0	0	3	0
5	A	28	0	36	6	0
5	B	28	0	35	6	0
5	C	28	0	37	8	0
5	D	28	0	36	8	1
6	A	8	0	6	0	0
6	B	8	0	6	1	0
6	C	8	0	6	2	0
6	D	8	0	6	3	0
7	A	24	0	32	6	0
7	B	6	0	8	0	0
7	C	12	0	16	1	0
7	D	12	0	16	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	1	0
8	D	1	0	0	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	151	0	0	5	0
12	B	225	0	0	13	0
12	C	131	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	228	0	0	7	0
All	All	14125	0	12887	280	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 11.

All (280) 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:B:97:ARG:HD2	12:B:700:HOH:O	1.21	1.34
1:A:277:HIS:HB3	1:A:302:LEU:HD11	1.36	1.07
1:C:192:LYS:HD3	1:C:192:LYS:C	1.80	1.02
1:C:242:ARG:NH2	1:C:479:PRO:HD3	1.77	0.99
1:C:242:ARG:HH21	1:C:479:PRO:HD3	1.34	0.91
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.58	0.84
7:A:514:GOL:O2	3:B:502:H4B:N5	2.12	0.83
1:A:365:ARG:HH22	7:A:510:GOL:H31	1.46	0.80
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.64	0.79
1:C:151:GLN:N	1:C:151:GLN:OE1	2.16	0.79
1:D:202:ARG:NH1	12:D:602:HOH:O	2.14	0.79
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.64	0.78
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.17	0.77
1:A:160:THR:HG23	1:A:162:THR:H	1.50	0.76
1:C:382:CYS:HA	5:C:506:BTB:H11	1.67	0.76
1:B:298:GLU:OE1	5:B:508:BTB:H42	1.87	0.74
1:D:144:GLN:NE2	12:D:604:HOH:O	2.16	0.74
1:A:76:VAL:HG23	1:A:78:SER:H	1.53	0.73
1:C:122:GLN:N	1:C:122:GLN:OE1	2.21	0.73
1:A:277:HIS:CB	1:A:302:LEU:HD11	2.18	0.73
1:A:156:GLU:O	1:A:160:THR:HG22	1.90	0.72
1:C:125:SER:HA	1:C:128:ARG:HE	1.53	0.71
5:D:507:BTB:O3	5:D:507:BTB:O1	2.06	0.71
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.72	0.70
1:C:88:ALA:O	1:D:97:ARG:NH2	2.24	0.70
1:D:336:VAL:HG21	4:D:503:A1BUH:C07	2.23	0.68
1:A:336:VAL:HG21	4:A:503:A1BUH:C07	2.24	0.68
1:B:474:ARG:HD2	12:B:601:HOH:O	1.93	0.67
1:D:144:GLN:OE1	12:D:601:HOH:O	2.13	0.67
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.77	0.67
1:B:90:GLN:OE1	12:B:601:HOH:O	2.13	0.67
6:C:505:ACT:O	12:C:601:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:N	1:A:272:GLU:OE1	2.28	0.66
1:D:206:GLU:OE2	12:D:602:HOH:O	2.13	0.66
1:B:397:LYS:NZ	12:B:602:HOH:O	2.28	0.65
5:D:506:BTB:O8	5:D:506:BTB:H62	1.95	0.65
1:D:128:ARG:HG3	1:D:150:LEU:HD22	1.78	0.65
1:C:271:THR:O	1:C:275:ILE:HG13	1.97	0.64
1:C:100:LEU:HB3	1:C:103:LEU:HD22	1.78	0.64
1:A:78:SER:OG	12:A:601:HOH:O	2.15	0.64
1:C:336:VAL:HG21	4:C:503:A1BUH:C07	2.28	0.64
1:B:342:GLU:OE2	1:B:474:ARG:NH1	2.30	0.64
1:C:429:LYS:NZ	1:C:432:GLU:OE1	2.31	0.64
1:B:336:VAL:HG21	4:B:503:A1BUH:C07	2.28	0.63
1:B:124:LEU:O	1:B:128:ARG:HG3	1.98	0.63
1:A:258:ASP:OD1	1:A:260:SER:OG	2.16	0.63
1:D:298:GLU:HG3	1:D:299:PRO:HD2	1.80	0.63
1:C:216:LYS:HB2	1:C:309:LEU:HD11	1.81	0.63
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.80	0.63
1:B:447:TRP:HA	3:B:502:H4B:N1	2.14	0.62
1:B:107:ARG:NH2	12:B:603:HOH:O	2.31	0.62
1:C:90:GLN:HB2	1:C:468:PHE:CD2	2.35	0.61
1:C:147:GLU:OE1	1:C:147:GLU:N	2.30	0.61
1:C:147:GLU:O	1:C:151:GLN:OE1	2.19	0.61
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.82	0.61
1:A:255:ARG:NH2	1:A:268:VAL:HG11	2.15	0.61
1:A:89:GLN:HG2	1:A:469:LEU:HA	1.83	0.61
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.83	0.61
1:D:256:GLN:O	12:D:603:HOH:O	2.16	0.60
1:B:221:ARG:NH1	12:B:605:HOH:O	2.34	0.60
1:C:242:ARG:NH2	1:C:479:PRO:CD	2.59	0.60
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.84	0.60
1:B:97:ARG:CD	12:B:700:HOH:O	2.02	0.59
1:C:147:GLU:O	1:C:148:GLN:C	2.46	0.59
1:C:377:GLU:OE1	5:C:507:BTB:O3	2.17	0.59
1:A:128:ARG:HB3	1:A:128:ARG:CZ	2.31	0.59
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.83	0.59
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.84	0.59
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.84	0.59
1:B:170:LEU:HD11	1:B:230:VAL:HG11	1.84	0.58
1:D:447:TRP:HA	3:D:502:H4B:N1	2.17	0.58
1:C:128:ARG:HG3	1:C:129:ASP:N	2.18	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:OE2	5:B:507:BTB:O4	2.23	0.56
1:C:97:ARG:HG3	1:C:98:ARG:HG2	1.85	0.56
1:C:167:GLU:OE2	7:C:508:GOL:O3	2.20	0.56
1:C:364:THR:O	1:C:368:CYS:HB2	2.06	0.56
1:C:90:GLN:HB2	1:C:468:PHE:CG	2.40	0.56
1:C:234:ARG:HA	1:C:238:ARG:HH21	1.71	0.56
1:D:202:ARG:NH2	12:D:608:HOH:O	2.29	0.56
1:C:143:SER:O	1:C:147:GLU:OE1	2.23	0.56
1:C:192:LYS:C	1:C:192:LYS:CD	2.69	0.56
1:D:138:ILE:HG13	1:D:140:ARG:HB2	1.87	0.56
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.88	0.55
1:A:302:LEU:N	1:A:302:LEU:HD12	2.20	0.55
5:A:505:BTB:O4	5:A:505:BTB:O3	2.21	0.55
1:A:364:THR:O	1:A:368:CYS:HB2	2.06	0.55
5:C:507:BTB:O3	5:C:507:BTB:O4	2.19	0.55
1:C:156:GLU:O	1:C:160:THR:OG1	2.24	0.55
1:D:144:GLN:NE2	1:D:145:ALA:H	2.05	0.54
1:D:70:ARG:HD2	1:D:79:ILE:HD13	1.89	0.54
1:D:256:GLN:HG3	1:D:257:GLN:H	1.73	0.54
1:C:135:TYR:HD1	1:C:140:ARG:HB2	1.73	0.53
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.90	0.53
4:A:503:A1BUH:N29	7:A:510:GOL:H12	2.23	0.53
1:C:384:ASP:OD1	5:C:506:BTB:O3	2.26	0.53
1:C:170:LEU:HD11	1:C:230:VAL:HG11	1.91	0.53
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.90	0.53
1:D:364:THR:O	1:D:368:CYS:HB2	2.09	0.52
1:A:329:ARG:NH1	12:A:603:HOH:O	2.37	0.52
1:A:388:ARG:NH1	5:A:505:BTB:H61	2.25	0.52
1:C:128:ARG:O	1:C:132:ASN:ND2	2.42	0.52
1:D:202:ARG:NH1	1:D:206:GLU:OE2	2.43	0.52
1:B:107:ARG:HG3	12:B:616:HOH:O	2.10	0.51
1:D:104:VAL:O	1:D:106:PRO:HD3	2.10	0.51
1:A:74:TRP:CB	7:A:514:GOL:H11	2.40	0.51
1:A:255:ARG:HB2	1:A:255:ARG:NH1	2.25	0.51
1:C:120:PRO:N	1:C:122:GLN:HE22	2.09	0.51
1:C:130:PHE:HB2	1:C:344:GLY:HA2	1.91	0.51
1:C:139:LYS:HD2	1:C:139:LYS:N	2.24	0.51
1:C:340:LEU:HD12	1:C:476:GLN:OE1	2.11	0.51
1:B:76:VAL:HG23	1:B:78:SER:H	1.76	0.51
1:A:97:ARG:HG3	1:B:88:ALA:HB3	1.94	0.50
7:A:514:GOL:HO2	3:B:502:H4B:HN5	1.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ALA:O	1:C:131:ILE:HG12	2.12	0.50
1:B:364:THR:O	1:B:368:CYS:HB2	2.12	0.50
1:C:307:PRO:HA	1:C:310:VAL:HG22	1.94	0.49
1:C:275:ILE:HD13	1:C:281:PRO:HB3	1.94	0.49
1:C:377:GLU:O	1:C:381:VAL:HG23	2.13	0.49
1:C:382:CYS:O	5:C:506:BTB:H51	2.12	0.49
1:B:107:ARG:NH1	12:B:616:HOH:O	2.46	0.49
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.95	0.49
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.95	0.49
1:B:106:PRO:HD2	12:B:714:HOH:O	2.12	0.49
1:C:122:GLN:CD	1:C:123:LEU:H	2.21	0.49
1:B:70:ARG:HB2	1:B:81:TYR:CE2	2.47	0.48
1:C:255:ARG:CZ	1:C:268:VAL:HG11	2.42	0.48
1:A:279:TRP:HB2	1:A:302:LEU:HD23	1.94	0.48
1:C:235:CYS:SG	1:C:238:ARG:NE	2.87	0.48
1:D:138:ILE:O	1:D:140:ARG:HG2	2.13	0.48
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.94	0.48
1:C:205:GLN:O	1:C:209:THR:HG23	2.14	0.48
1:A:94:CYS:HB3	1:B:94:CYS:HB3	1.96	0.48
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.54	0.48
1:B:250:ARG:NH2	6:B:505:ACT:OXT	2.44	0.48
