



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 01:56 AM EDT

PDB ID : 8FGR  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(5-(2-aminoethyl)-2,3-difluorophenethyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2022-12-12  
Resolution : 1.98 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

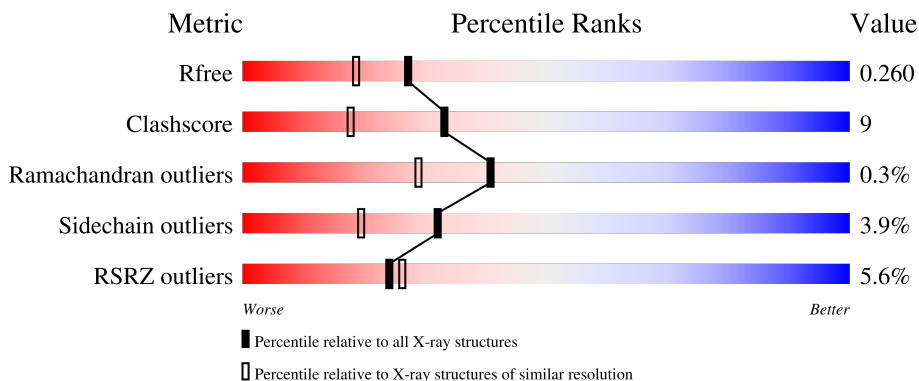
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	 11% 70% 19% • 9%
1	B	440	 2% 77% 13% • 9%
1	C	440	 6% 70% 20% • 9%
1	D	440	 % 74% 17% 9%

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	GOL	A	512	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13960 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.

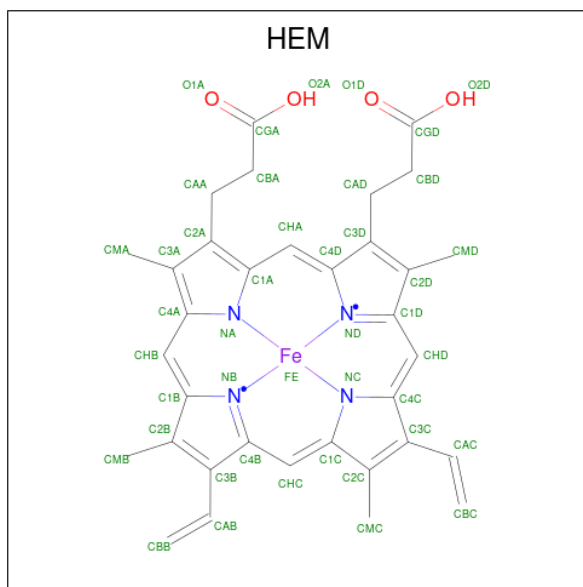
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3207	2043	564	584	16	0	1	0
1	B	402	3222	2051	568	587	16	0	3	0
1	C	402	3212	2046	565	585	16	0	1	0
1	D	402	3214	2046	567	585	16	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

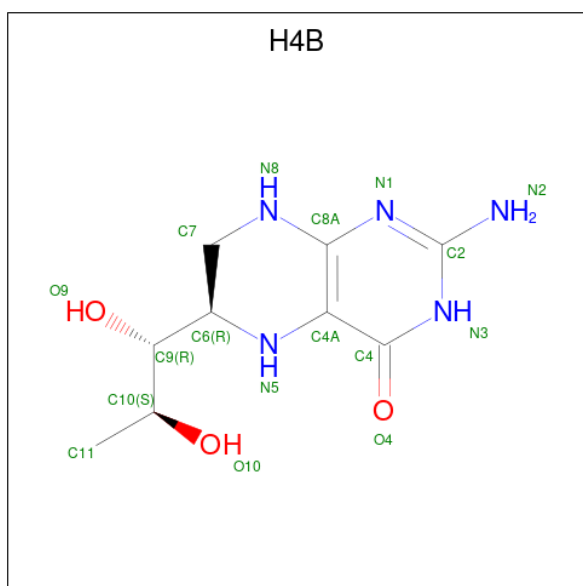
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



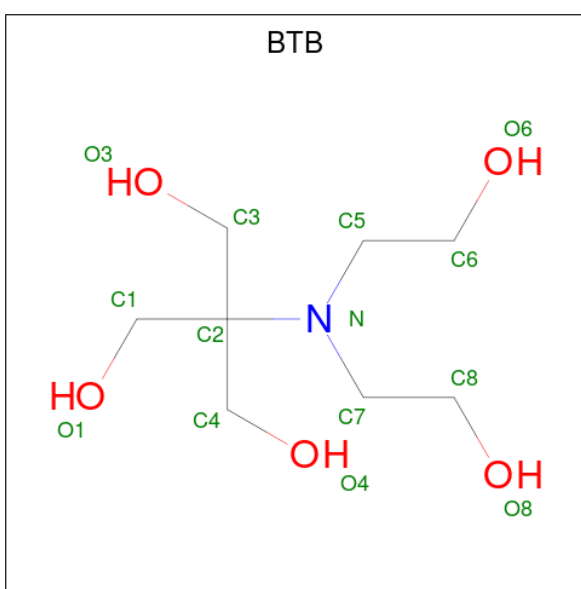
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Fe	N			O	
2	A	1	Total	43	34	1	4	4	0	0
2	B	1	Total	43	34	1	4	4	0	0
2	C	1	Total	43	34	1	4	4	0	0
2	D	1	Total	43	34	1	4	4	0	0

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



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

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



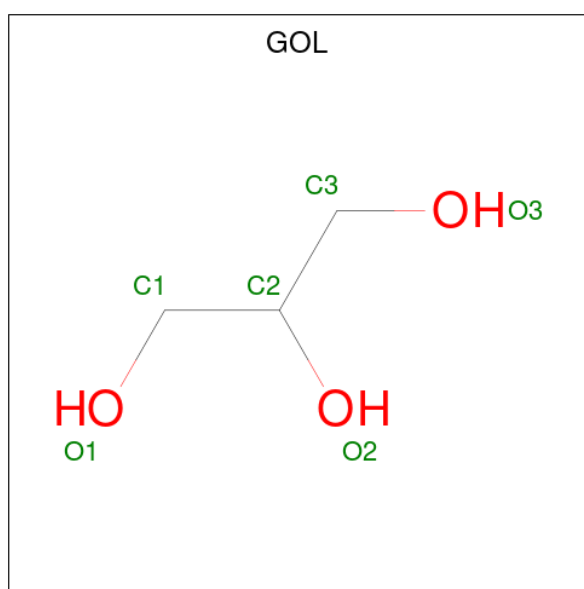
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

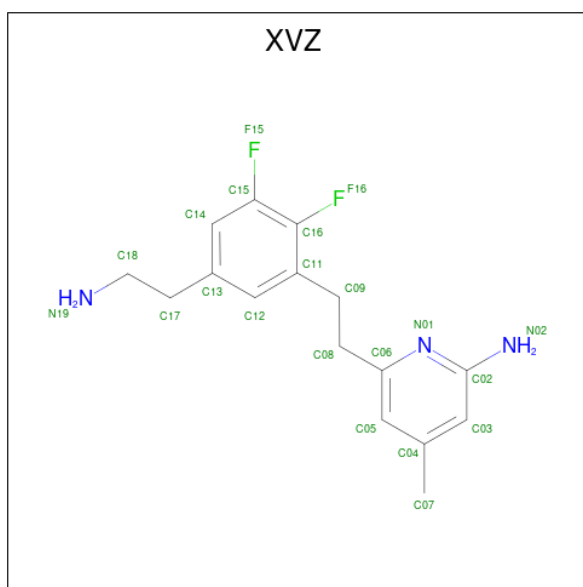
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Gd 1 1	0	0
7	B	1	Total Gd 1 1	0	0
7	C	1	Total Gd 1 1	0	0
7	D	1	Total Gd 1 1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is 6-{2-[5-(2-aminoethyl)-2,3-difluorophenyl]ethyl}-4-methylpyridin-2-amine (three-letter code: XVZ) (formula: C<sub>16</sub>H<sub>19</sub>F<sub>2</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
9	A	1	21	16	2	3	0	0
9	B	1	21	16	2	3	0	0
9	C	1	21	16	2	3	0	0
9	D	1	21	16	2	3	0	0

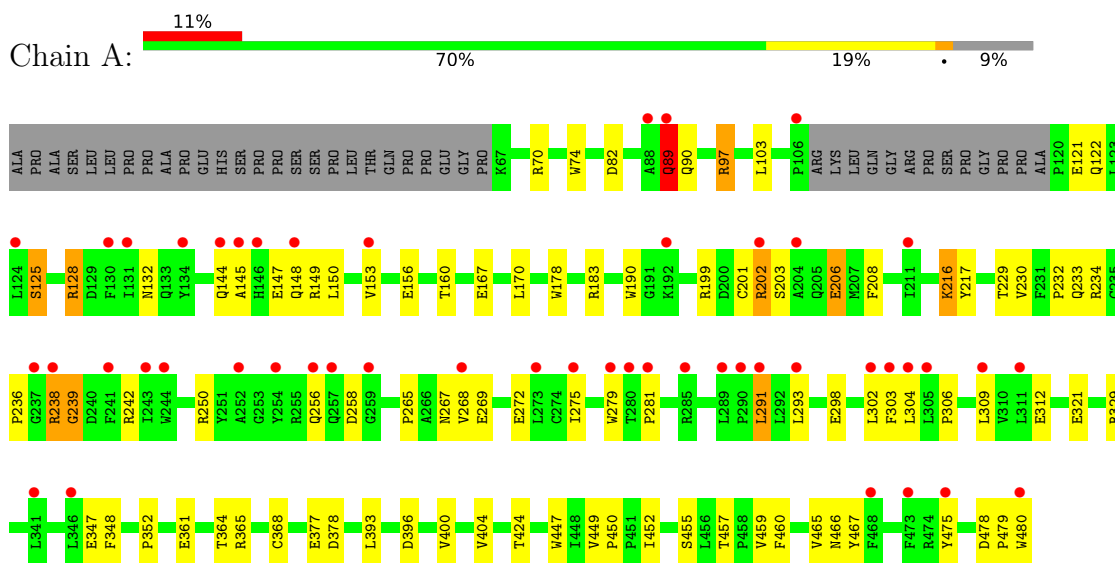
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	100	100	100	0	0
10	B	169	169	169	0	0
10	C	126	126	126	0	0
10	D	168	168	168	0	0

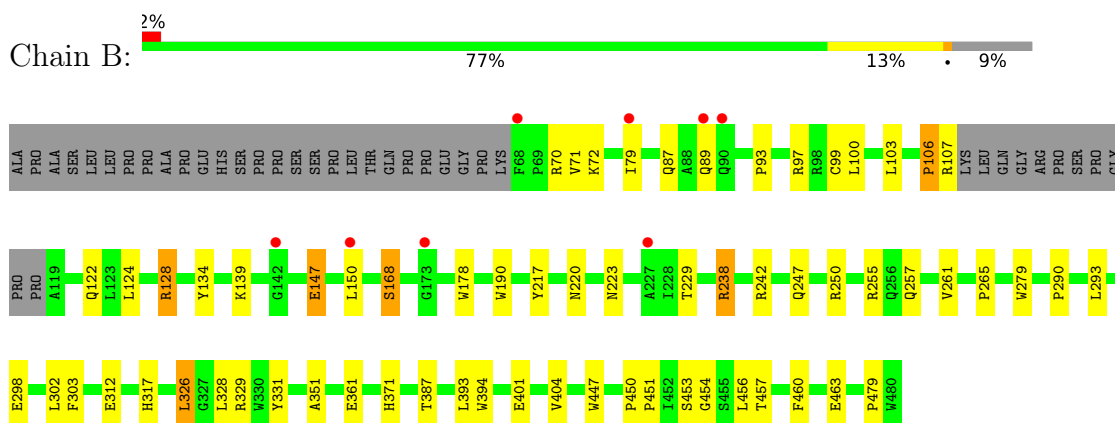
### 3 Residue-property plots

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.

