



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2025 – 06:19 PM EDT

PDB ID : 9C1Z / pdb_00009c1z
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-((3-(((4-(6-aminopyridin-2-yl)butyl)amino)methyl)phenoxy)methyl)quinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2024-05-30
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

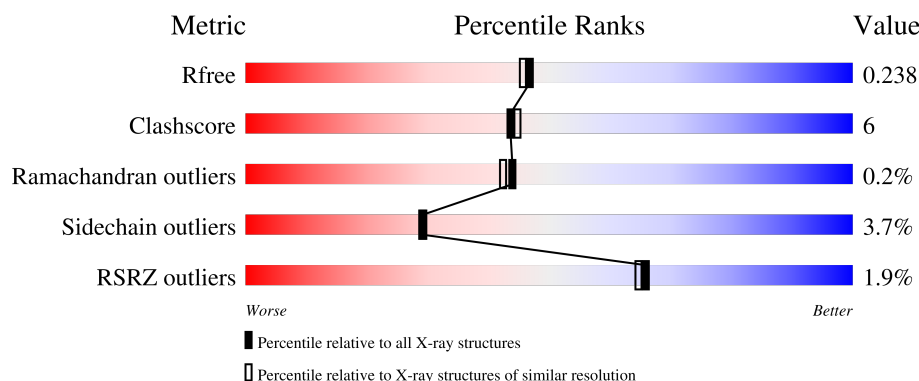
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

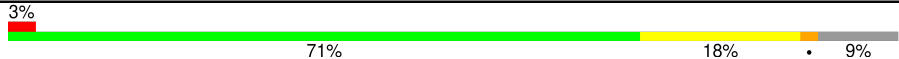



The reported resolution of this entry is 2.00 Å.

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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	440	
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
4	BTB	B	507	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14169 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.

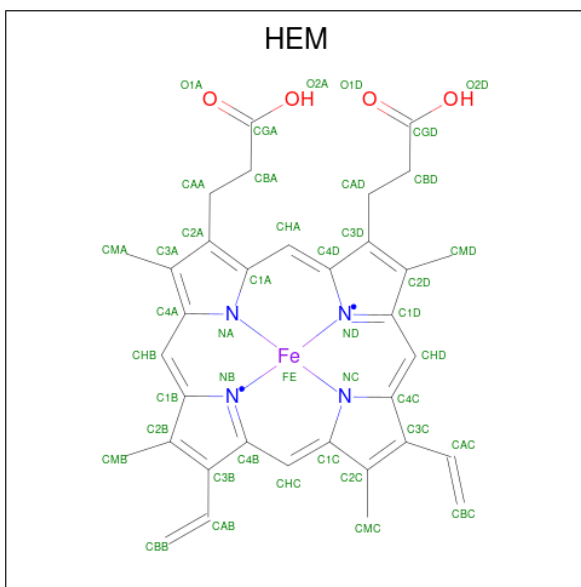
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	1	0
			3214	2046	567	585	16			

There are 4 discrepancies between the modelled and reference sequences:

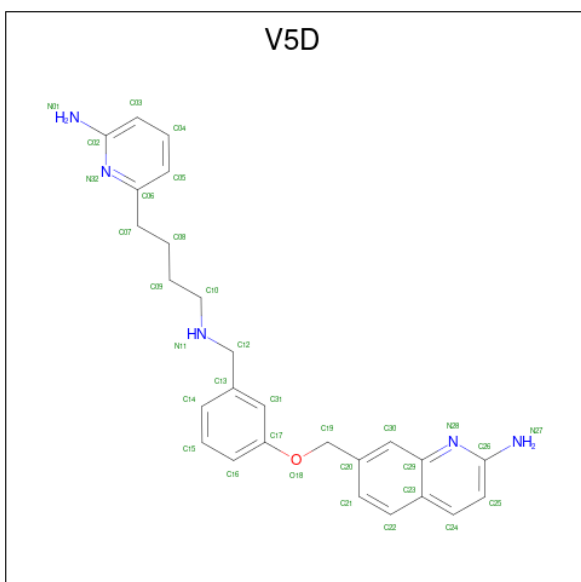
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