1:D:131:ILE:HD11	1:D:153:VAL:HG21	1.96	0.48
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.28	0.47
1:C:88:ALA:N	1:D:97:ARG:HH21	2.12	0.47
1:C:153:VAL:HG13	1:C:163:TYR:CG	2.49	0.47
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.32	0.47
1:B:89:GLN:HB3	1:B:90:GLN:H	1.43	0.47
1:C:238:ARG:HG2	1:C:239:GLY:N	2.29	0.47
1:D:361:GLU:OE1	4:D:503:A1BUH:N01	2.47	0.47
1:B:143:SER:O	1:B:147:GLU:HG2	2.15	0.47
1:C:367:LEU:HB3	1:C:375:ILE:HD13	1.97	0.47
1:C:163:TYR:CE1	1:C:346:LEU:HD21	2.49	0.47
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.70	0.47
1:A:70:ARG:HG3	1:A:81:TYR:CE2	2.50	0.46
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.50	0.46
1:B:336:VAL:HG21	4:B:503:A1BUH:F07	2.06	0.46
1:A:89:GLN:HE21	1:A:470:SER:HB3	1.81	0.46
1:A:267:ASN:O	1:A:268:VAL:C	2.55	0.46
2:C:501:HEM:HBA1	4:C:503:A1BUH:C09	2.45	0.46
1:D:436:LYS:N	1:D:436:LYS:HE2	2.31	0.46
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:O	1:C:351:ALA:HA	2.15	0.46
5:C:506:BTB:H41	5:C:506:BTB:H72	1.55	0.46
1:A:200:ASP:OD2	1:A:200:ASP:N	2.46	0.46
1:B:221:ARG:CZ	12:B:605:HOH:O	2.62	0.46
1:C:263:GLY:O	1:C:265:PRO:HD3	2.15	0.46
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.29	0.46
1:A:89:GLN:NE2	12:A:605:HOH:O	2.37	0.45
1:A:238:ARG:HG2	1:A:239:GLY:O	2.15	0.45
1:A:447:TRP:HA	3:A:502:H4B:N1	2.31	0.45
7:A:514:GOL:H2	1:B:365:ARG:HH22	1.82	0.45
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.98	0.45
1:D:202:ARG:NH1	12:D:608:HOH:O	2.46	0.45
1:D:250:ARG:HA	1:D:250:ARG:HD2	1.71	0.45
5:A:505:BTB:H72	5:A:505:BTB:H41	1.28	0.45
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.51	0.45
1:B:387:THR:HA	1:B:394:TRP:CD1	2.52	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.52	0.45
1:B:229:THR:O	1:B:351:ALA:HA	2.17	0.45
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.99	0.45
1:D:262:ARG:NE	1:D:283:ASN:O	2.44	0.45
1:A:387:THR:HA	1:A:394:TRP:CD1	2.52	0.44
1:C:86:ALA:O	1:D:97:ARG:NH2	2.51	0.44
5:A:505:BTB:H51	5:A:505:BTB:H11	1.33	0.44
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.53	0.44
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.53	0.44
1:B:127:ALA:O	1:B:131:ILE:HG12	2.17	0.44
1:D:89:GLN:NE2	1:D:129:ASP:OD2	2.51	0.44
2:D:501:HEM:HMB3	6:D:504:ACT:H2	1.99	0.44
1:D:342:GLU:OE2	1:D:470:SER:OG	2.26	0.44
1:A:229:THR:O	1:A:351:ALA:HA	2.18	0.44
1:A:379:VAL:HG21	1:A:402:ILE:HD11	1.99	0.44
1:D:298:GLU:OE2	5:D:507:BTB:H31	2.17	0.44
1:C:148:GLN:O	1:C:152:GLU:OE1	2.36	0.43
1:C:221:ARG:HE	1:C:221:ARG:HB3	1.58	0.43
5:C:507:BTB:H41	5:C:507:BTB:H72	1.42	0.43
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.53	0.43
1:A:70:ARG:HG3	1:A:81:TYR:CZ	2.53	0.43
1:B:290:PRO:HB3	1:B:304:LEU:HD23	2.00	0.43
1:A:414:LYS:HA	1:A:414:LYS:HD3	1.75	0.43
1:D:365:ARG:HH22	7:D:509:GOL:H31	1.82	0.43
1:A:133:GLN:NE2	12:A:618:HOH:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:O	1:A:203:SER:OG	2.32	0.43
1:C:202:ARG:HA	1:C:241:PHE:HZ	1.84	0.43
5:B:507:BTB:H32	5:B:507:BTB:H51	1.85	0.43
1:C:279:TRP:HB2	1:C:302:LEU:HD13	2.01	0.43
1:B:455:SER:HA	1:B:460:PHE:CG	2.54	0.43
1:C:255:ARG:NH2	1:C:268:VAL:HG11	2.34	0.43
1:D:144:GLN:CD	1:D:144:GLN:H	2.27	0.43
1:D:336:VAL:HG21	4:D:503:A1BUH:F07	2.09	0.43
1:C:99:CYS:HB3	1:D:466:ASN:HB3	2.00	0.43
1:C:120:PRO:N	1:C:122:GLN:OE1	2.52	0.43
1:C:322:TRP:CD1	5:C:506:BTB:H52	2.54	0.43
1:A:233:GLN:NE2	12:A:609:HOH:O	2.40	0.43
1:C:199:ARG:O	1:C:232:PRO:HG3	2.19	0.43
5:D:507:BTB:H61	5:D:507:BTB:H11	2.01	0.43
1:A:207:MET:HG3	1:A:231:PHE:CE1	2.54	0.42
1:D:312:GLU:CD	1:D:329:ARG:HH21	2.27	0.42
1:C:153:VAL:O	1:C:157:VAL:HG23	2.20	0.42
1:C:275:ILE:CD1	1:C:281:PRO:HB3	2.49	0.42
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.41	0.42
1:C:233:GLN:OE1	12:C:602:HOH:O	2.21	0.42
1:C:342:GLU:OE2	1:C:470:SER:OG	2.35	0.42
1:C:357:TYR:OH	8:C:510:CL:CL	2.67	0.42
1:D:285:ARG:NH2	1:D:326:LEU:O	2.51	0.42
1:B:70:ARG:HG3	1:B:79:ILE:HG23	2.02	0.42
1:B:97:ARG:HG3	12:B:700:HOH:O	2.18	0.42
1:D:140:ARG:HH11	1:D:140:ARG:HD2	1.52	0.42
1:C:428:MET:HG3	1:C:458:PRO:HB2	2.01	0.42
1:D:290:PRO:HB3	1:D:304:LEU:HD23	2.01	0.42
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.50	0.42
1:A:269:GLU:HA	1:A:272:GLU:OE1	2.18	0.42
1:B:470:SER:HA	1:B:471:PRO:C	2.45	0.42
1:C:455:SER:HA	1:C:460:PHE:CG	2.54	0.42
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.60	0.42
1:C:103:LEU:HD12	1:D:463:GLU:HB3	2.01	0.42
1:C:171:VAL:HA	1:C:195:VAL:HG21	2.02	0.42
1:A:124:LEU:O	1:A:128:ARG:HG3	2.19	0.42
1:A:383:MET:HB2	1:A:385:LEU:HG	2.01	0.42
1:C:336:VAL:HG21	4:C:503:A1BUH:F07	2.09	0.42
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	2.02	0.41
1:C:400:VAL:HG11	1:D:397:LYS:HG2	2.02	0.41
1:D:214:HIS:CD2	1:D:214:HIS:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:507:BTB:H11	5:D:507:BTB:C6	2.49	0.41
1:C:216:LYS:HB2	1:C:309:LEU:CD1	2.47	0.41
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.02	0.41
1:D:445:TRP:CE2	1:D:449:VAL:HG21	2.55	0.41
1:A:219:THR:O	1:A:224:LEU:HD12	2.21	0.41
1:A:361:GLU:OE2	4:A:503:A1BUH:N02	2.53	0.41
1:C:265:PRO:HA	1:C:268:VAL:HG23	2.03	0.41
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.53	0.41
1:A:445:TRP:CE2	1:A:449:VAL:HG21	2.56	0.41
1:A:149:ARG:NH2	1:A:164:GLN:O	2.38	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.96	0.41
1:A:382:CYS:HA	5:A:504:BTB:C1	2.51	0.41
1:C:96:PRO:O	1:D:92:GLY:N	2.50	0.41
1:C:242:ARG:HA	1:C:242:ARG:HD2	1.93	0.41
1:C:292:LEU:HA	1:C:292:LEU:HD23	1.79	0.41
1:C:454:GLY:O	1:C:460:PHE:HB2	2.20	0.41
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.55	0.41
1:B:218:ALA:HB1	12:B:666:HOH:O	2.21	0.41
1:B:298:GLU:CD	5:B:508:BTB:H42	2.46	0.41
5:B:507:BTB:O1	5:B:507:BTB:H72	2.21	0.41
1:C:246:SER:OG	1:C:250:ARG:HD2	2.20	0.41
1:C:250:ARG:HD3	1:C:267:ASN:OD1	2.21	0.41
1:B:319:THR:HB	5:B:507:BTB:O3	2.21	0.40
1:C:367:LEU:HA	1:C:373:TYR:HB2	2.02	0.40
1:D:250:ARG:NH2	6:D:505:ACT:O	2.47	0.40
1:D:298:GLU:CD	5:D:507:BTB:H31	2.46	0.40
1:A:132:ASN:O	1:A:136:SER:OG	2.34	0.40
1:B:244:TRP:CH2	1:B:300:PRO:HG3	2.56	0.40
1:C:121:GLU:CD	1:C:121:GLU:H	2.29	0.40
1:C:455:SER:HA	1:C:460:PHE:CB	2.51	0.40
1:D:202:ARG:HH11	1:D:206:GLU:CD	2.29	0.40
6:D:505:ACT:H1	8:D:510:CL:CL	2.58	0.40
1:C:269:GLU:OE2	1:C:480:TRP:HZ2	2.05	0.40
1:C:372:ARG:HH12	6:C:505:ACT:C	2.34	0.40
1:D:321:GLU:OE2	5:D:506:BTB:O4	2.40	0.40
5:D:507:BTB:H72	5:D:507:BTB:H41	1.54	0.40
1:A:470:SER:HA	1:A:471:PRO:C	2.46	0.40
1:B:124:LEU:HD21	1:B:154:GLU:HA	2.03	0.40
1:C:275:ILE:HG23	1:C:279:TRP:O	2.21	0.40
1:C:135:TYR:HB3	1:C:140:ARG:O	2.21	0.40
1:C:208:PHE:CE1	1:C:303:PHE:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LEU:HG	1:D:346:LEU:HD12	2.03	0.40
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.57	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:B:167:GLU:OE2	5:D:507:BTB:O8[1_556]	2.18	0.02