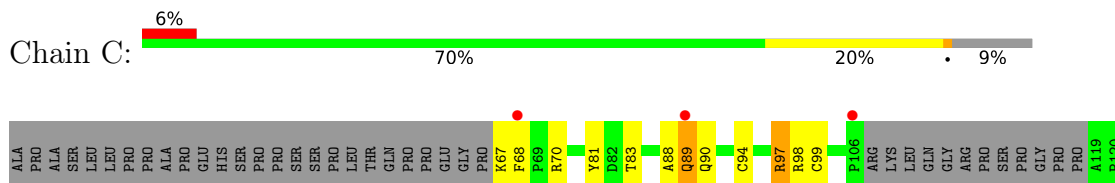
- Molecule 1: Nitric oxide synthase, endothelial

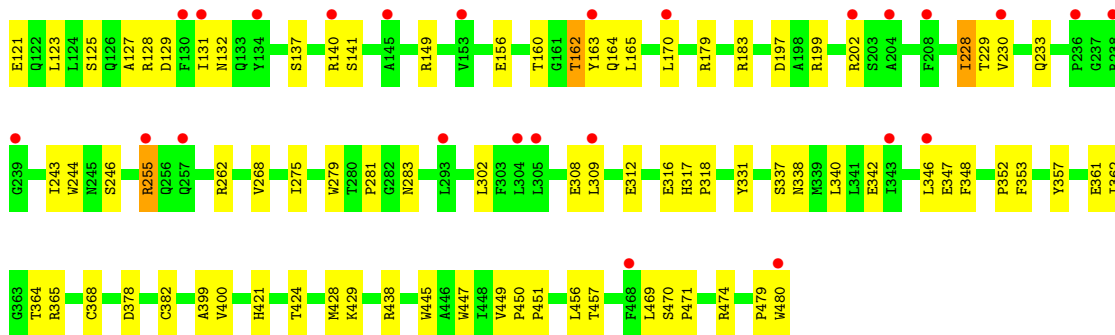


- Molecule 1: Nitric oxide synthase, endothelial

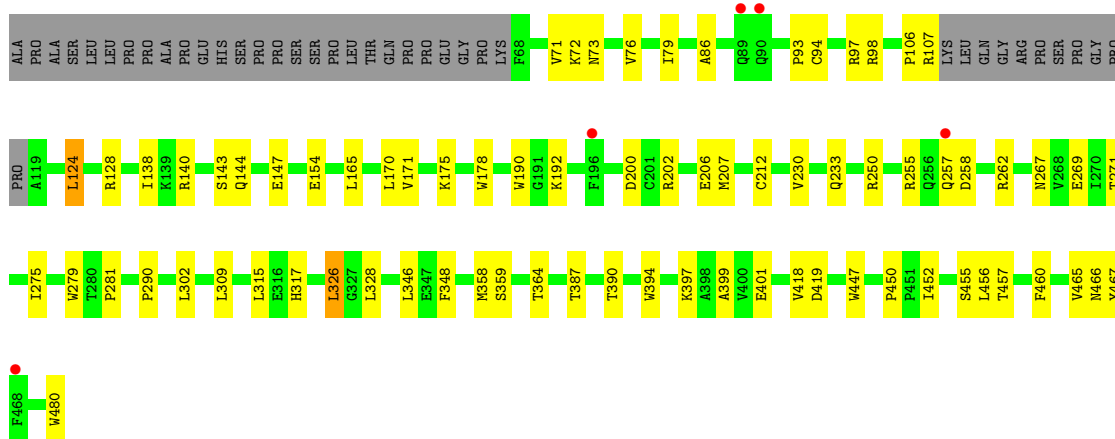
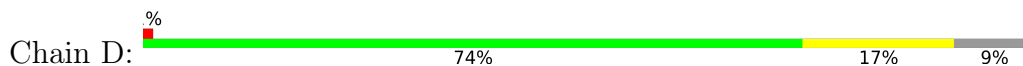


- Molecule 1: Nitric oxide synthase, endothelial





• Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.78Å 150.90Å 107.43Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	48.60 – 1.98 48.99 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.60-1.98) 96.8 (48.99-1.98)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.208 , 0.263 0.202 , 0.260	Depositor DCC
$R_{free}$ test set	6554 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtrriage
Anisotropy	0.941	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.226 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: ZN, HEM, GOL, XVZ, GD, H4B, CL, BTB

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	0.35	0/3302	0.52	0/4498
1	B	0.42	0/3323	0.55	0/4528
1	C	0.36	0/3307	0.51	0/4506
1	D	0.42	0/3309	0.57	0/4509
All	All	0.39	0/13241	0.54	0/18041

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3207	0	3112	63	0
1	B	3222	0	3127	46	0
1	C	3212	0	3116	57	0
1	D	3214	0	3116	43	0
2	A	43	0	30	6	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	2	0
3	C	17	0	15	2	0
3	D	17	0	15	1	0
4	A	42	0	57	5	0
4	B	28	0	37	9	0
4	C	42	0	56	8	0
4	D	42	0	56	5	0
5	A	18	0	24	2	0
5	B	12	0	16	1	0
5	C	18	0	24	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	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	C	1	0	0	0	0
9	A	21	0	0	1	0
9	B	21	0	0	2	0
9	C	21	0	0	3	0
9	D	21	0	0	1	0
10	A	100	0	0	5	0
10	B	169	0	0	2	0
10	C	126	0	0	4	0
10	D	168	0	0	3	0
All	All	13960	0	12929	225	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 (225) 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:247:GLN:HB2	1:B:250:ARG:HD3	1.53	0.87
1:C:382:CYS:HA	4:C:504:BTB:H12	1.62	0.80
1:C:378:ASP:OD1	10:C:601:HOH:O	2.05	0.74
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:OD2	10:A:601:HOH:O	2.06	0.73
2:C:501:HEM:O2A	9:C:503:XVZ:N19	2.21	0.73
1:A:378:ASP:OD1	10:A:602:HOH:O	2.07	0.72
4:B:505:BTB:O8	4:B:505:BTB:O3	2.07	0.72
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.71	0.72
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.58	0.69
1:C:128:ARG:O	1:C:132:ASN:ND2	2.26	0.68
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.77	0.66
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.59	0.66
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.76	0.65
4:B:505:BTB:HO3	4:B:505:BTB:HO8	1.44	0.65
2:A:501:HEM:HHA	2:A:501:HEM:HBA1	1.78	0.65
1:C:160:THR:HG23	1:C:162:THR:H	1.62	0.65
1:A:321:GLU:H	1:A:321:GLU:CD	2.00	0.65
1:C:316:GLU:OE2	10:C:602:HOH:O	2.14	0.64
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.79	0.63
4:C:506:BTB:O1	4:C:506:BTB:O4	2.16	0.63
2:B:502:HEM:HBB2	2:B:502:HEM:HHC	1.81	0.63
1:C:255:ARG:HH12	1:C:268:VAL:HG11	1.66	0.61
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.14	0.61
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.83	0.60
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.14	0.60
1:A:312:GLU:OE2	1:A:329:ARG:NH2	2.35	0.59
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.37	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.83	0.59
1:B:298:GLU:OE1	4:B:505:BTB:H42	2.02	0.58
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.86	0.58
1:D:170:LEU:HD11	1:D:230:VAL:HG11	1.86	0.58
4:D:506:BTB:O4	4:D:506:BTB:O3	2.11	0.58
1:B:106:PRO:O	1:B:107:ARG:HG3	2.04	0.57
1:A:70:ARG:NH2	10:A:603:HOH:O	2.10	0.57
1:A:447:TRP:HE3	2:A:501:HEM:HBA2	1.68	0.57
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.87	0.57
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.86	0.57
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.40	0.57
4:D:505:BTB:O4	4:D:505:BTB:H52	2.04	0.56
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.86	0.56
1:A:89:GLN:HG3	1:A:90:GLN:N	2.21	0.56
1:D:447:TRP:HA	3:D:502:H4B:N1	2.21	0.56
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.88	0.55
1:A:145:ALA:HA	1:A:148:GLN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.41	0.55
1:D:271:THR:O	1:D:275:ILE:HG12	2.06	0.55
2:A:501:HEM:HBA1	2:A:501:HEM:CHA	2.35	0.55
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.42	0.55
1:A:156:GLU:O	1:A:160:THR:OG1	2.25	0.55
1:B:217:TYR:OH	10:B:601:HOH:O	2.09	0.55
1:C:364:THR:O	1:C:368:CYS:HB2	2.07	0.54
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.89	0.54
1:B:447:TRP:HA	3:B:503:H4B:N1	2.23	0.54
1:C:255:ARG:NH1	1:C:268:VAL:HG11	2.22	0.54
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.24	0.53
1:B:450:PRO:HG3	1:B:457:THR:HG21	1.90	0.53
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.43	0.53
1:B:371:HIS:HD1	1:B:371:HIS:H	1.55	0.52
4:C:505:BTB:O4	4:C:505:BTB:H51	2.08	0.52
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.90	0.52
3:A:502:H4B:H113	1:B:463:GLU:HG2	1.92	0.52
1:C:342:GLU:HG3	1:C:474:ARG:NH2	2.24	0.52
1:C:97:ARG:NH2	10:C:609:HOH:O	2.41	0.52
1:B:298:GLU:OE1	4:B:505:BTB:H72	2.10	0.52
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.45	0.51
1:C:90:GLN:NE2	10:C:610:HOH:O	2.42	0.51
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.45	0.51
1:B:298:GLU:CD	4:B:505:BTB:H42	2.31	0.51
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.45	0.51
1:A:125:SER:HA	1:A:128:ARG:NH1	2.26	0.51
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.92	0.51
1:B:387:THR:HA	1:B:394:TRP:CD1	2.46	0.51
4:C:504:BTB:O3	4:C:504:BTB:O4	2.28	0.50
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.50
9:B:501:XVZ:N19	3:B:503:H4B:O4	2.44	0.50
1:A:298:GLU:OE1	4:A:505:BTB:O4	2.26	0.50
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.46	0.50
1:A:238:ARG:NH2	1:A:239:GLY:O	2.45	0.50
1:D:72:LYS:NZ	10:D:608:HOH:O	2.41	0.49
1:C:197:ASP:OD2	1:C:199:ARG:NH2	2.33	0.49
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.29	0.49
1:C:246:SER:HA	1:C:338:ASN:HB3	1.93	0.49
1:C:421:HIS:HB2	1:D:390:THR:HB	1.94	0.49
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.94	0.49
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:HEM:O2D	9:C:503:XVZ:F15	2.20	0.49
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.95	0.49
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.27	0.49
4:B:504:BTB:O4	4:B:504:BTB:O3	2.26	0.49
1:C:170:LEU:HD11	1:C:230:VAL:HG21	1.94	0.49
1:D:275:ILE:HD12	1:D:281:PRO:HB3	1.95	0.49
1:C:156:GLU:O	1:C:160:THR:HG22	2.13	0.49
1:C:228:ILE:HG13	1:C:353:PHE:HB3	1.95	0.49
1:C:262:ARG:NH1	1:C:283:ASN:O	2.45	0.49
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.48	0.49
1:B:72:LYS:O	1:B:463:GLU:HG3	2.13	0.48
1:D:143:SER:O	1:D:147:GLU:HG2	2.14	0.48
4:A:503:BTB:O8	10:A:604:HOH:O	2.20	0.47
1:A:144:GLN:HG3	1:A:145:ALA:N	2.30	0.47
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.95	0.47
4:B:504:BTB:O8	1:C:378:ASP:OD2	2.32	0.47
1:A:216:LYS:HG3	1:A:217:TYR:N	2.29	0.47
1:A:90:GLN:NE2	10:A:606:HOH:O	2.27	0.47
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.97	0.47
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.49	0.47
1:C:162:THR:OG1	1:C:163:TYR:N	2.48	0.47
1:C:312:GLU:HA	1:C:331:TYR:HA	1.96	0.47
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.50	0.47
1:B:238:ARG:NH2	10:B:613:HOH:O	2.48	0.47
1:C:129:ASP:HA	1:C:132:ASN:HD22	1.79	0.47
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.96	0.47
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.97	0.47
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.48	0.47
1:C:89:GLN:HG2	1:C:469:LEU:HA	1.97	0.47
1:A:269:GLU:O	1:A:272:GLU:HG2	2.15	0.46
1:C:97:ARG:NH2	1:D:86:ALA:HA	2.30	0.46
1:C:149:ARG:NH2	1:C:164:GLN:O	2.45	0.46
1:A:404:VAL:HG23	1:B:393:LEU:HD12	1.97	0.46
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.98	0.46
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.97	0.46
1:A:377:GLU:OE1	4:A:504:BTB:H32	2.15	0.46
1:A:74:TRP:HB3	5:B:507:GOL:H32	1.98	0.45
1:A:291:LEU:HD23	1:A:293:LEU:HD21	1.98	0.45
1:C:70:ARG:HG3	1:C:81:TYR:CE2	2.51	0.45
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.29	0.45
4:B:505:BTB:H42	4:B:505:BTB:H72	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ARG:NH2	1:C:438:ARG:HG3	2.31	0.45
1:B:178:TRP:CZ3	2:B:502:HEM:HMC3	2.50	0.45
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.52	0.45
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.97	0.45
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.52	0.45
1:C:340:LEU:HD21	1:C:347:GLU:HB3	1.98	0.45
1:C:361:GLU:OE2	9:C:503:XVZ:N02	2.49	0.45
1:D:465:VAL:HG12	1:D:467:TYR:HD1	1.80	0.45
1:B:147:GLU:H	1:B:147:GLU:HG2	1.45	0.45
1:C:456:LEU:HD11	1:D:399:ALA:CB	2.47	0.45
1:A:455:SER:HA	1:A:460:PHE:CG	2.52	0.45
1:B:293:LEU:HD12	1:B:303:PHE:CD1	2.52	0.44
1:A:393:LEU:HD12	1:B:404:VAL:HG23	1.99	0.44
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.77	0.44
1:D:138:ILE:HD12	1:D:140:ARG:HE	1.82	0.44
4:D:504:BTB:H32	4:D:504:BTB:H51	1.79	0.44
4:C:506:BTB:H72	4:C:506:BTB:H31	1.51	0.44
1:A:149:ARG:O	1:A:153:VAL:HG22	2.18	0.44
1:C:123:LEU:HD21	1:C:162:THR:HA	1.99	0.44
4:B:504:BTB:H32	4:B:504:BTB:H51	1.74	0.44
1:D:387:THR:HA	1:D:394:TRP:CD1	2.52	0.44
1:A:167:GLU:CD	5:A:506:GOL:H2	2.38	0.44
1:A:279:TRP:HB2	1:A:302:LEU:HD11	2.00	0.44
1:C:445:TRP:CZ2	1:C:449:VAL:HG21	2.53	0.44
4:C:505:BTB:H52	4:C:505:BTB:H81	1.37	0.44
1:D:450:PRO:HG2	1:D:457:THR:HG21	2.00	0.44
1:C:447:TRP:HA	3:C:502:H4B:N1	2.33	0.44
1:A:250:ARG:HD3	1:A:267:ASN:OD1	2.18	0.43
1:B:261:VAL:HG11	1:B:265:PRO:HA	2.00	0.43
1:A:256:GLN:C	1:A:258:ASP:H	2.21	0.43
1:A:455:SER:OG	1:B:451:PRO:HB2	2.17	0.43
1:B:220:ASN:HB3	1:B:223:ASN:O	2.18	0.43
1:C:399:ALA:CB	1:D:456:LEU:HD11	2.47	0.43
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.53	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.17	0.43
1:D:144:GLN:HG2	10:D:741:HOH:O	2.18	0.43
1:A:202:ARG:NH1	1:A:202:ARG:HB2	2.33	0.43
1:A:361:GLU:OE2	9:A:511:XVZ:N02	2.52	0.43
1:D:358:MET:HA	1:D:418:VAL:O	2.19	0.43
1:A:298:GLU:OE2	4:A:505:BTB:H32	2.19	0.43
1:A:396:ASP:O	1:A:400:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:PHE:CD1	1:C:83:THR:HG22	2.54	0.43
1:A:128:ARG:O	1:A:132:ASN:ND2	2.52	0.43
1:A:449:VAL:HG22	1:A:459:VAL:HG23	2.00	0.43
1:A:103:LEU:HG	1:B:463:GLU:OE1	2.19	0.42
1:A:178:TRP:CZ3	2:A:501:HEM:HMC3	2.54	0.42
1:A:229:THR:O	1:A:352:PRO:HD2	2.19	0.42
1:C:451:PRO:HB2	1:D:455:SER:OG	2.19	0.42
1:D:212:CYS:HA	1:D:309:LEU:HD21	2.01	0.42
1:C:255:ARG:NH1	1:C:255:ARG:HB2	2.34	0.42
1:D:269:GLU:OE2	1:D:480:TRP:NE1	2.44	0.42
1:D:359:SER:OG	1:D:419:ASP:HA	2.18	0.42
1:B:134:TYR:OH	1:B:168[A]:SER:HB3	2.19	0.42
1:B:124:LEU:HB3	1:B:128:ARG:NH1	2.32	0.42
1:A:465:VAL:HG12	1:A:467:TYR:HD1	1.84	0.42
1:B:147:GLU:HA	1:B:150:LEU:HD12	2.00	0.42
1:C:127:ALA:O	1:C:131:ILE:HG12	2.19	0.42
1:D:124:LEU:HD22	1:D:128:ARG:CZ	2.49	0.42
1:A:424:THR:HB	1:A:459:VAL:HG13	2.01	0.42
1:A:306:PRO:HB2	1:A:309:LEU:HB2	2.02	0.42
1:C:424:THR:O	1:C:428:MET:HG2	2.20	0.42
1:A:478:ASP:O	1:A:480:TRP:N	2.44	0.42
4:C:505:BTB:H32	4:C:505:BTB:H71	1.81	0.42
1:D:315:LEU:HD12	1:D:328:LEU:HB3	2.02	0.42
4:A:504:BTB:H51	4:A:504:BTB:H11	1.75	0.42
1:B:71:VAL:HG13	1:B:463:GLU:HB2	2.02	0.42
1:B:312:GLU:HA	1:B:331:TYR:HA	2.02	0.42
1:C:229:THR:O	1:C:352:PRO:HD2	2.20	0.42
1:D:255:ARG:HD2	1:D:255:ARG:HA	1.85	0.42
1:A:199:ARG:O	1:A:232:PRO:HG3	2.20	0.41
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.60	0.41
1:C:470:SER:HA	1:C:471:PRO:C	2.41	0.41
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.51	0.41
1:C:243:ILE:HB	1:C:337:SER:O	2.20	0.41
1:B:229:THR:O	1:B:351:ALA:HA	2.21	0.41
1:C:400:VAL:HG11	1:D:397:LYS:HG3	2.02	0.41
1:D:250:ARG:HD3	1:D:267:ASN:OD1	2.20	0.41
1:B:361:GLU:OE2	9:B:501:XVZ:N02	2.53	0.41
1:D:73:ASN:OD1	1:D:76:VAL:HG23	2.21	0.41
1:A:167:GLU:OE2	5:A:506:GOL:H2	2.20	0.41
1:A:170:LEU:HD11	1:A:230:VAL:HG21	2.03	0.41
1:C:94:CYS:HB3	1:D:94:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:506:BTB:H51	4:C:506:BTB:H42	1.46	0.41
1:D:165:LEU:HG	1:D:346:LEU:HD12	2.03	0.41
1:A:466:ASN:HB3	1:B:99:CYS:HB3	2.02	0.41
1:D:79:ILE:HD11	10:D:608:HOH:O	2.21	0.41
4:D:506:BTB:H11	4:D:506:BTB:H72	1.54	0.41
1:D:275:ILE:CD1	1:D:281:PRO:HB3	2.51	0.40
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.38	0.40
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.86	0.40
1:B:454:GLY:O	1:B:460:PHE:HB2	2.21	0.40
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.03	0.40
4:D:504:BTB:O8	4:D:504:BTB:O6	2.33	0.40
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.57	0.40
1:A:236:PRO:C	1:A:238:ARG:H	2.25	0.40
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.03	0.40
1:D:171:VAL:CG1	1:D:175:LYS:HE3	2.52	0.40
2:D:501:HEM:O2A	9:D:503:XVZ:N19	2.55	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	398/440 (90%)	377 (95%)	18 (4%)	3 (1%)	19 9
1	B	401/440 (91%)	387 (96%)	13 (3%)	1 (0%)	47 38
1	C	399/440 (91%)	383 (96%)	16 (4%)	0	100 100
1	D	399/440 (91%)	390 (98%)	9 (2%)	0	100 100
All	All	1597/1760 (91%)	1537 (96%)	56 (4%)	4 (0%)	41 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	PRO
1	A	89	GLN
1	A	203	SER
1	A	239	GLY