## 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	398/440 (90%)	381 (96%)	17 (4%)	0	100	100
1	B	400/440 (91%)	391 (98%)	7 (2%)	2 (0%)	25	16
1	C	398/440 (90%)	379 (95%)	16 (4%)	3 (1%)	16	8
1	D	400/440 (91%)	389 (97%)	11 (3%)	0	100	100
All	All	1596/1760 (91%)	1540 (96%)	51 (3%)	5 (0%)	37	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	B	120	PRO
1	C	203	SER
1	C	260	SER
1	C	239	GLY



### 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	342/373 (92%)	338 (99%)	4 (1%)	67	65
1	B	343/373 (92%)	341 (99%)	2 (1%)	84	83
1	C	342/373 (92%)	340 (99%)	2 (1%)	84	83
1	D	343/373 (92%)	338 (98%)	5 (2%)	60	57
All	All	1370/1492 (92%)	1357 (99%)	13 (1%)	79	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	151	GLN
1	A	188	ILE
1	A	258	ASP
1	B	125	SER
1	B	207	MET
1	C	192	LYS
1	C	417	ILE
1	D	168[A]	SER
1	D	168[B]	SER
1	D	213[A]	ASN
1	D	213[B]	ASN
1	D	417	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	133	GLN
1	A	151	GLN
1	A	194	GLN
1	A	233	GLN
1	A	408	HIS

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Mol	Chain	Res	Type
1	A	433	ASN
1	B	408	HIS
1	C	126	GLN
1	C	164	GLN
1	C	256	GLN
1	D	144	GLN
1	D	256	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 12 are monoatomic - leaving 37 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	$\# Z  > 2$
7	GOL	A	510	-	5,5,5	0.35	0	5,5,5	0.49	0
5	BTB	B	508	-	13,13,13	0.51	0	7,16,16	1.13	1 (14%)
7	GOL	D	509	-	5,5,5	0.44	0	5,5,5	0.21	0
6	ACT	B	505	-	3,3,3	0.78	0	3,3,3	0.81	0
4	A1BUH	D	503	-	25,25,25	1.02	2 (8%)	35,36,36	1.80	7 (20%)
7	GOL	C	508	-	5,5,5	0.31	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ACT	C	505	-	3,3,3	0.86	0	3,3,3	0.86	0
4	A1BUH	A	503	-	25,25,25	0.99	2 (8%)	35,36,36	1.74	6 (17%)
3	H4B	B	502	-	16,18,18	0.72	0	14,26,26	2.39	5 (35%)
3	H4B	D	502	-	16,18,18	0.79	0	14,26,26	2.84	7 (50%)
6	ACT	D	505	-	3,3,3	0.87	0	3,3,3	0.86	0
5	BTB	A	504	9	13,13,13	0.44	0	7,16,16	1.36	1 (14%)
4	A1BUH	B	503	-	25,25,25	1.11	2 (8%)	35,36,36	1.83	7 (20%)
2	HEM	D	501	1	42,50,50	1.44	5 (11%)	46,82,82	1.71	9 (19%)
7	GOL	A	508	-	5,5,5	0.35	0	5,5,5	0.60	0
7	GOL	D	508	-	5,5,5	0.36	0	5,5,5	0.55	0
4	A1BUH	C	503	-	25,25,25	1.06	3 (12%)	35,36,36	1.67	6 (17%)
6	ACT	C	504	-	3,3,3	0.79	0	3,3,3	0.88	0
2	HEM	A	501	1	42,50,50	1.42	6 (14%)	46,82,82	1.76	9 (19%)
5	BTB	A	505	-	13,13,13	0.80	0	7,16,16	1.37	0
3	H4B	A	502	-	16,18,18	0.76	0	14,26,26	2.31	4 (28%)
5	BTB	D	507	-	13,13,13	0.49	0	7,16,16	0.93	0
7	GOL	A	509	-	5,5,5	0.34	0	5,5,5	0.37	0
7	GOL	C	509	-	5,5,5	0.41	0	5,5,5	0.20	0
6	ACT	D	504	-	3,3,3	0.81	0	3,3,3	0.74	0
2	HEM	C	501	1	42,50,50	1.47	6 (14%)	46,82,82	1.62	10 (21%)
6	ACT	A	506	-	3,3,3	0.73	0	3,3,3	0.96	0
2	HEM	B	501	1	42,50,50	1.49	7 (16%)	46,82,82	1.78	9 (19%)
3	H4B	C	502	-	16,18,18	0.70	0	14,26,26	2.27	5 (35%)
7	GOL	A	514	-	5,5,5	0.46	0	5,5,5	0.92	0
5	BTB	D	506	9	13,13,13	0.50	0	7,16,16	0.63	0
6	ACT	B	504	-	3,3,3	0.80	0	3,3,3	0.78	0
7	GOL	B	506	-	5,5,5	0.33	0	5,5,5	0.35	0
5	BTB	C	507	-	13,13,13	0.53	0	7,16,16	1.20	1 (14%)
5	BTB	C	506	9	13,13,13	0.43	0	7,16,16	1.26	1 (14%)
6	ACT	A	507	-	3,3,3	0.89	0	3,3,3	0.47	0
5	BTB	B	507	9	13,13,13	0.44	0	7,16,16	0.58	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
7	GOL	A	510	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	B	508	-	-	8/21/21/21	-
7	GOL	D	509	-	-	2/4/4/4	-
4	A1BUH	D	503	-	-	2/7/7/7	0/3/3/3
7	GOL	C	508	-	-	4/4/4/4	-
4	A1BUH	A	503	-	-	2/7/7/7	0/3/3/3
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	504	9	-	5/21/21/21	-
4	A1BUH	B	503	-	-	2/7/7/7	0/3/3/3
2	HEM	D	501	1	-	4/12/54/54	-
7	GOL	A	508	-	-	4/4/4/4	-
4	A1BUH	C	503	-	-	2/7/7/7	0/3/3/3
2	HEM	A	501	1	-	3/12/54/54	-
5	BTB	A	505	-	-	12/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	D	507	-	-	11/21/21/21	-
7	GOL	A	509	-	-	2/4/4/4	-
7	GOL	C	509	-	-	4/4/4/4	-
2	HEM	C	501	1	-	5/12/54/54	-
2	HEM	B	501	1	-	5/12/54/54	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
7	GOL	A	514	-	-	1/4/4/4	-
5	BTB	D	506	9	-	1/21/21/21	-
7	GOL	B	506	-	-	3/4/4/4	-
5	BTB	C	507	-	-	11/21/21/21	-
5	BTB	C	506	9	-	6/21/21/21	-
7	GOL	D	508	-	-	2/4/4/4	-
5	BTB	B	507	9	-	6/21/21/21	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-3.80	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.65	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.53	1.35	1.40
2	A	501	HEM	C3C-CAC	3.48	1.55	1.47
2	D	501	HEM	C3C-CAC	3.44	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-CAC	3.39	1.55	1.47
2	D	501	HEM	CAB-C3B	3.34	1.56	1.47
2	B	501	HEM	C3C-CAC	3.33	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.33	1.35	1.40
2	C	501	HEM	CAB-C3B	3.32	1.56	1.47
2	A	501	HEM	CAB-C3B	3.22	1.56	1.47
2	B	501	HEM	CAB-C3B	2.92	1.55	1.47
2	B	501	HEM	CMD-C2D	2.87	1.56	1.50
2	C	501	HEM	C3C-C4C	2.79	1.45	1.41
2	B	501	HEM	CMA-C3A	2.74	1.57	1.51
4	A	503	A1BUH	C06-C07	2.56	1.40	1.35
2	A	501	HEM	C3C-C4C	2.53	1.45	1.41
2	D	501	HEM	C3C-C4C	2.50	1.45	1.41
2	D	501	HEM	CMB-C2B	2.44	1.55	1.50
4	C	503	A1BUH	C05-C10	-2.35	1.38	1.42
4	B	503	A1BUH	C10-N01	-2.31	1.34	1.37
2	C	501	HEM	FE-NB	2.29	2.10	1.98
2	B	501	HEM	C3C-C4C	2.28	1.44	1.41
2	C	501	HEM	CMD-C2D	2.24	1.55	1.50
4	D	503	A1BUH	C06-C07	2.22	1.39	1.35
2	B	501	HEM	FE-NB	2.18	2.10	1.98
4	D	503	A1BUH	C09-C10	-2.17	1.38	1.41
4	B	503	A1BUH	C06-C07	2.16	1.39	1.35
2	A	501	HEM	CMD-C2D	2.15	1.55	1.50
4	C	503	A1BUH	C10-N01	-2.13	1.34	1.37
4	A	503	A1BUH	C05-C10	-2.11	1.39	1.42
4	C	503	A1BUH	C06-C07	2.06	1.39	1.35
2	A	501	HEM	CMB-C2B	2.04	1.54	1.50

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	A1BUH	C21-C08-C07	-7.02	116.10	122.45
4	B	503	A1BUH	C21-C08-C07	-6.85	116.25	122.45
4	A	503	A1BUH	C21-C08-C07	-6.81	116.29	122.45
2	B	501	HEM	CBA-CAA-C2A	-6.15	102.20	112.54
2	A	501	HEM	CBA-CAA-C2A	-5.90	102.61	112.54
3	A	502	H4B	C8A-C4A-C4	5.47	119.48	114.50
2	D	501	HEM	CBA-CAA-C2A	-5.34	103.55	112.54
4	C	503	A1BUH	C21-C08-C07	-5.34	117.62	122.45
3	B	502	H4B	C8A-C4A-C4	5.04	119.09	114.50
3	D	502	H4B	C11-C10-C9	-4.94	106.06	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4B-CHC-C1C	4.72	128.79	122.56
3	D	502	H4B	C8A-C4A-C4	4.71	118.79	114.50
3	C	502	H4B	C8A-C4A-C4	4.71	118.78	114.50
3	D	502	H4B	C2-N3-C4	4.52	122.25	115.96
4	B	503	A1BUH	C09-C08-C07	4.47	121.23	116.03
2	C	501	HEM	C4B-CHC-C1C	4.23	128.14	122.56
3	D	502	H4B	N1-C2-N3	-4.08	119.23	125.48
3	C	502	H4B	C2-N3-C4	3.88	121.36	115.96
3	B	502	H4B	C2-N3-C4	3.85	121.32	115.96
2	B	501	HEM	CAD-CBD-CGD	-3.65	103.98	113.67
2	C	501	HEM	C3B-C2B-C1B	3.61	109.12	106.41
3	B	502	H4B	N1-C2-N3	-3.57	120.00	125.48
2	D	501	HEM	CAD-CBD-CGD	-3.52	104.34	113.67
3	A	502	H4B	C2-N3-C4	3.51	120.84	115.96
4	D	503	A1BUH	C09-C08-C07	3.50	120.10	116.03
4	A	503	A1BUH	C05-C10-N01	-3.47	119.12	122.80
4	C	503	A1BUH	C05-C10-N01	-3.47	119.12	122.80
3	A	502	H4B	N1-C2-N3	-3.35	120.34	125.48
2	B	501	HEM	CMC-C2C-C3C	3.34	131.35	124.68
3	C	502	H4B	N1-C2-N3	-3.32	120.39	125.48
2	B	501	HEM	C4B-CHC-C1C	3.27	126.87	122.56
5	A	504	BTB	O3-C3-C2	3.25	119.04	111.40
2	C	501	HEM	CBA-CAA-C2A	-3.15	107.24	112.54
4	A	503	A1BUH	C09-C08-C21	3.09	124.53	117.47
2	D	501	HEM	CMC-C2C-C3C	3.06	130.80	124.68
2	D	501	HEM	C4B-CHC-C1C	3.06	126.59	122.56
4	B	503	A1BUH	C22-C21-C08	-3.04	112.61	118.74
2	A	501	HEM	CAD-CBD-CGD	-3.02	105.66	113.67
4	C	503	A1BUH	C09-C08-C07	3.01	119.53	116.03
4	D	503	A1BUH	C05-C10-N01	-3.00	119.62	122.80
4	C	503	A1BUH	C04-C05-C10	2.97	119.81	118.00
5	C	506	BTB	O3-C3-C2	2.95	118.35	111.40
2	A	501	HEM	C3B-C4B-NB	-2.89	107.39	109.47
2	B	501	HEM	CMA-C3A-C4A	-2.84	124.30	128.46
4	A	503	A1BUH	C04-C05-C10	2.81	119.71	118.00
3	D	502	H4B	C2-N1-C8A	2.79	121.21	114.59
2	D	501	HEM	CHA-C4D-ND	2.76	127.79	124.37
3	B	502	H4B	C2-N1-C8A	2.73	121.07	114.59
4	D	503	A1BUH	C09-C08-C21	2.66	123.56	117.47
4	A	503	A1BUH	C09-C08-C07	2.66	119.12	116.03
2	C	501	HEM	CAD-CBD-CGD	-2.66	106.62	113.67
2	C	501	HEM	C1B-NB-C4B	2.63	108.32	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C2B-C1B	2.59	108.36	106.41
2	A	501	HEM	C1B-NB-C4B	2.54	108.21	105.21
3	A	502	H4B	C2-N1-C8A	2.52	120.59	114.59
3	C	502	H4B	C2-N1-C8A	2.50	120.54	114.59
5	B	508	BTB	O1-C1-C2	-2.48	105.56	111.40
2	C	501	HEM	CMA-C3A-C4A	-2.48	124.82	128.46
3	D	502	H4B	C4-C4A-N5	2.48	122.11	118.57
3	D	502	H4B	N2-C2-N1	2.46	120.91	117.22
2	B	501	HEM	C1B-NB-C4B	2.46	108.12	105.21
2	A	501	HEM	C3D-C4D-ND	-2.46	107.48	110.17
2	B	501	HEM	C3B-C2B-C1B	2.45	108.25	106.41
4	C	503	A1BUH	C03-C04-C05	2.42	120.28	117.84
4	D	503	A1BUH	C04-C05-C10	2.38	119.45	118.00
4	C	503	A1BUH	C09-C08-C21	2.35	122.84	117.47
2	C	501	HEM	CHD-C1D-ND	2.33	126.94	124.44
2	A	501	HEM	C3B-C2B-C1B	2.32	108.15	106.41
2	C	501	HEM	C4A-C3A-C2A	2.32	108.61	107.00
2	D	501	HEM	CHD-C1D-ND	2.31	126.92	124.44
4	A	503	A1BUH	C03-C04-C05	2.23	120.09	117.84
2	B	501	HEM	CMA-C3A-C2A	2.22	129.13	124.94
2	A	501	HEM	CHA-C4D-ND	2.21	127.11	124.37
4	B	503	A1BUH	C04-C05-C10	2.18	119.33	118.00
5	C	507	BTB	O3-C3-C2	-2.15	106.34	111.40
4	D	503	A1BUH	C06-C07-C08	-2.14	120.18	123.59
2	C	501	HEM	C2B-C1B-NB	-2.14	107.38	109.84
2	B	501	HEM	CHC-C4B-C3B	2.14	127.85	124.57
3	B	502	H4B	C4-C4A-N5	2.13	121.61	118.57
4	D	503	A1BUH	C22-C21-C08	-2.12	114.45	118.74
2	D	501	HEM	C3D-C4D-ND	-2.12	107.84	110.17
2	D	501	HEM	C4A-C3A-C2A	2.12	108.47	107.00
2	A	501	HEM	C4D-ND-C1D	2.08	107.67	105.21
4	B	503	A1BUH	C06-C07-C08	-2.06	120.31	123.59
4	B	503	A1BUH	C09-C08-C21	2.06	122.19	117.47
4	B	503	A1BUH	C05-C10-N01	-2.04	120.64	122.80
3	C	502	H4B	C4-C4A-N5	2.01	121.45	118.57
2	C	501	HEM	C3D-C4D-ND	-2.00	107.97	110.17

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C4-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	507	BTB	O1-C1-C2-C3
5	B	507	BTB	O1-C1-C2-C4
5	B	507	BTB	O1-C1-C2-N
5	B	507	BTB	C1-C2-C4-O4
5	B	507	BTB	C3-C2-C4-O4
5	B	507	BTB	N-C2-C4-O4
5	B	508	BTB	C1-C2-C3-O3
5	B	508	BTB	C4-C2-C3-O3
5	B	508	BTB	N-C2-C3-O3
5	B	508	BTB	C3-C2-C4-O4
5	B	508	BTB	N-C2-C4-O4
5	C	506	BTB	O1-C1-C2-C3
5	C	506	BTB	O1-C1-C2-C4
5	C	506	BTB	O1-C1-C2-N
5	C	506	BTB	C1-C2-C4-O4
5	C	506	BTB	C3-C2-C4-O4
5	C	506	BTB	N-C2-C4-O4
5	C	507	BTB	C1-C2-C4-O4
5	C	507	BTB	C3-C2-C4-O4
5	C	507	BTB	C1-C2-N-C5
5	C	507	BTB	C1-C2-N-C7
5	C	507	BTB	C3-C2-N-C5
5	C	507	BTB	C3-C2-N-C7
5	C	507	BTB	C4-C2-N-C5
5	C	507	BTB	C4-C2-N-C7
5	D	507	BTB	O1-C1-C2-C3
5	D	507	BTB	O1-C1-C2-C4
5	D	507	BTB	O1-C1-C2-N
5	D	507	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	507	BTB	C1-C2-C4-O4
5	D	507	BTB	C3-C2-C4-O4
5	D	507	BTB	N-C2-C4-O4
7	A	508	GOL	O1-C1-C2-C3
7	A	508	GOL	C1-C2-C3-O3
7	A	509	GOL	O1-C1-C2-C3
7	A	510	GOL	O1-C1-C2-C3
7	A	510	GOL	C1-C2-C3-O3
7	A	510	GOL	O2-C2-C3-O3
7	C	508	GOL	C1-C2-C3-O3
7	C	508	GOL	O2-C2-C3-O3
7	C	509	GOL	O1-C1-C2-C3
7	C	509	GOL	C1-C2-C3-O3
7	D	508	GOL	C1-C2-C3-O3
7	D	508	GOL	O2-C2-C3-O3
5	D	507	BTB	N-C7-C8-O8
5	D	506	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
5	C	507	BTB	N-C7-C8-O8
5	A	505	BTB	N-C7-C8-O8
7	B	506	GOL	O1-C1-C2-C3
7	B	506	GOL	C1-C2-C3-O3
7	C	508	GOL	O1-C1-C2-C3
5	C	507	BTB	O1-C1-C2-C4
7	A	509	GOL	O1-C1-C2-O2
7	A	510	GOL	O1-C1-C2-O2
7	C	508	GOL	O1-C1-C2-O2
7	C	509	GOL	O1-C1-C2-O2
7	C	509	GOL	O2-C2-C3-O3
5	B	508	BTB	N-C5-C6-O6
2	D	501	HEM	C4D-C3D-CAD-CBD
7	A	508	GOL	O1-C1-C2-O2
7	B	506	GOL	O2-C2-C3-O3
2	D	501	HEM	C2D-C3D-CAD-CBD
5	B	508	BTB	N-C7-C8-O8
7	A	508	GOL	O2-C2-C3-O3
4	C	503	A1BUH	C23-C24-C27-C28
4	C	503	A1BUH	C25-C24-C27-C28
4	D	503	A1BUH	C23-C24-C27-C28
4	D	503	A1BUH	C25-C24-C27-C28
7	A	514	GOL	O2-C2-C3-O3
7	D	509	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	507	BTB	N-C5-C6-O6
2	B	501	HEM	C4B-C3B-CAB-CBB
5	A	505	BTB	N-C2-C4-O4
5	C	507	BTB	N-C2-C4-O4
5	D	507	BTB	C1-C2-N-C5
5	D	507	BTB	C4-C2-N-C7
7	D	509	GOL	O2-C2-C3-O3
2	C	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C4D-C3D-CAD-CBD
5	A	504	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
4	A	503	A1BUH	C23-C24-C27-C28
2	D	501	HEM	CAD-CBD-CGD-O2D
4	A	503	A1BUH	C25-C24-C27-C28
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	C4D-C3D-CAD-CBD
4	B	503	A1BUH	C25-C24-C27-C28
4	B	503	A1BUH	C23-C24-C27-C28
5	B	508	BTB	C1-C2-C4-O4
2	B	501	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

28 monomers are involved in 65 short contacts:

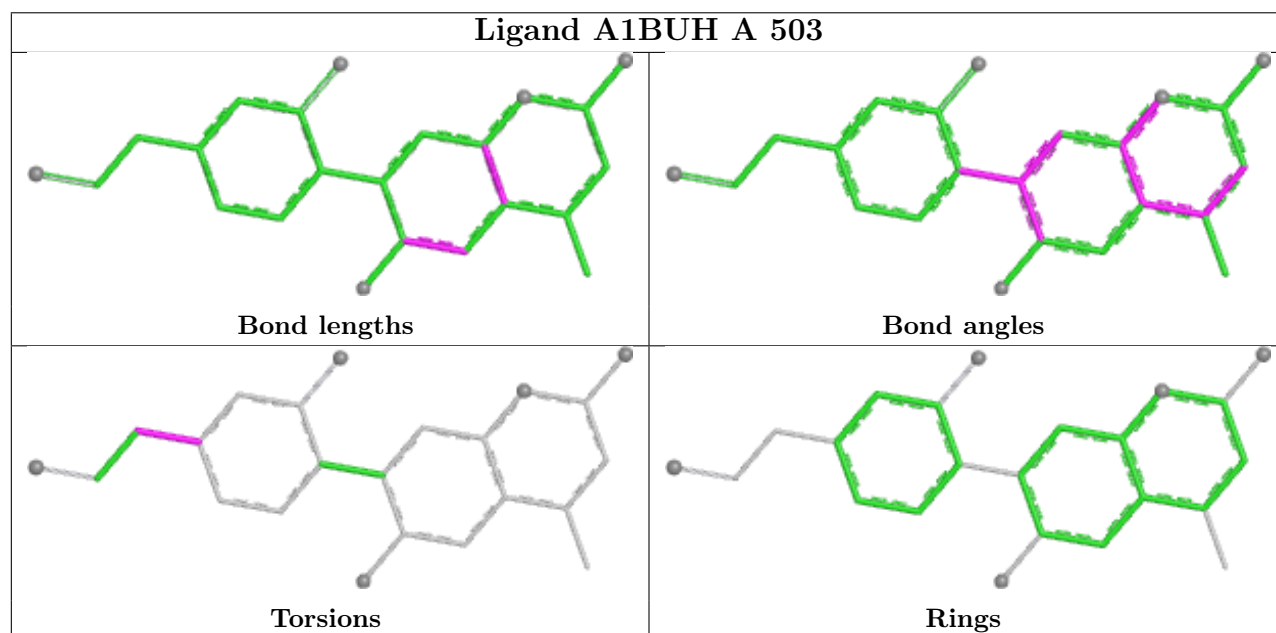
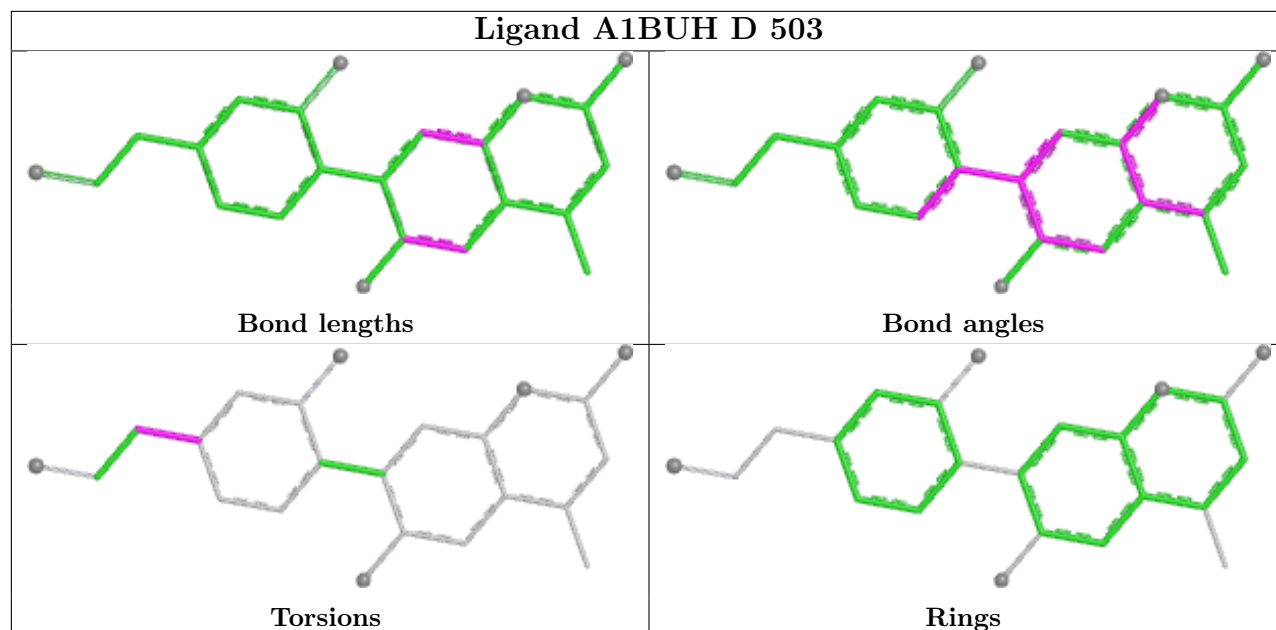
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	510	GOL	2	0
5	B	508	BTB	2	0
7	D	509	GOL	1	0
6	B	505	ACT	1	0
4	D	503	A1BUH	3	0
7	C	508	GOL	1	0
6	C	505	ACT	2	0
4	A	503	A1BUH	3	0
3	B	502	H4B	3	0
3	D	502	H4B	1	0
6	D	505	ACT	2	0

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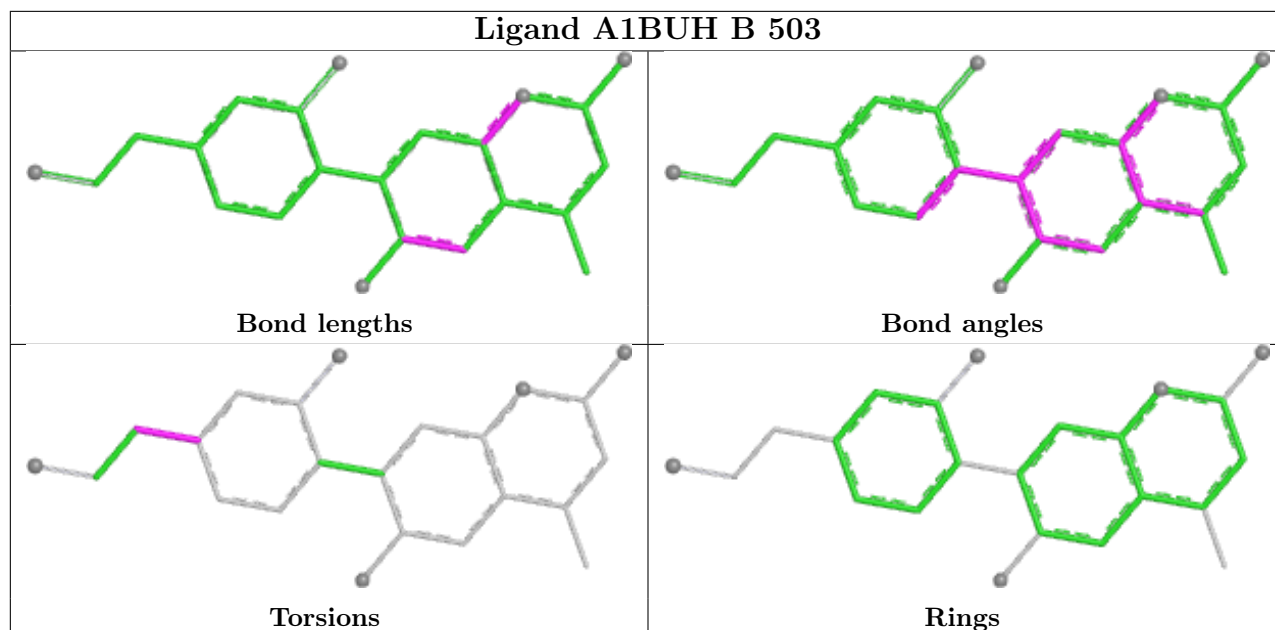
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	2	0
4	B	503	A1BUH	2	0
2	D	501	HEM	3	0
4	C	503	A1BUH	3	0
2	A	501	HEM	2	0
5	A	505	BTB	4	0
3	A	502	H4B	1	0
5	D	507	BTB	6	1
6	D	504	ACT	1	0
2	C	501	HEM	3	0
2	B	501	HEM	2	0
3	C	502	H4B	1	0
7	A	514	GOL	4	0
5	D	506	BTB	2	0
5	C	507	BTB	3	0
5	C	506	BTB	5	0
5	B	507	BTB	4	0

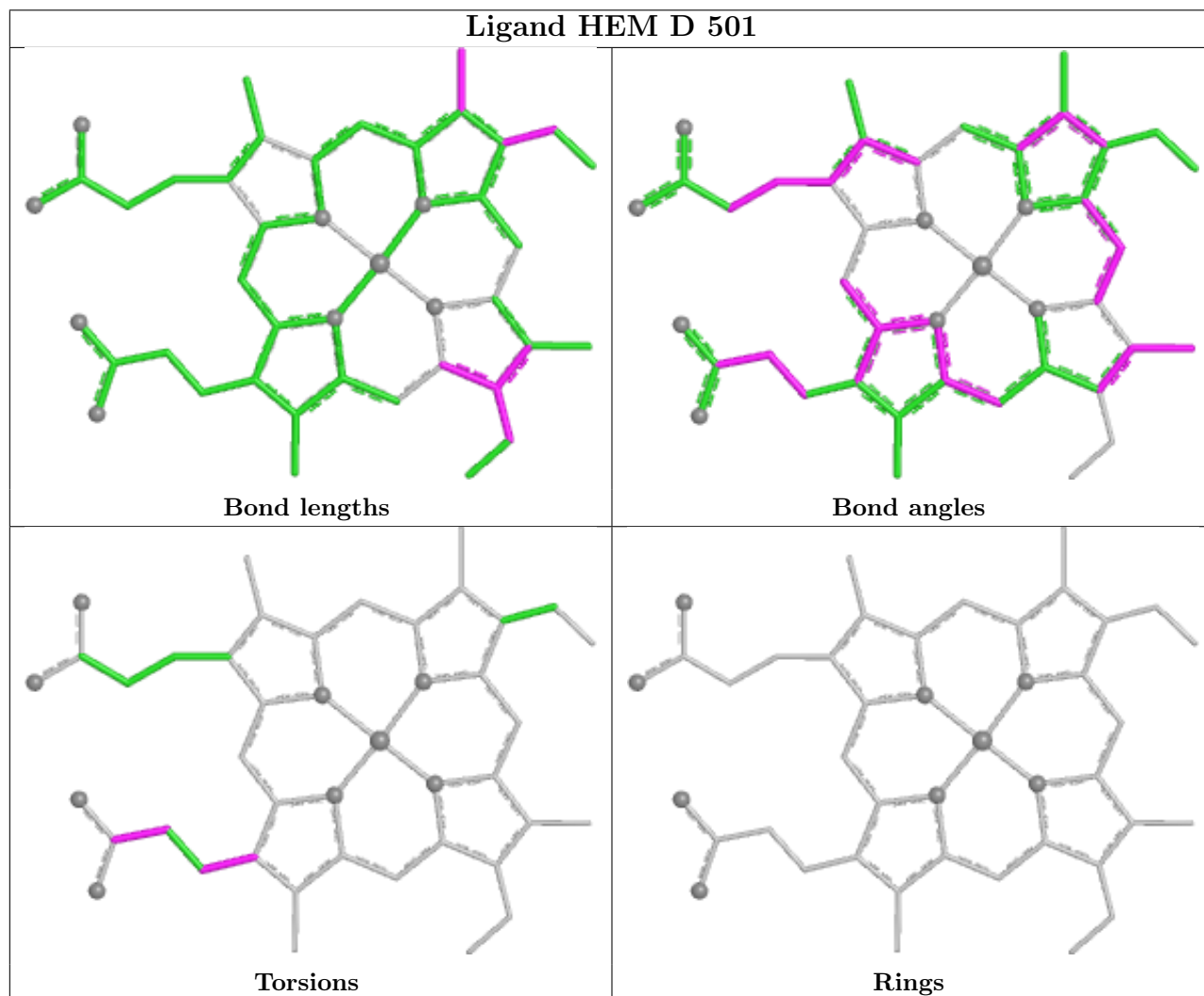
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