### 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	342/373 (92%)	330 (96%)	12 (4%)	36	24
1	B	344/373 (92%)	331 (96%)	13 (4%)	33	21
1	C	342/373 (92%)	326 (95%)	16 (5%)	26	13
1	D	342/373 (92%)	329 (96%)	13 (4%)	33	21
All	All	1370/1492 (92%)	1316 (96%)	54 (4%)	32	19

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	122	GLN
1	A	125	SER
1	A	128	ARG
1	A	202	ARG
1	A	206	GLU
1	A	216	LYS
1	A	238	ARG
1	A	291	LEU
1	A	304	LEU
1	B	87	GLN
1	B	89	GLN
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG
1	B	139	LYS

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Mol	Chain	Res	Type
1	B	147	GLU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	238	ARG
1	B	255	ARG
1	B	257	GLN
1	B	326	LEU
1	C	67	LYS
1	C	89	GLN
1	C	97	ARG
1	C	98	ARG
1	C	121	GLU
1	C	125	SER
1	C	137	SER
1	C	140	ARG
1	C	141	SER
1	C	162	THR
1	C	202	ARG
1	C	228	ILE
1	C	255	ARG
1	C	308	GLU
1	C	309	LEU
1	C	429	LYS
1	D	71	VAL
1	D	98	ARG
1	D	107	ARG
1	D	124	LEU
1	D	192	LYS
1	D	200	ASP
1	D	202	ARG
1	D	206	GLU
1	D	207	MET
1	D	257	GLN
1	D	258	ASP
1	D	262	ARG
1	D	326	LEU

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

Mol	Chain	Res	Type
1	C	132	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 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
5	GOL	B	507	-	5,5,5	0.39	0	5,5,5	0.40	0
9	XVZ	D	503	-	21,22,22	0.42	0	28,30,30	1.74	6 (21%)
4	BTB	C	505	-	13,13,13	0.48	0	7,16,16	0.87	0
4	BTB	B	504	7	13,13,13	0.53	0	7,16,16	0.58	0
5	GOL	D	507	-	5,5,5	0.35	0	5,5,5	0.33	0
4	BTB	A	505	-	13,13,13	0.35	0	7,16,16	0.51	0
3	H4B	C	502	-	16,18,18	0.82	0	11,26,26	2.81	5 (45%)
5	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	A	512	-	5,5,5	0.55	0	5,5,5	1.98	2 (40%)
9	XVZ	B	501	-	21,22,22	0.55	0	28,30,30	1.60	5 (17%)
5	GOL	C	507	-	5,5,5	0.41	0	5,5,5	0.50	0
4	BTB	A	503	7	13,13,13	0.34	0	7,16,16	0.58	0
5	GOL	C	509	-	5,5,5	0.35	0	5,5,5	0.30	0
4	BTB	D	505	-	13,13,13	0.63	0	7,16,16	1.10	1 (14%)
4	BTB	A	504	-	13,13,13	0.72	0	7,16,16	1.12	0
3	H4B	A	502	-	16,18,18	0.91	0	11,26,26	2.58	6 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BTB	B	505	-	13,13,13	0.43	0	7,16,16	1.07	0
9	XVZ	C	503	-	21,22,22	0.34	0	28,30,30	1.72	6 (21%)
5	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.30	0
2	HEM	A	501	1	41,50,50	1.55	5 (12%)	45,82,82	1.67	8 (17%)
3	H4B	D	502	-	16,18,18	0.88	0	11,26,26	2.89	6 (54%)
9	XVZ	A	511	-	21,22,22	0.39	0	28,30,30	1.73	6 (21%)
2	HEM	D	501	1	41,50,50	1.36	5 (12%)	45,82,82	2.08	11 (24%)
4	BTB	D	504	7	13,13,13	0.38	0	7,16,16	0.50	0
3	H4B	B	503	-	16,18,18	0.82	0	11,26,26	3.01	6 (54%)
4	BTB	C	506	-	13,13,13	0.46	0	7,16,16	0.49	0
5	GOL	A	507	-	5,5,5	0.54	0	5,5,5	1.66	2 (40%)
4	BTB	D	506	-	13,13,13	0.70	0	7,16,16	1.03	1 (14%)
5	GOL	C	508	-	5,5,5	0.35	0	5,5,5	0.36	0
2	HEM	C	501	1	41,50,50	1.47	6 (14%)	45,82,82	1.74	8 (17%)
4	BTB	C	504	7	13,13,13	0.45	0	7,16,16	1.03	0
2	HEM	B	502	1	41,50,50	1.44	5 (12%)	45,82,82	1.99	14 (31%)