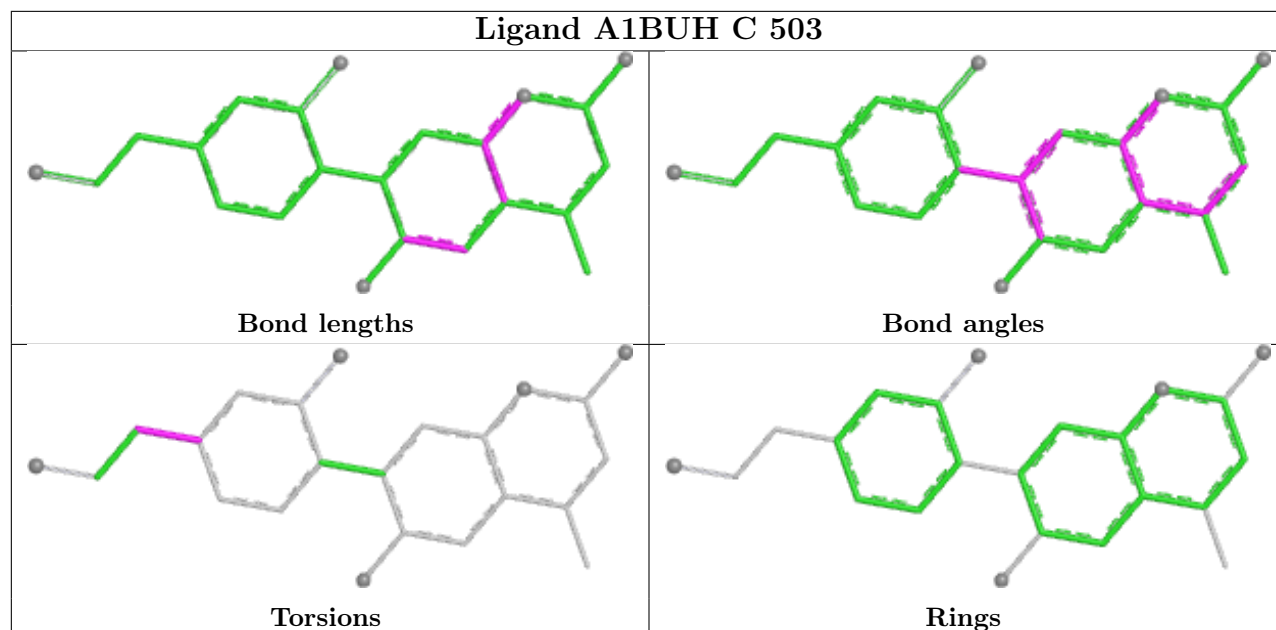
## Ligand A1BUH B 503



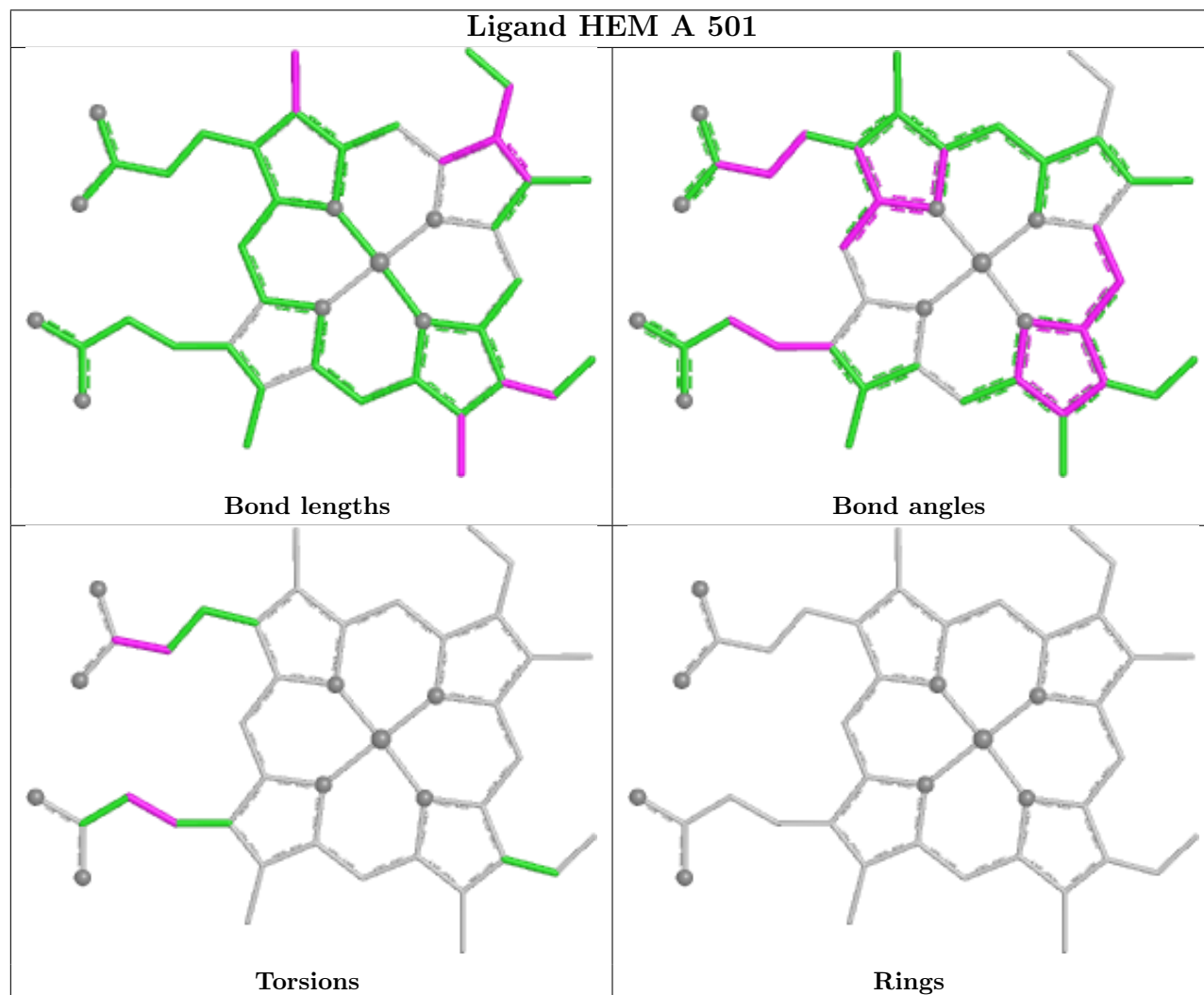
## Ligand HEM D 501

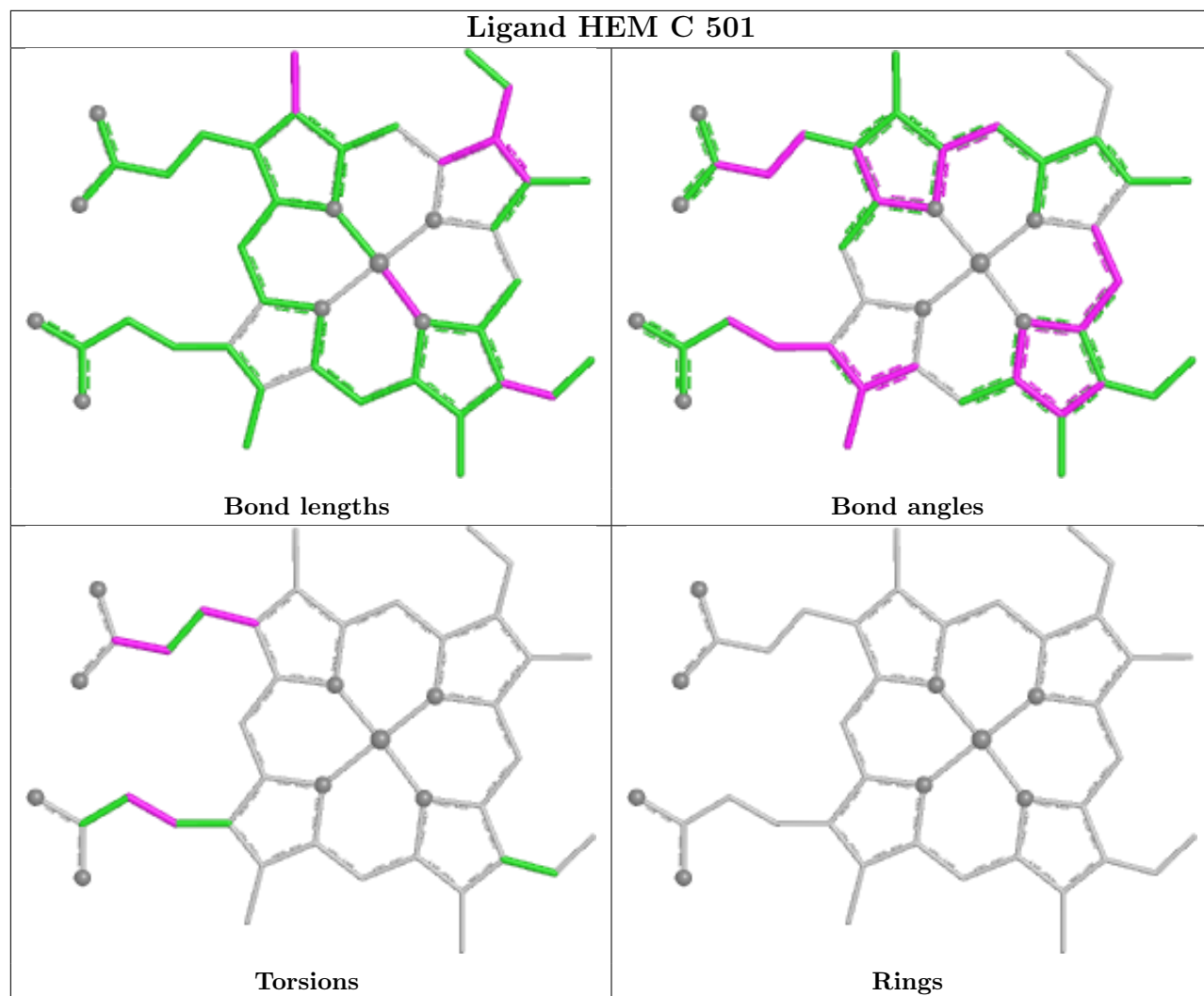


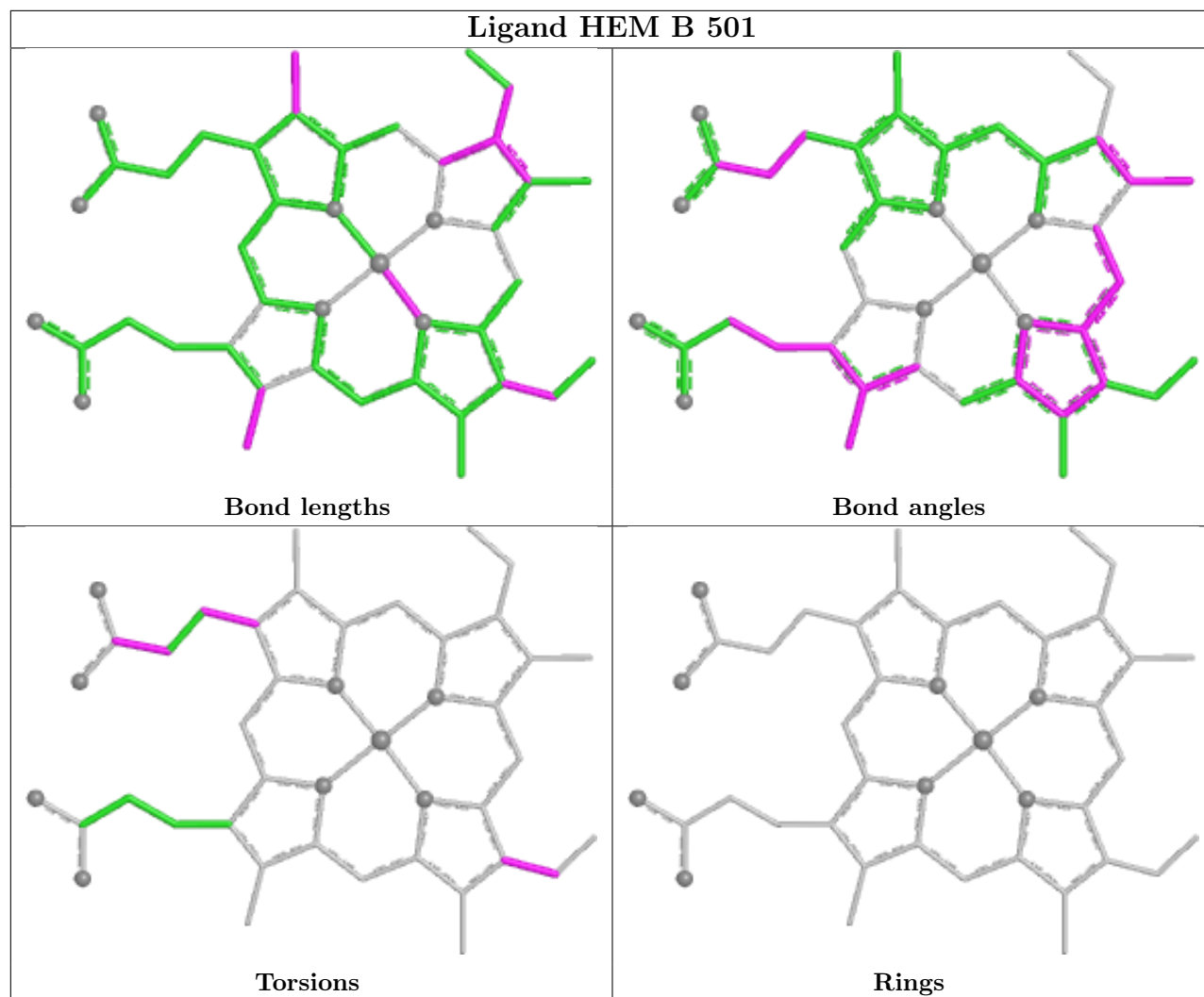
## Ligand A1BUH C 503



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	401/440 (91%)	-1.13	0 100 100	23, 44, 79, 108	1 (0%)
1	B	402/440 (91%)	-1.25	0 100 100	23, 37, 62, 95	2 (0%)
1	C	401/440 (91%)	-1.01	0 100 100	23, 49, 89, 103	1 (0%)
1	D	402/440 (91%)	-1.22	0 100 100	19, 37, 66, 93	2 (0%)
All	All	1606/1760 (91%)	-1.15	0 100 100	19, 42, 80, 108	6 (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	GOL	C	509	6/6	0.93	0.04	80,82,85,87	0
7	GOL	B	506	6/6	0.94	0.04	63,67,70,71	0
7	GOL	A	509	6/6	0.94	0.05	78,82,82,84	0
6	ACT	B	505	4/4	0.97	0.09	40,42,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BTB	B	508	14/14	0.97	0.04	70,75,77,80	0
7	GOL	A	514	6/6	0.97	0.06	48,58,59,67	0
5	BTB	C	507	14/14	0.97	0.04	65,68,73,73	0
6	ACT	A	506	4/4	0.97	0.08	41,45,46,46	0
5	BTB	D	507	14/14	0.98	0.04	61,73,78,78	0
7	GOL	C	508	6/6	0.98	0.04	52,69,71,74	0
6	ACT	D	504	4/4	0.98	0.08	36,38,39,46	0
7	GOL	D	508	6/6	0.98	0.04	71,73,78,83	0
7	GOL	D	509	6/6	0.98	0.06	48,66,68,73	0
5	BTB	C	506	14/14	0.99	0.04	51,67,74,75	0
3	H4B	A	502	17/17	0.99	0.03	27,32,44,44	0
5	BTB	D	506	14/14	0.99	0.04	35,44,54,67	0
3	H4B	B	502	17/17	0.99	0.03	27,36,46,47	0
3	H4B	C	502	17/17	0.99	0.04	36,39,42,42	0
6	ACT	A	507	4/4	0.99	0.05	43,44,48,52	0
6	ACT	B	504	4/4	0.99	0.04	39,40,44,54	0
3	H4B	D	502	17/17	0.99	0.03	28,34,41,44	0
6	ACT	C	504	4/4	0.99	0.07	44,46,49,52	0
6	ACT	C	505	4/4	0.99	0.04	48,50,58,59	0
4	A1BUH	A	503	23/23	0.99	0.04	33,44,57,61	0