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
5	GOL	B	507	-	-	2/4/4/4	-
9	XVZ	D	503	-	-	2/8/8/8	0/2/2/2
4	BTB	C	505	-	-	14/21/21/21	-
4	BTB	B	504	7	-	3/21/21/21	-
5	GOL	D	507	-	-	0/4/4/4	-
4	BTB	A	505	-	-	5/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	GOL	B	506	-	-	0/4/4/4	-
5	GOL	A	512	-	-	4/4/4/4	-
9	XVZ	B	501	-	-	2/8/8/8	0/2/2/2
5	GOL	C	507	-	-	2/4/4/4	-
4	BTB	A	503	7	-	3/21/21/21	-
5	GOL	C	509	-	-	0/4/4/4	-
4	BTB	D	505	-	-	6/21/21/21	-
4	BTB	A	504	-	-	7/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
4	BTB	B	505	-	-	11/21/21/21	-
9	XVZ	C	503	-	-	0/8/8/8	0/2/2/2
5	GOL	A	506	-	-	2/4/4/4	-
2	HEM	A	501	1	-	4/12/54/54	-
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
9	XVZ	A	511	-	-	1/8/8/8	0/2/2/2
2	HEM	D	501	1	-	6/12/54/54	-
4	BTB	D	504	7	-	3/21/21/21	-
3	H4B	B	503	-	-	0/8/17/17	0/2/2/2
4	BTB	C	506	-	-	9/21/21/21	-
5	GOL	A	507	-	-	3/4/4/4	-
4	BTB	D	506	-	-	6/21/21/21	-
5	GOL	C	508	-	-	2/4/4/4	-
2	HEM	C	501	1	-	4/12/54/54	-
4	BTB	C	504	7	-	3/21/21/21	-
2	HEM	B	502	1	-	6/12/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-3.91	1.34	1.40
2	C	501	HEM	C3C-CAC	3.83	1.55	1.47
2	A	501	HEM	C3C-CAC	3.70	1.55	1.47
2	B	502	HEM	C3C-CAC	3.69	1.55	1.47
2	A	501	HEM	FE-NB	3.57	2.14	1.96
2	C	501	HEM	C3C-C2C	-3.49	1.35	1.40
2	B	502	HEM	C3C-C2C	-3.31	1.35	1.40
2	A	501	HEM	CAB-C3B	3.26	1.56	1.47
2	B	502	HEM	CAB-C3B	3.25	1.56	1.47
2	D	501	HEM	C3C-CAC	3.06	1.54	1.47
2	C	501	HEM	CAB-C3B	3.02	1.55	1.47
2	D	501	HEM	CAB-C3B	2.89	1.55	1.47
2	D	501	HEM	C3C-C2C	-2.75	1.36	1.40
2	B	502	HEM	FE-NB	2.69	2.10	1.96
2	C	501	HEM	FE-ND	2.46	2.09	1.96
2	A	501	HEM	CAA-C2A	2.34	1.55	1.52
2	D	501	HEM	FE-NB	2.32	2.08	1.96
2	B	502	HEM	C3B-C2B	-2.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CMB-C2B	2.11	1.55	1.50
2	D	501	HEM	CMD-C2D	2.04	1.55	1.50
2	C	501	HEM	CAA-C2A	2.04	1.55	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBA-CAA-C2A	-5.80	102.72	112.62
3	A	502	H4B	C8A-C4A-C4	5.60	119.55	114.57
2	B	502	HEM	CBA-CAA-C2A	-5.60	103.06	112.62
3	C	502	H4B	C8A-C4A-C4	5.48	119.44	114.57
9	D	503	XVZ	C02-N01-C06	5.23	122.06	118.10
3	D	502	H4B	C8A-C4A-C4	5.01	119.02	114.57
3	B	503	H4B	C8A-C4A-C4	4.81	118.84	114.57
2	C	501	HEM	CBA-CAA-C2A	-4.78	104.46	112.62
9	C	503	XVZ	C02-N01-C06	4.65	121.62	118.10
2	D	501	HEM	C4B-CHC-C1C	4.64	128.68	122.56
9	B	501	XVZ	C02-N01-C06	4.54	121.54	118.10
9	A	511	XVZ	C02-N01-C06	4.38	121.42	118.10
3	B	503	H4B	C2-N3-C4	4.36	122.86	115.93
2	C	501	HEM	C4B-CHC-C1C	4.35	128.29	122.56
2	A	501	HEM	C3B-C2B-C1B	4.21	109.61	106.49
3	B	503	H4B	N1-C2-N3	-4.18	118.87	125.42
3	D	502	H4B	C2-N3-C4	4.16	122.53	115.93
2	B	502	HEM	CMA-C3A-C4A	-4.05	122.23	128.46
3	D	502	H4B	N1-C2-N3	-4.04	119.09	125.42
3	B	503	H4B	C4-C4A-N5	3.98	122.46	119.12
9	B	501	XVZ	F16-C16-C11	3.70	121.76	117.85
3	C	502	H4B	C2-N3-C4	3.65	121.73	115.93
5	A	512	GOL	O1-C1-C2	-3.64	92.75	110.20
2	D	501	HEM	CHD-C1D-ND	3.61	128.35	124.43
2	A	501	HEM	C4A-C3A-C2A	3.60	109.50	107.00
2	D	501	HEM	C4C-CHD-C1D	3.57	127.27	122.56
2	D	501	HEM	CAD-CBD-CGD	-3.56	105.94	113.60
2	B	502	HEM	C4D-ND-C1D	3.55	108.74	105.07
2	A	501	HEM	C4B-CHC-C1C	3.55	127.24	122.56
2	C	501	HEM	C1B-NB-C4B	3.54	108.73	105.07
3	C	502	H4B	N1-C2-N3	-3.49	119.94	125.42
2	D	501	HEM	C1B-NB-C4B	3.48	108.67	105.07
9	A	511	XVZ	F16-C16-C11	3.48	121.52	117.85
2	B	502	HEM	C4B-CHC-C1C	3.43	127.08	122.56
2	B	502	HEM	CAD-CBD-CGD	-3.42	106.24	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	503	XVZ	C08-C06-N01	3.36	120.95	115.95
2	D	501	HEM	C4D-ND-C1D	3.35	108.54	105.07
3	A	502	H4B	N1-C2-N3	-3.11	120.54	125.42
2	C	501	HEM	CBD-CAD-C3D	-3.11	103.99	112.63
2	D	501	HEM	C3D-C4D-ND	-3.11	106.71	110.17
9	C	503	XVZ	F16-C16-C11	3.06	121.08	117.85
3	C	502	H4B	C4-C4A-N5	3.06	121.69	119.12
3	D	502	H4B	C4-C4A-N5	3.04	121.67	119.12
2	B	502	HEM	C3B-C2B-C1B	3.00	108.71	106.49
9	A	511	XVZ	C08-C06-N01	2.99	120.41	115.95
2	A	501	HEM	C1B-NB-C4B	2.94	108.11	105.07
2	B	502	HEM	C4C-CHD-C1D	2.93	126.42	122.56
3	B	503	H4B	C2-N1-C8A	2.93	121.10	114.54
9	D	503	XVZ	C05-C06-N01	-2.91	119.82	122.90
3	A	502	H4B	C2-N3-C4	2.89	120.52	115.93
3	D	502	H4B	C2-N1-C8A	2.86	120.95	114.54
9	C	503	XVZ	C05-C06-N01	-2.80	119.94	122.90
3	A	502	H4B	C2-N1-C8A	2.78	120.78	114.54
3	C	502	H4B	C2-N1-C8A	2.77	120.75	114.54
9	A	511	XVZ	C05-C06-N01	-2.76	119.98	122.90
9	D	503	XVZ	C08-C09-C11	-2.76	108.35	112.81
2	B	502	HEM	CMA-C3A-C2A	2.74	130.11	124.94
9	A	511	XVZ	C12-C11-C16	2.73	119.26	116.76
2	C	501	HEM	C4D-ND-C1D	2.72	107.88	105.07
9	D	503	XVZ	C08-C06-N01	2.67	119.93	115.95
2	B	502	HEM	C1B-NB-C4B	2.67	107.83	105.07
3	B	503	H4B	N2-C2-N1	2.66	121.40	117.25
9	C	503	XVZ	N02-C02-N01	2.66	120.70	116.49
9	D	503	XVZ	C12-C11-C16	2.65	119.19	116.76
2	D	501	HEM	CMC-C2C-C3C	2.65	129.63	124.68
2	A	501	HEM	CBD-CAD-C3D	-2.65	105.28	112.63
5	A	507	GOL	O2-C2-C3	-2.58	97.74	109.12
9	B	501	XVZ	C08-C09-C11	-2.54	108.70	112.81
2	D	501	HEM	C3B-C2B-C1B	2.53	108.37	106.49
2	C	501	HEM	C3D-C4D-ND	-2.53	107.35	110.17
9	C	503	XVZ	C12-C11-C16	2.53	119.08	116.76
2	B	502	HEM	CHA-C4D-ND	2.52	127.49	124.38
2	B	502	HEM	C2D-C1D-ND	-2.51	106.87	109.88
9	B	501	XVZ	C05-C06-N01	-2.51	120.24	122.90
3	A	502	H4B	C4-C4A-N5	2.49	121.21	119.12
4	D	506	BTB	C6-C5-N	2.47	121.25	111.59
2	A	501	HEM	C4D-ND-C1D	2.46	107.62	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	N2-C2-N1	2.43	121.03	117.25
5	A	512	GOL	O2-C2-C1	-2.40	98.55	109.12
2	B	502	HEM	C3D-C4D-ND	-2.39	107.50	110.17
2	C	501	HEM	C3B-C2B-C1B	2.37	108.24	106.49
5	A	507	GOL	O3-C3-C2	-2.33	99.04	110.20
9	D	503	XVZ	F16-C16-C11	2.30	120.28	117.85
9	A	511	XVZ	N02-C02-N01	2.28	120.10	116.49
2	A	501	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
4	D	505	BTB	O1-C1-C2	-2.25	105.28	111.44
9	B	501	XVZ	C08-C06-N01	2.24	119.29	115.95
2	B	502	HEM	CHC-C4B-NB	2.19	126.81	124.43
2	B	502	HEM	CMC-C2C-C3C	2.16	128.71	124.68
2	C	501	HEM	C4A-C3A-C2A	2.13	108.48	107.00
2	A	501	HEM	C2B-C1B-NB	-2.12	107.33	109.84
3	A	502	H4B	N2-C2-N3	2.10	120.52	117.25
2	D	501	HEM	CHA-C4D-C3D	2.07	129.21	125.33

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3D-CAD-CBD-CGD
4	A	504	BTB	C1-C2-C4-O4
4	A	504	BTB	C3-C2-C4-O4
4	A	505	BTB	C1-C2-C3-O3
4	A	505	BTB	C4-C2-C3-O3
4	B	504	BTB	O1-C1-C2-C3
4	B	505	BTB	C1-C2-C3-O3
4	B	505	BTB	C4-C2-C3-O3
4	B	505	BTB	N-C2-C3-O3
4	B	505	BTB	C1-C2-N-C5
4	B	505	BTB	C1-C2-N-C7
4	B	505	BTB	C3-C2-N-C5
4	B	505	BTB	C3-C2-N-C7
4	B	505	BTB	C4-C2-N-C5
4	B	505	BTB	C4-C2-N-C7
4	C	504	BTB	C1-C2-C4-O4
4	C	504	BTB	C3-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
4	C	504	BTB	N-C2-C4-O4
4	C	505	BTB	C3-C2-C4-O4
4	C	505	BTB	C1-C2-N-C5
4	C	505	BTB	C1-C2-N-C7
4	C	505	BTB	C3-C2-N-C7
4	C	505	BTB	C4-C2-N-C7
4	C	505	BTB	C8-C7-N-C5
4	C	506	BTB	C1-C2-C4-O4
4	C	506	BTB	C3-C2-C4-O4
4	C	506	BTB	N-C2-C4-O4
4	C	506	BTB	C1-C2-N-C5
4	C	506	BTB	C1-C2-N-C7
4	C	506	BTB	C3-C2-N-C5
4	C	506	BTB	C3-C2-N-C7
4	C	506	BTB	C4-C2-N-C5
4	C	506	BTB	C4-C2-N-C7
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	O1-C1-C2-N
4	D	505	BTB	C1-C2-C3-O3
4	D	505	BTB	C4-C2-C3-O3
4	D	505	BTB	N-C2-C3-O3
4	D	505	BTB	N-C5-C6-O6
4	D	506	BTB	C1-C2-C4-O4
4	D	506	BTB	C3-C2-C4-O4
4	D	506	BTB	N-C2-C4-O4
5	A	506	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	512	GOL	O1-C1-C2-C3
5	A	512	GOL	C1-C2-C3-O3
5	A	512	GOL	O2-C2-C3-O3
5	B	507	GOL	C1-C2-C3-O3
5	C	507	GOL	O1-C1-C2-C3
5	C	508	GOL	O1-C1-C2-C3
4	B	505	BTB	N-C5-C6-O6
5	C	507	GOL	O1-C1-C2-O2
2	B	502	HEM	C3D-CAD-CBD-CGD
4	A	504	BTB	N-C7-C8-O8
4	A	505	BTB	N-C7-C8-O8
4	C	505	BTB	N-C5-C6-O6
4	D	506	BTB	N-C7-C8-O8
5	A	506	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	507	GOL	O2-C2-C3-O3
5	C	508	GOL	O1-C1-C2-O2
4	D	505	BTB	C6-C5-N-C7
4	D	506	BTB	C6-C5-N-C7
4	B	505	BTB	N-C7-C8-O8
4	C	505	BTB	N-C7-C8-O8
5	A	512	GOL	O1-C1-C2-O2
4	A	503	BTB	N-C7-C8-O8
4	A	505	BTB	N-C5-C6-O6
5	A	507	GOL	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	502	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	A	503	BTB	C1-C2-C4-O4
4	A	504	BTB	C1-C2-C3-O3
4	B	504	BTB	O1-C1-C2-C4
4	C	505	BTB	C1-C2-C4-O4
2	C	501	HEM	C3A-C2A-CAA-CBA
4	A	504	BTB	N-C2-C4-O4
4	A	505	BTB	N-C2-C3-O3
4	B	504	BTB	O1-C1-C2-N
4	C	505	BTB	N-C2-C3-O3
4	C	505	BTB	N-C2-C4-O4
4	C	505	BTB	C3-C2-N-C5
4	C	505	BTB	C4-C2-N-C5
4	A	504	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
3	A	502	H4B	C7-C6-C9-C10
9	B	501	XVZ	C14-C13-C17-C18
9	D	503	XVZ	C14-C13-C17-C18
9	B	501	XVZ	C12-C13-C17-C18
2	B	502	HEM	CAD-CBD-CGD-O1D
3	A	502	H4B	C7-C6-C9-O9
2	B	502	HEM	CAD-CBD-CGD-O2D
9	D	503	XVZ	C12-C13-C17-C18
2	B	502	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O2D
2	B	502	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	D	501	HEM	CAA-CBA-CGA-O1A
3	A	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
4	A	503	BTB	C3-C2-C4-O4
4	A	504	BTB	C4-C2-C3-O3
4	C	505	BTB	C4-C2-C3-O3
4	D	505	BTB	C3-C2-C4-O4
4	D	506	BTB	C1-C2-C3-O3
9	A	511	XVZ	C14-C13-C17-C18

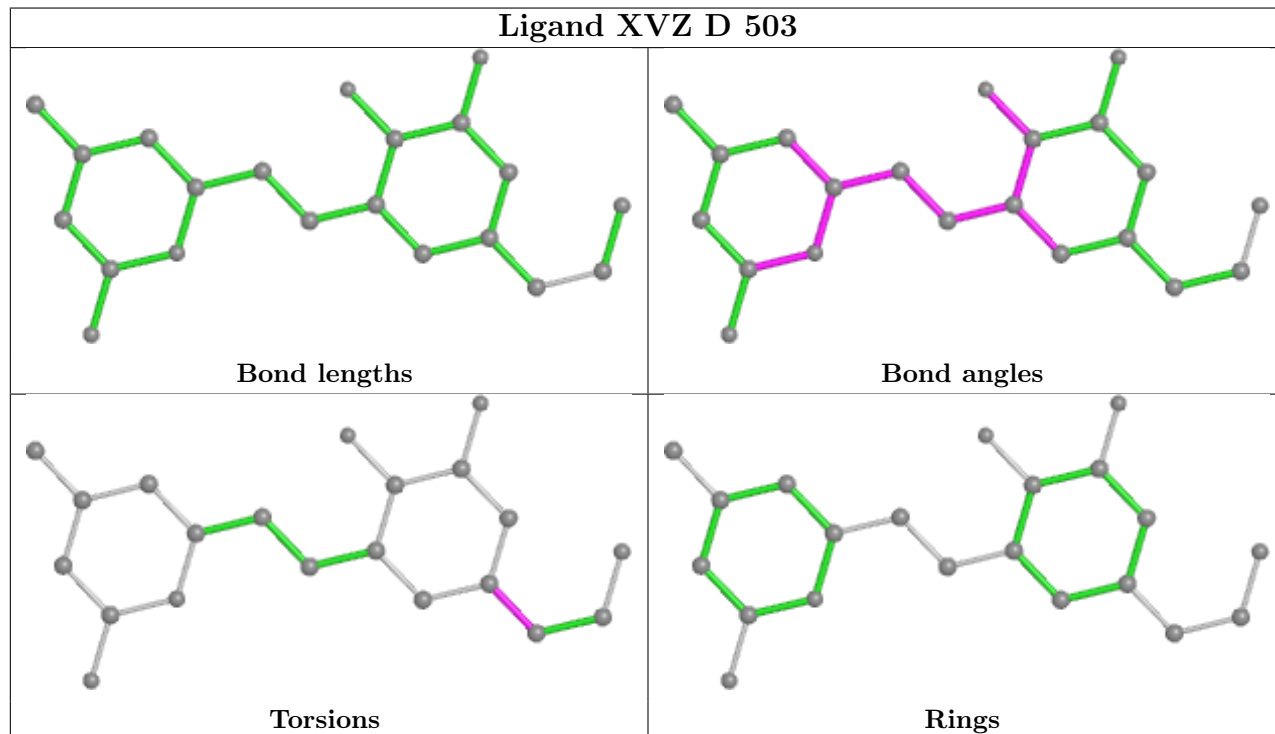
There are no ring outliers.

25 monomers are involved in 54 short contacts:

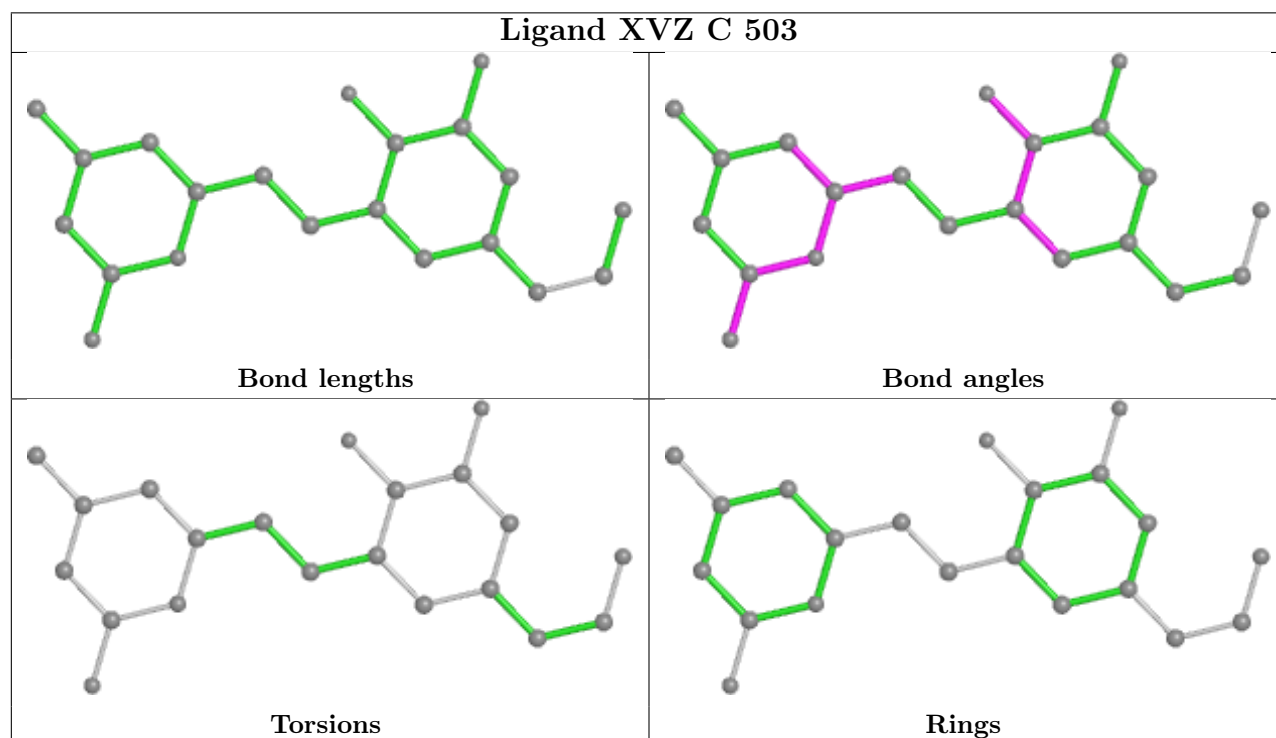
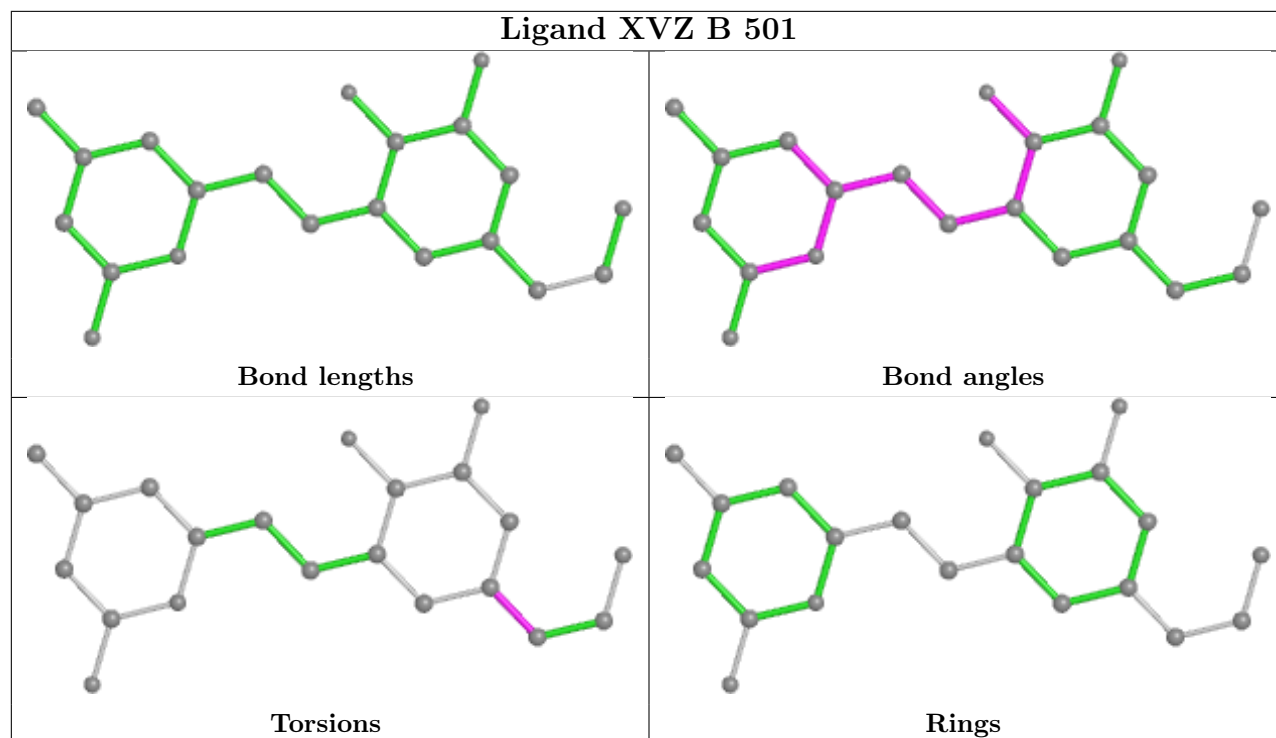
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	507	GOL	1	0
9	D	503	XVZ	1	0
4	C	505	BTB	3	0
4	B	504	BTB	3	0
4	A	505	BTB	2	0
3	C	502	H4B	2	0
9	B	501	XVZ	2	0
4	A	503	BTB	1	0
4	D	505	BTB	1	0
4	A	504	BTB	2	0
3	A	502	H4B	2	0
4	B	505	BTB	6	0
9	C	503	XVZ	3	0
5	A	506	GOL	2	0
2	A	501	HEM	6	0
3	D	502	H4B	1	0
9	A	511	XVZ	1	0
2	D	501	HEM	3	0
4	D	504	BTB	2	0
3	B	503	H4B	2	0
4	C	506	BTB	3	0
4	D	506	BTB	2	0
2	C	501	HEM	3	0
4	C	504	BTB	2	0
2	B	502	HEM	2	0

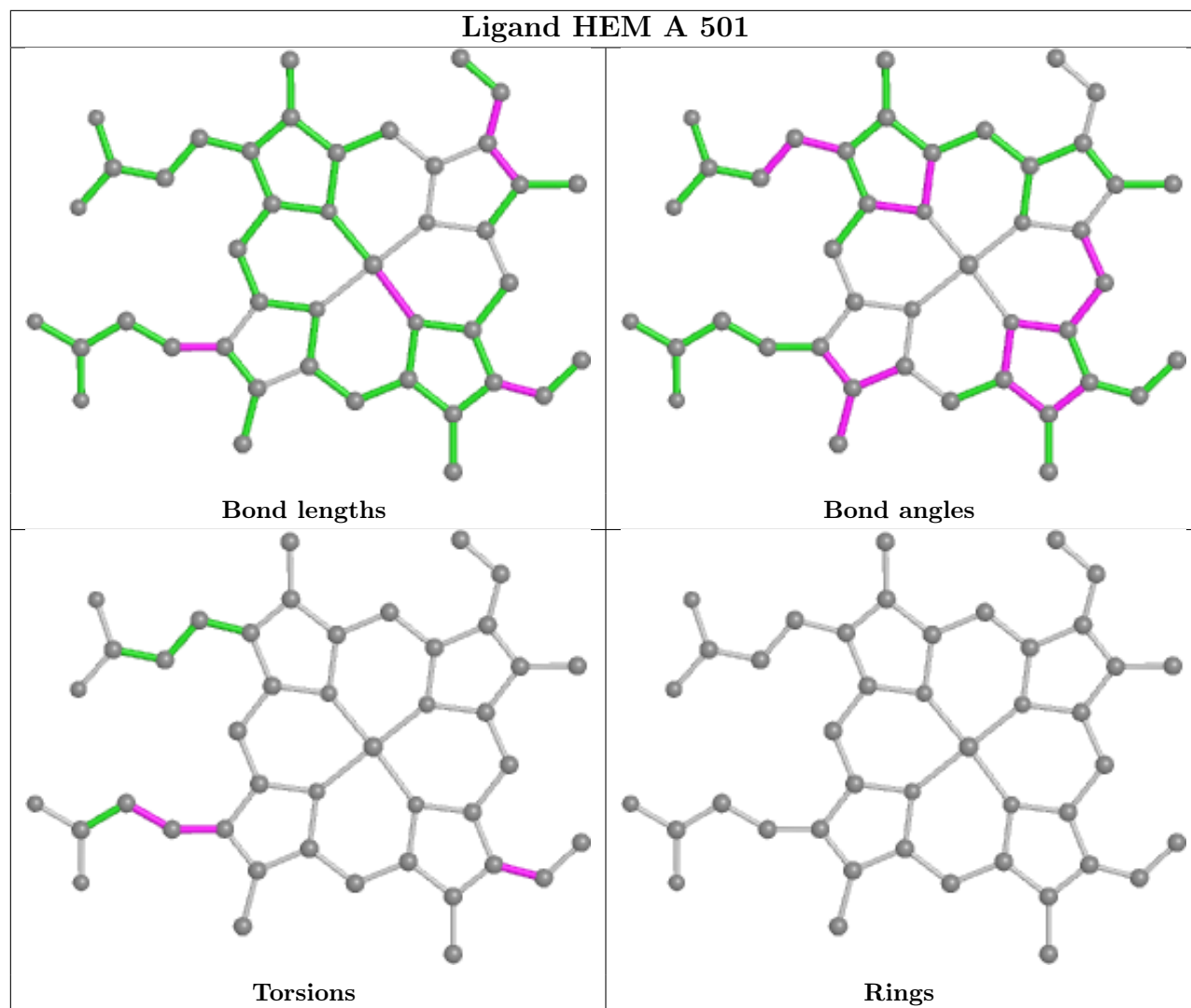
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

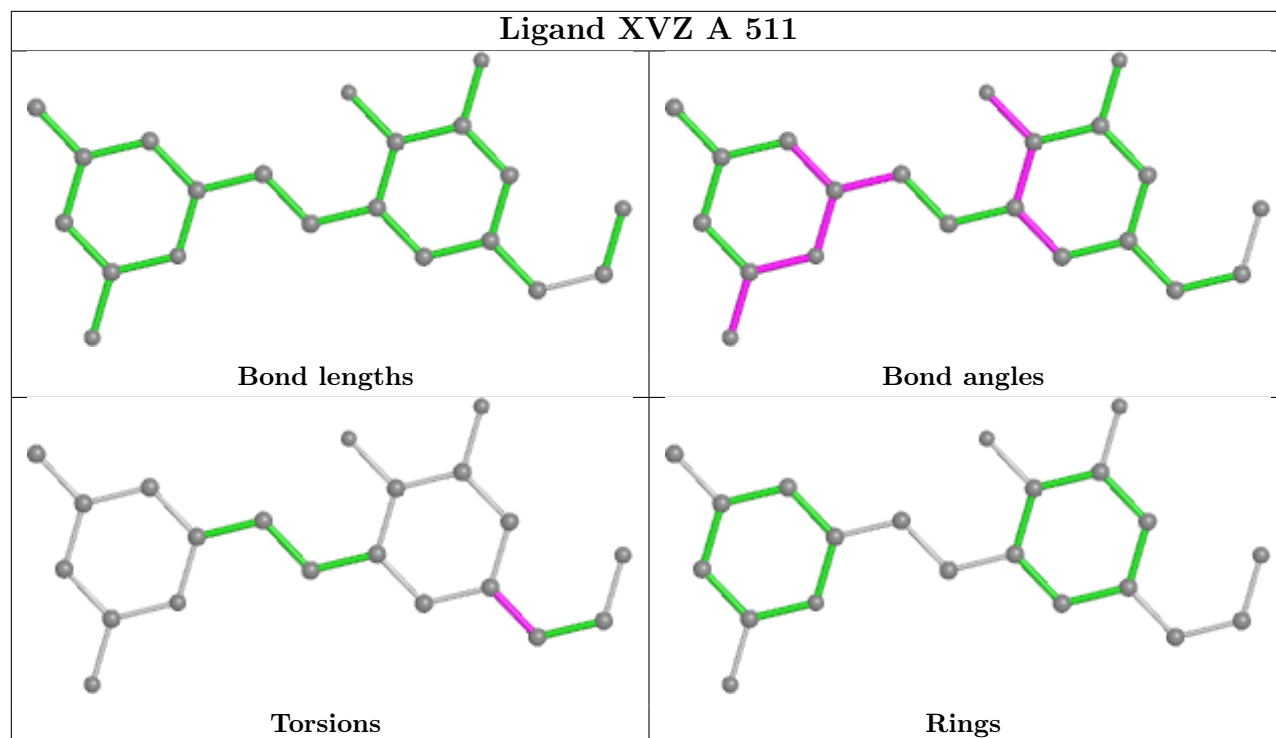
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