6	ACT	D	505	4/4	0.99	0.08	37,39,41,44	0
7	GOL	A	508	6/6	0.99	0.03	46,55,62,65	0
4	A1BUH	B	503	23/23	0.99	0.03	23,31,49,54	0
7	GOL	A	510	6/6	0.99	0.07	71,77,80,83	0
4	A1BUH	C	503	23/23	0.99	0.04	39,50,56,62	0
4	A1BUH	D	503	23/23	0.99	0.04	26,33,52,56	0
5	BTB	A	504	14/14	0.99	0.04	28,54,58,59	0
5	BTB	A	505	14/14	0.99	0.03	35,63,70,71	0
5	BTB	B	507	14/14	0.99	0.04	34,53,62,72	0
2	HEM	C	501	43/43	0.99	0.04	31,41,47,50	0
8	CL	B	509	1/1	0.99	0.06	49,49,49,49	0
8	CL	D	510	1/1	0.99	0.07	46,46,46,46	0
11	CA	B	511	1/1	0.99	0.02	34,34,34,34	0
8	CL	A	511	1/1	1.00	0.06	48,48,48,48	0
2	HEM	B	501	43/43	1.00	0.03	20,25,33,39	0
8	CL	C	510	1/1	1.00	0.05	58,58,58,58	0
2	HEM	A	501	43/43	1.00	0.03	29,36,40,44	0
9	GD	A	512	1/1	1.00	0.04	71,71,71,71	0
9	GD	B	510	1/1	1.00	0.02	44,44,44,44	0
9	GD	C	511	1/1	1.00	0.03	100,100,100,100	0
9	GD	D	511	1/1	1.00	0.01	41,41,41,41	0
10	ZN	A	513	1/1	1.00	0.01	31,31,31,31	0

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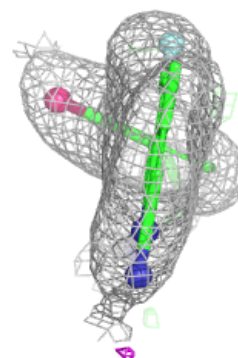
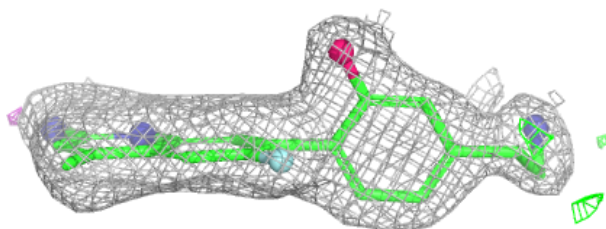
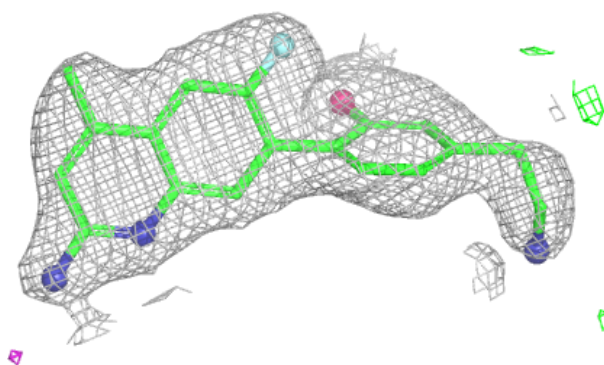
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	ZN	C	512	1/1	1.00	0.01	36,36,36,36	0
11	CA	A	515	1/1	1.00	0.02	49,49,49,49	0
2	HEM	D	501	43/43	1.00	0.03	21,27,37,38	0

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.

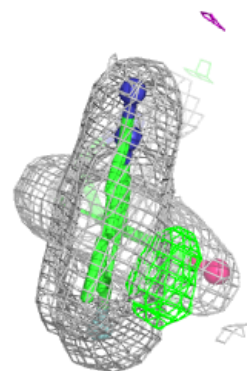
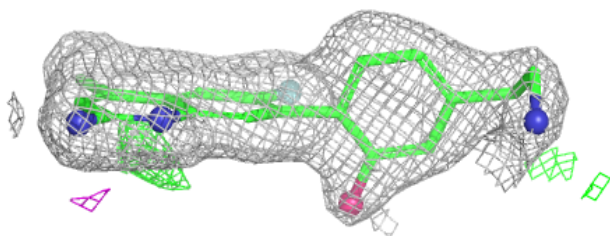
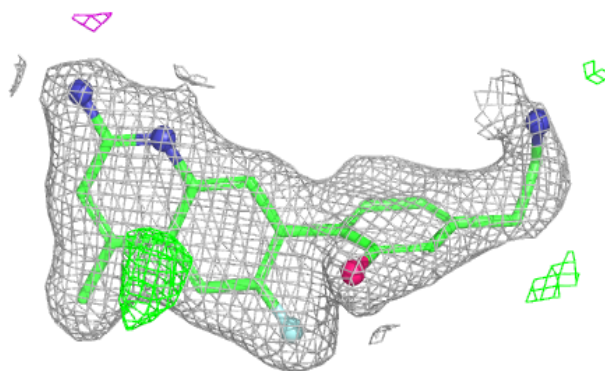
**Electron density around A1BUH A 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

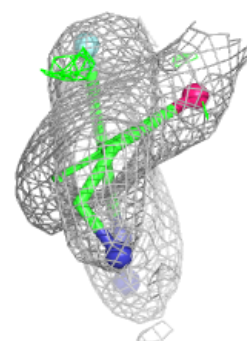
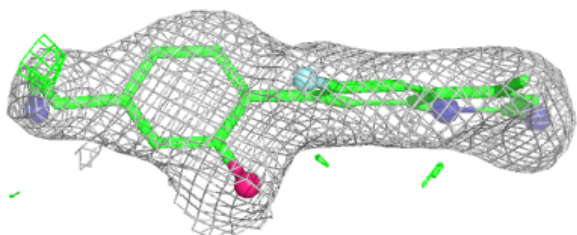
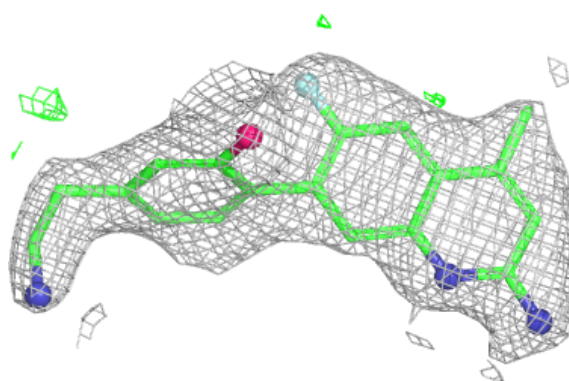