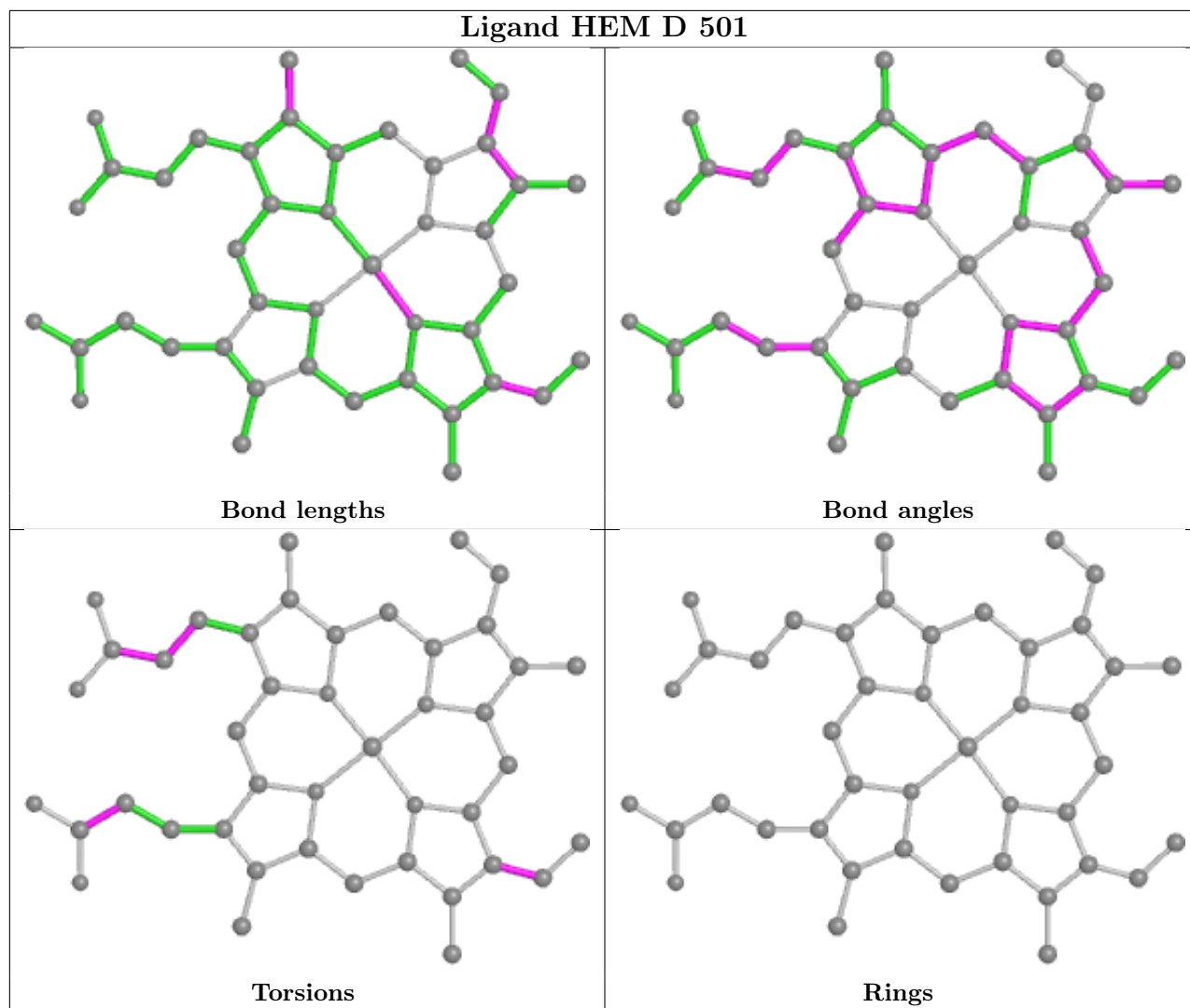


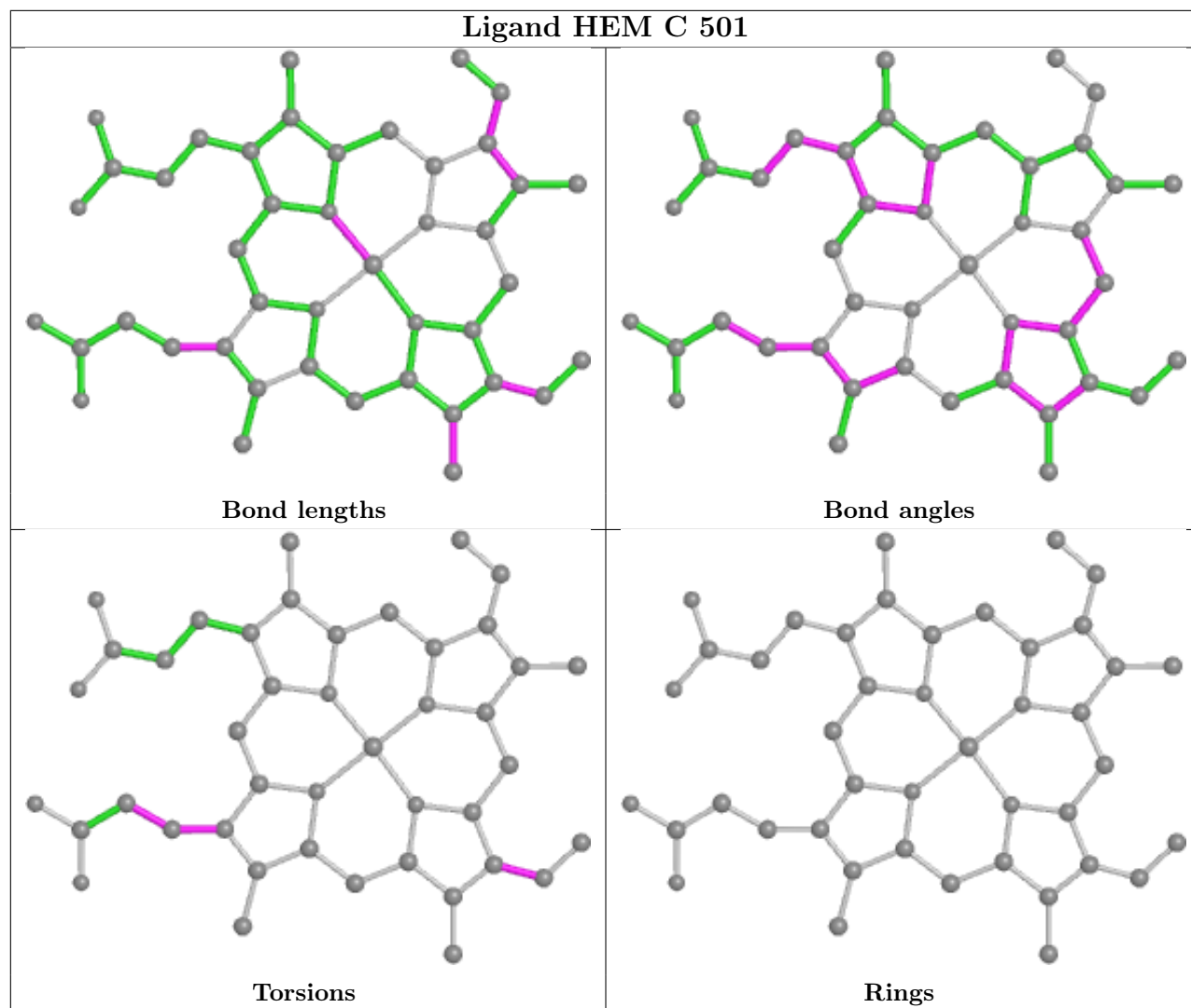


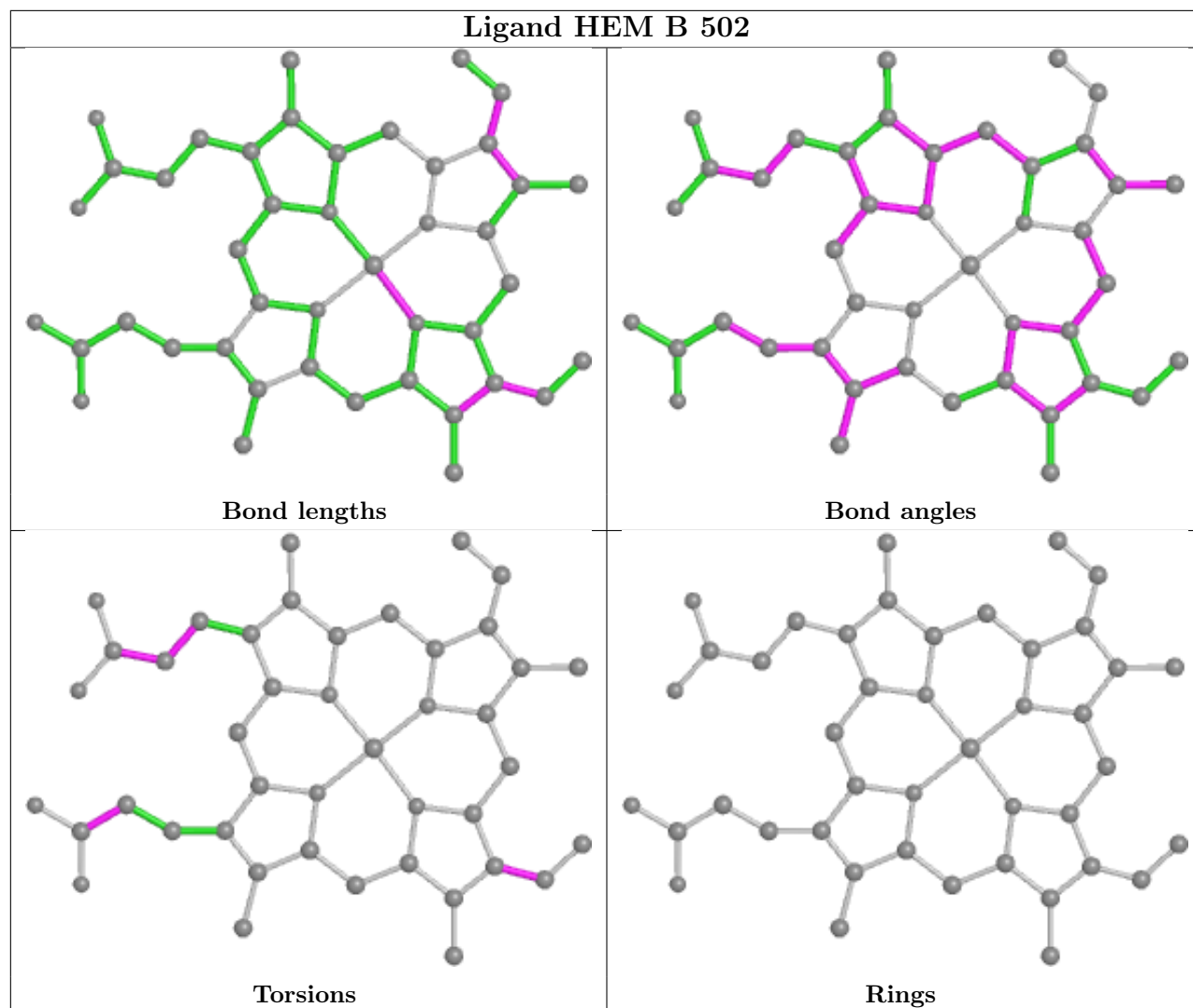












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.82	49 (12%) 4 4	28, 60, 106, 137	0
1	B	402/440 (91%)	0.35	8 (1%) 65 66	25, 42, 78, 109	0
1	C	402/440 (91%)	0.63	28 (6%) 16 18	29, 56, 98, 124	0
1	D	402/440 (91%)	0.31	5 (1%) 79 80	28, 41, 69, 117	0
All	All	1607/1760 (91%)	0.53	90 (5%) 24 26	25, 49, 95, 137	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	7.9
1	C	480	TRP	6.3
1	A	204	ALA	5.1
1	A	480	TRP	4.7
1	A	254	TYR	4.4
1	C	202	ARG	4.2
1	C	238	ARG	4.2
1	C	293	LEU	4.1
1	A	238	ARG	4.0
1	C	304	LEU	3.9
1	C	204	ALA	3.8
1	B	150	LEU	3.8
1	C	468	PHE	3.6
1	A	124	LEU	3.5
1	C	89	GLN	3.5
1	C	343	ILE	3.4
1	C	305	LEU	3.4
1	A	291	LEU	3.3
1	A	237	GLY	3.2
1	A	305	LEU	3.2
1	C	106	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	473	PHE	3.1
1	C	130	PHE	3.0
1	A	293	LEU	3.0
1	C	257	GLN	3.0
1	A	268	VAL	2.9
1	D	468	PHE	2.9
1	D	90	GLN	2.9
1	C	134	TYR	2.8
1	A	304	LEU	2.8
1	C	131	ILE	2.8
1	A	106	PRO	2.8
1	A	202	ARG	2.8
1	B	89	GLN	2.8
1	A	280	THR	2.7
1	A	130	PHE	2.7
1	A	146	HIS	2.7
1	A	134	TYR	2.7
1	D	257	GLN	2.6
1	A	275	ILE	2.6
1	C	68	PHE	2.6
1	A	211	ILE	2.6
1	C	208	PHE	2.6
1	B	90	GLN	2.6
1	D	89	GLN	2.6
1	A	89	GLN	2.6
1	A	259	GLY	2.6
1	A	145	ALA	2.5
1	A	346	LEU	2.5
1	B	142	GLY	2.5
1	C	230	VAL	2.5
1	A	279	TRP	2.5
1	A	303	PHE	2.5
1	A	468	PHE	2.5
1	C	140	ARG	2.5
1	A	131	ILE	2.4
1	B	68	PHE	2.3
1	C	153	VAL	2.3
1	A	88	ALA	2.3
1	A	281	PRO	2.3
1	A	290	PRO	2.3
1	A	273	LEU	2.3
1	A	192	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	79	ILE	2.2
1	A	243	ILE	2.2
1	A	244	TRP	2.2
1	A	309	LEU	2.2
1	C	346	LEU	2.2
1	A	148	GLN	2.2
1	C	145	ALA	2.2
1	A	256	GLN	2.2
1	A	241	PHE	2.2
1	C	163	TYR	2.1
1	A	311	LEU	2.1
1	A	341	LEU	2.1
1	D	196	PHE	2.1
1	A	144	GLN	2.1
1	C	309	LEU	2.1
1	C	236	PRO	2.1
1	A	252	ALA	2.1
1	A	302	LEU	2.1
1	A	257	GLN	2.1
1	C	239	GLY	2.1
1	C	255	ARG	2.1
1	B	227	ALA	2.1
1	A	289	LEU	2.1
1	A	475	TYR	2.0
1	B	173	GLY	2.0
1	A	285	ARG	2.0
1	C	170	LEU	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 monosaccharides 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.

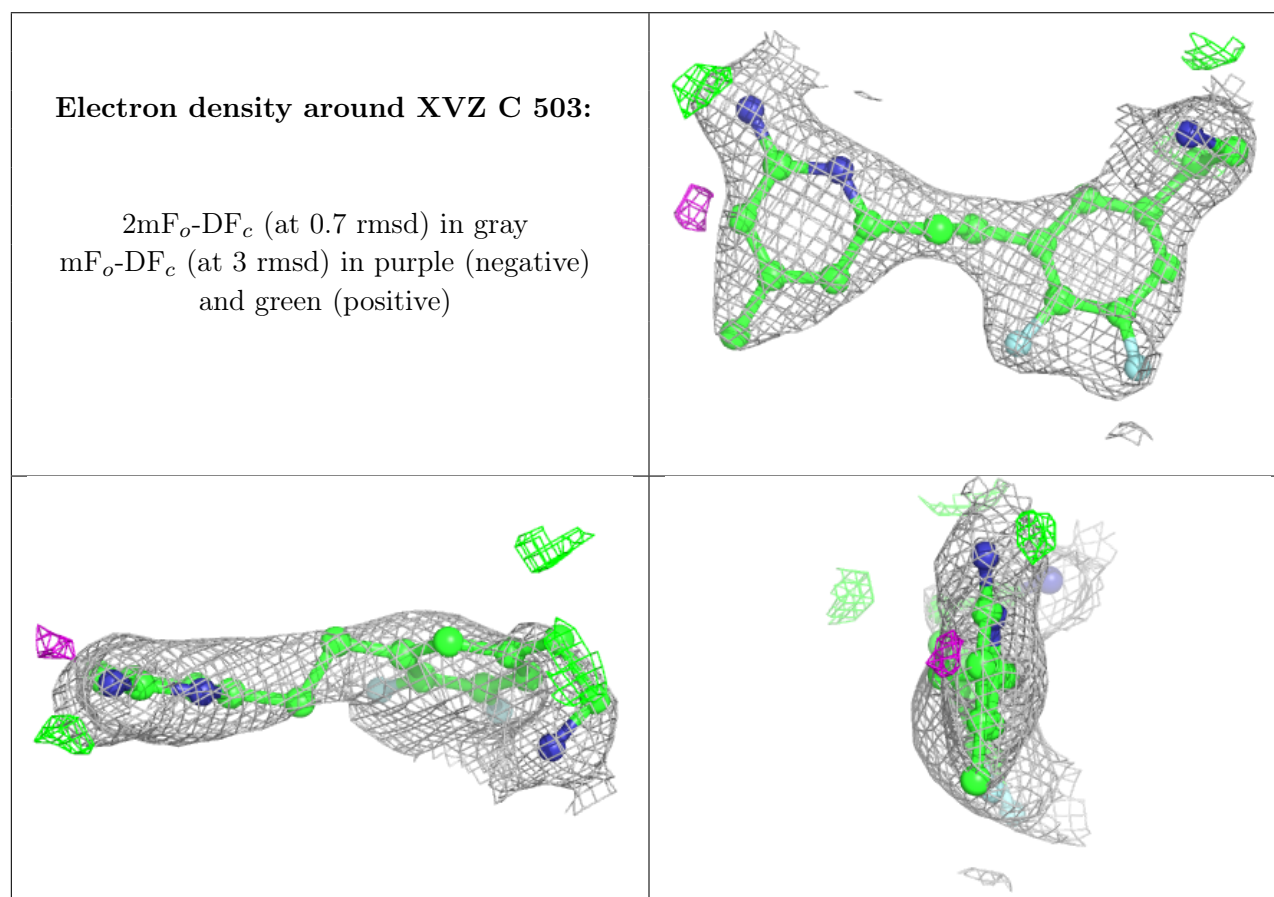