**Electron density around A1BUH B 503:**

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

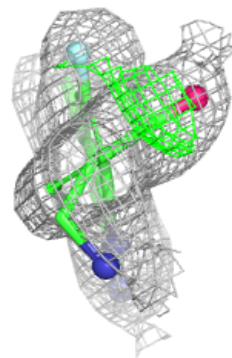
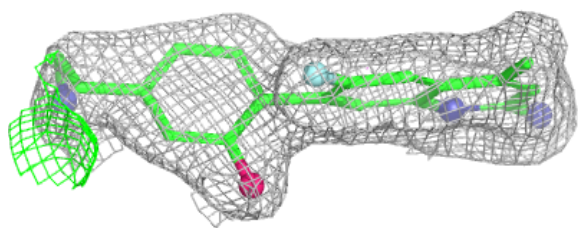
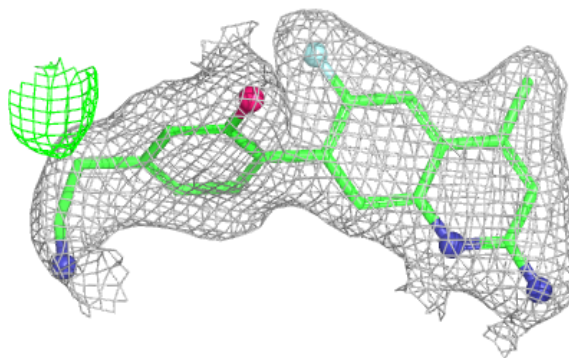
**Electron density around A1BUH C 503:**

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



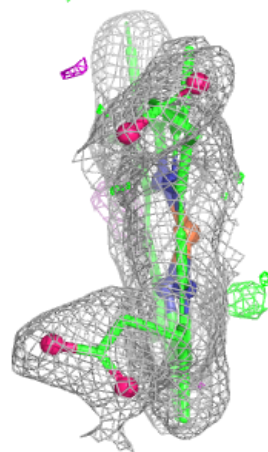
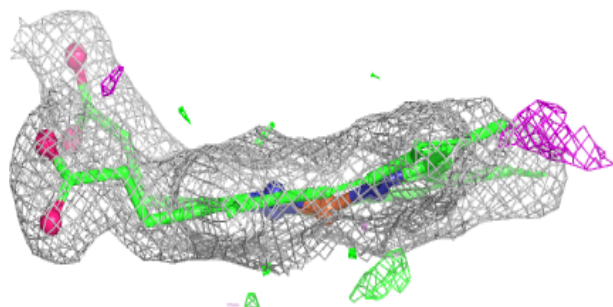
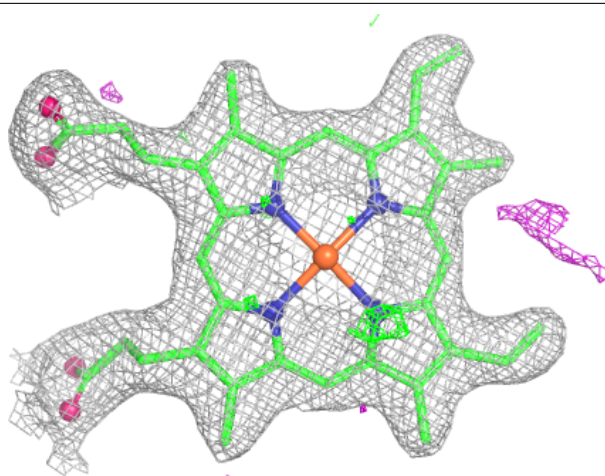
**Electron density around A1BUH D 503:**

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



**Electron density around HEM C 501:**

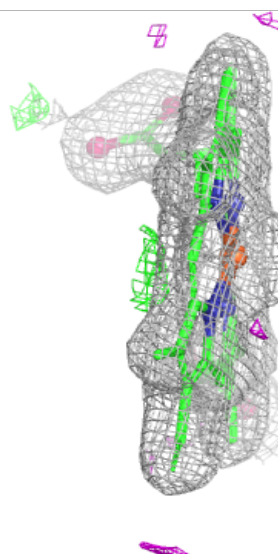
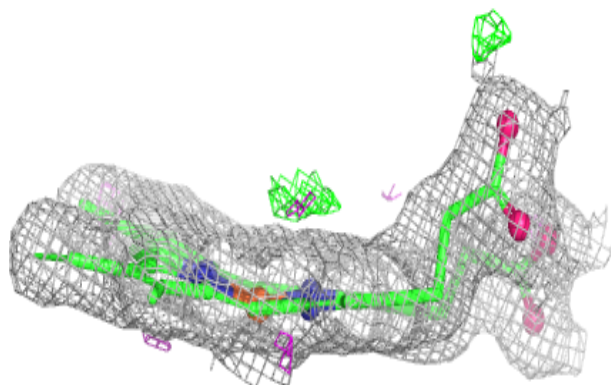
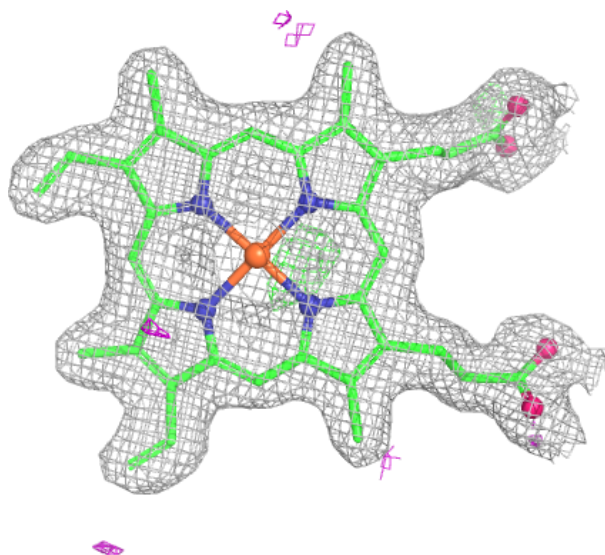
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





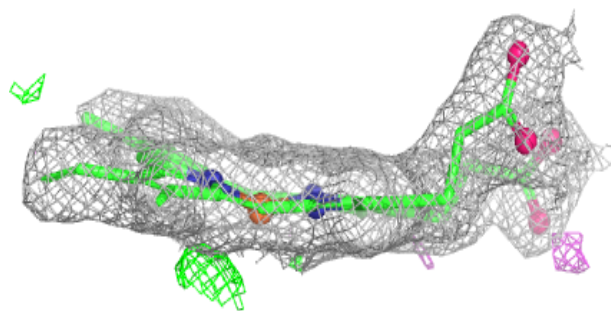
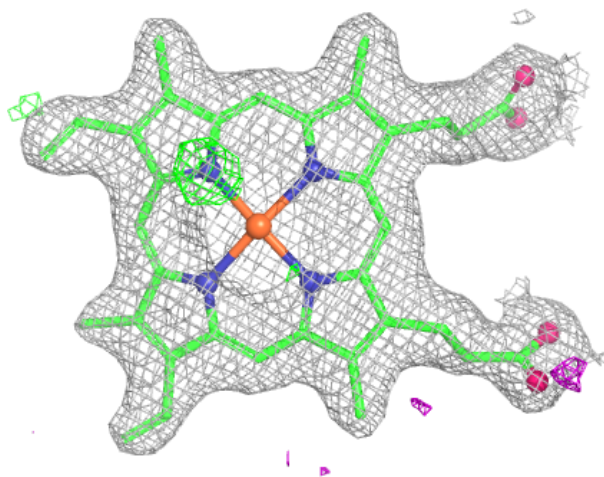
**Electron density around HEM B 501:**

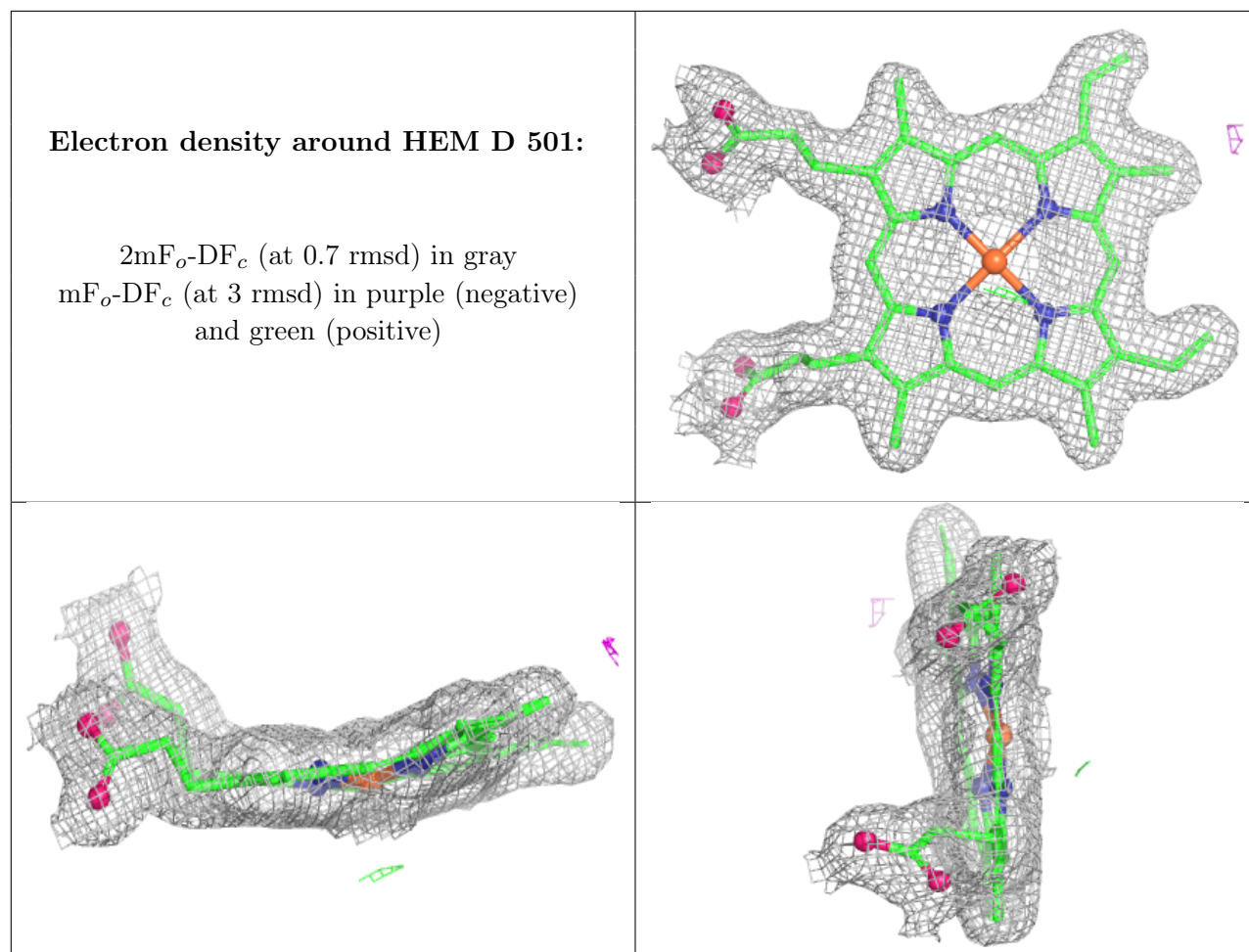
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 [i](#)

There are no such residues in this entry.