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GD	A	509	1/1	0.52	0.16	126,126,126,126	1
4	BTB	C	506	14/14	0.69	0.16	72,94,99,102	0
5	GOL	C	509	6/6	0.77	0.13	71,73,74,79	0
5	GOL	C	508	6/6	0.81	0.15	50,57,58,68	0
4	BTB	D	505	14/14	0.83	0.22	53,70,85,92	0
5	GOL	D	507	6/6	0.84	0.14	52,73,79,87	0
4	BTB	A	505	14/14	0.86	0.12	77,85,92,92	0
5	GOL	B	506	6/6	0.87	0.14	65,67,68,71	0
4	BTB	A	503	14/14	0.88	0.14	55,82,86,90	0
5	GOL	B	507	6/6	0.88	0.19	59,65,68,75	0
5	GOL	A	506	6/6	0.88	0.20	49,63,71,71	0
4	BTB	D	506	14/14	0.89	0.14	77,80,83,85	0
4	BTB	B	505	14/14	0.89	0.19	30,62,73,73	0
4	BTB	C	504	14/14	0.90	0.20	36,71,84,89	0
4	BTB	D	504	14/14	0.91	0.16	33,71,85,86	0
4	BTB	A	504	14/14	0.91	0.20	39,67,72,73	0
3	H4B	C	502	17/17	0.92	0.22	43,55,63,64	0
5	GOL	A	507	6/6	0.92	0.20	37,43,63,69	0
9	XVZ	C	503	21/21	0.92	0.20	35,64,82,90	0
3	H4B	A	502	17/17	0.94	0.18	49,55,63,71	0
4	BTB	C	505	14/14	0.94	0.22	21,57,72,77	0
5	GOL	C	507	6/6	0.94	0.20	44,52,59,60	0
9	XVZ	A	511	21/21	0.94	0.17	41,60,80,95	0
5	GOL	A	512	6/6	0.94	0.22	17,33,54,55	0
9	XVZ	D	503	21/21	0.94	0.15	18,41,64,67	0
3	H4B	B	503	17/17	0.95	0.12	30,51,58,60	0
4	BTB	B	504	14/14	0.95	0.12	31,50,67,69	0
9	XVZ	B	501	21/21	0.96	0.15	23,37,54,57	0
2	HEM	A	501	43/43	0.96	0.17	39,58,79,88	0
3	H4B	D	502	17/17	0.96	0.15	32,49,57,59	0
2	HEM	C	501	43/43	0.97	0.13	27,47,68,80	0
2	HEM	D	501	43/43	0.98	0.14	23,31,50,62	0
6	CL	A	508	1/1	0.98	0.09	49,49,49,49	0
2	HEM	B	502	43/43	0.98	0.13	21,32,53,58	0
7	GD	C	511	1/1	0.98	0.10	70,70,70,70	1
8	ZN	A	510	1/1	0.99	0.13	42,42,42,42	0
6	CL	C	510	1/1	0.99	0.06	46,46,46,46	0
7	GD	B	509	1/1	0.99	0.18	45,45,45,45	0
6	CL	D	508	1/1	0.99	0.11	38,38,38,38	0
7	GD	D	509	1/1	0.99	0.18	47,47,47,47	0
6	CL	B	508	1/1	1.00	0.10	37,37,37,37	0

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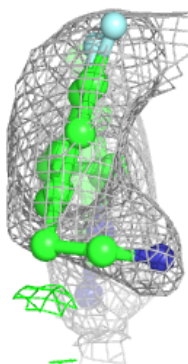
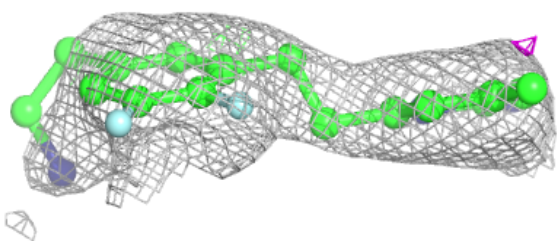
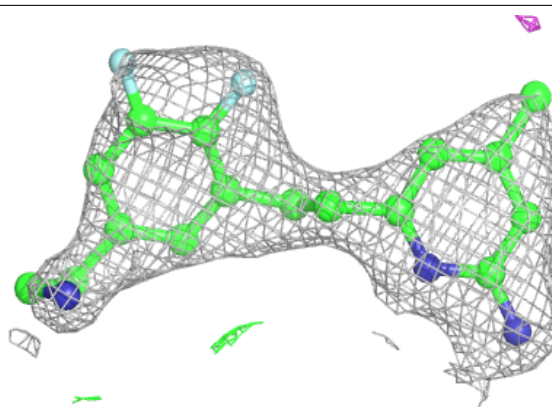
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	C	512	1/1	1.00	0.10	36,36,36,36	0

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.

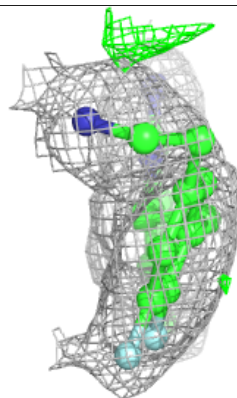
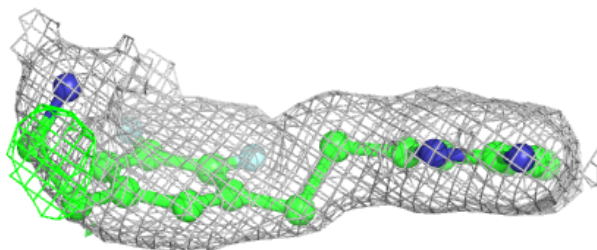
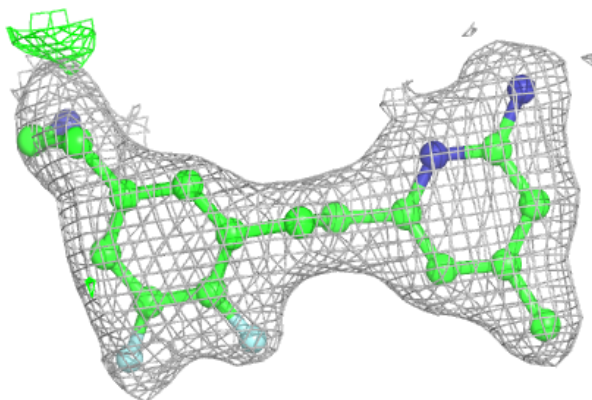


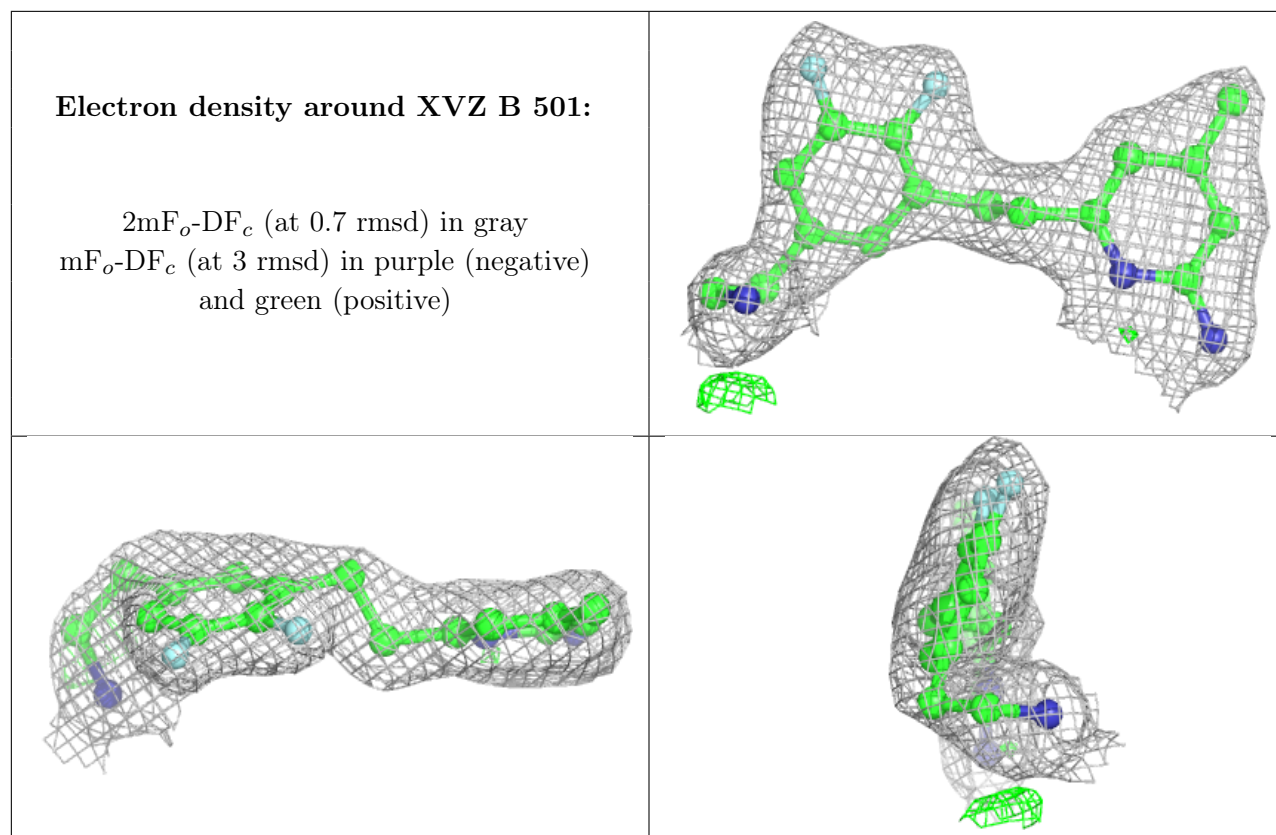
**Electron density around XVZ A 511:**

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

**Electron density around XVZ D 503:**

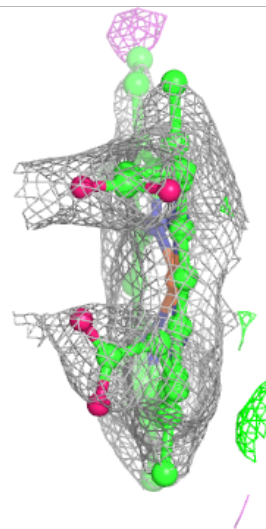
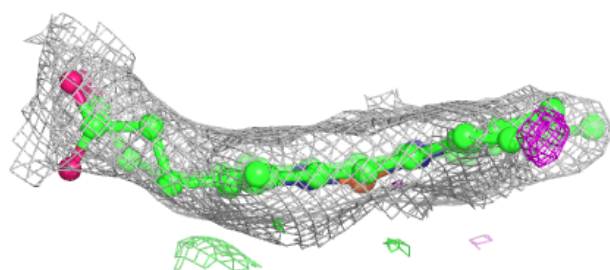
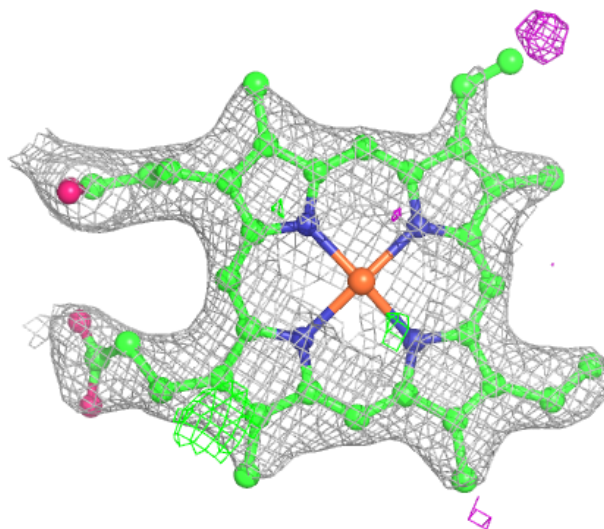
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





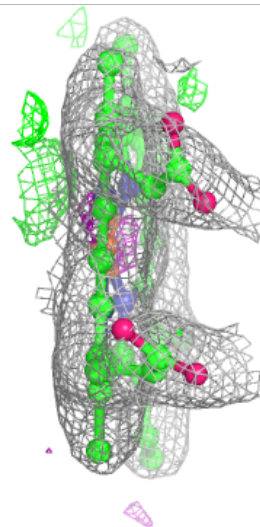
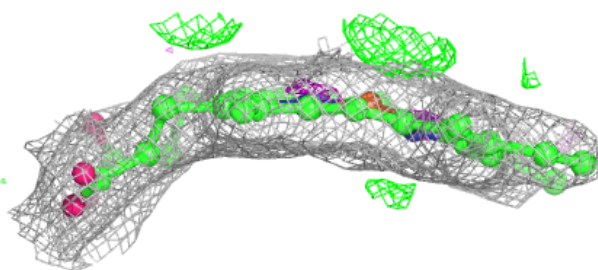
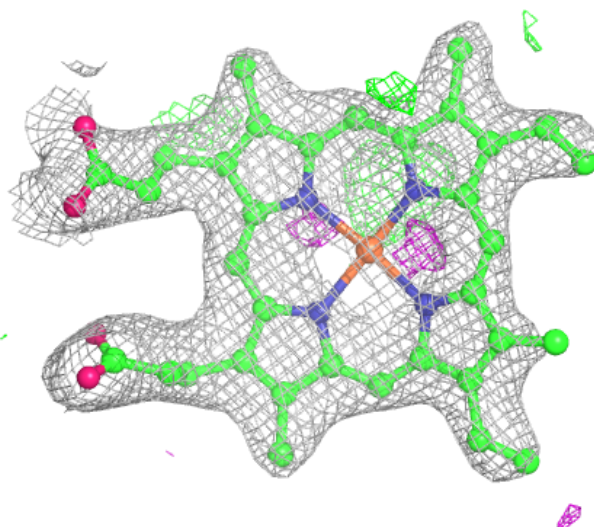
**Electron density around HEM A 501:**

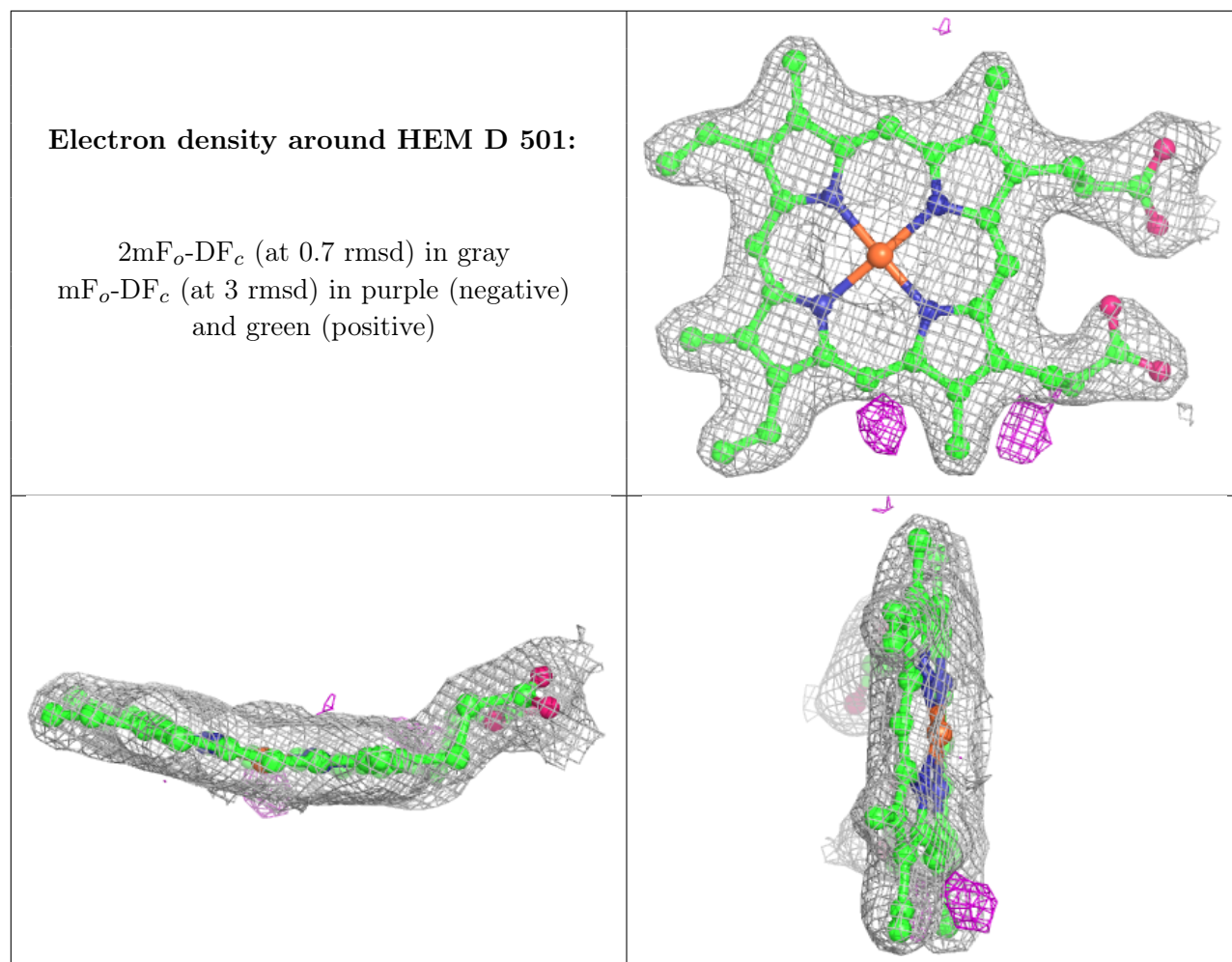
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



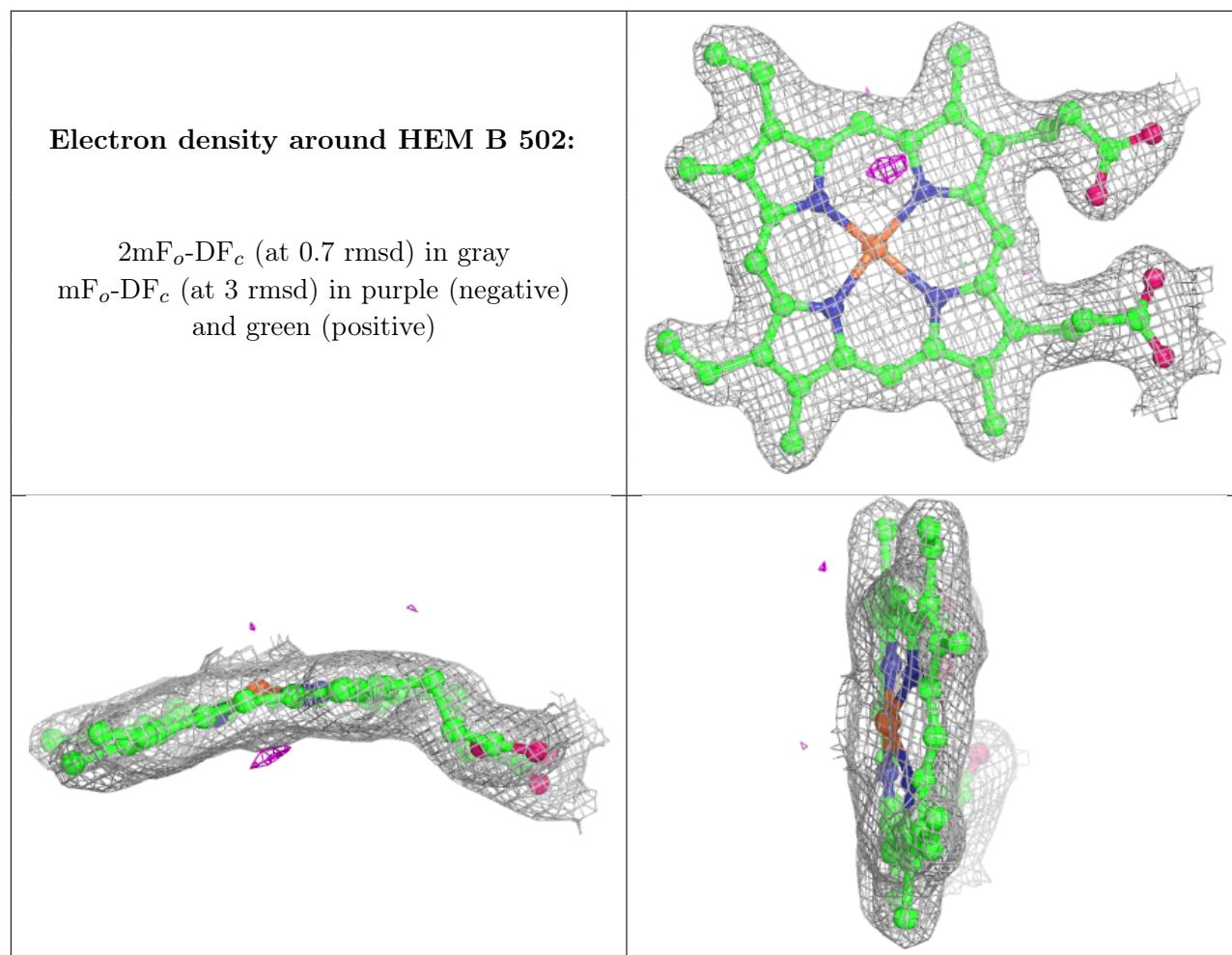
**Electron density around HEM C 501:**

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









## 6.5 Other polymers [i](#)

There are no such residues in this entry.