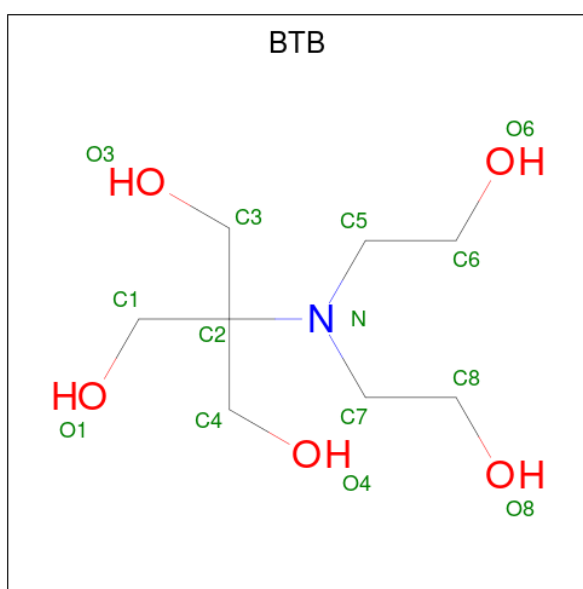
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 7-{{3-({[4-(6-aminopyridin-2-yl)butyl]amino}methyl)phenoxy}methyl}quinolin-2-amine (CCD ID: V5D) (formula: C₂₆H₂₉N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	26	5	1		
3	B	1	Total	C	N	O	0	0
			32	26	5	1		
3	C	1	Total	C	N	O	0	0
			32	26	5	1		
3	D	1	Total	C	N	O	0	0
			32	26	5	1		

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



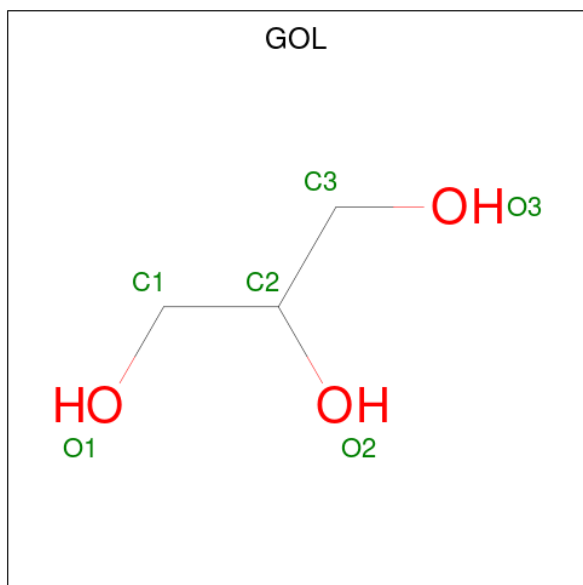
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

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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		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

- Molecule 7 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Gd 1	0	0
7	B	2	Total 2	Gd 2	0	0
7	D	1	Total 1	Gd 1	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

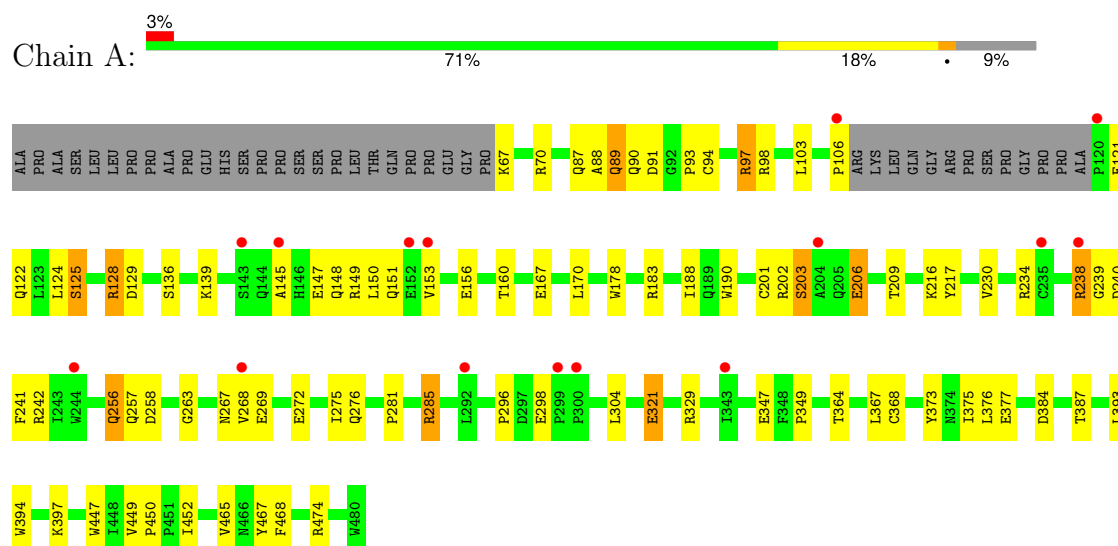
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	148	Total 148	O 148	0	0
9	B	243	Total 243	O 243	0	0
9	C	185	Total 185	O 185	0	0
9	D	269	Total 269	O 269	0	0

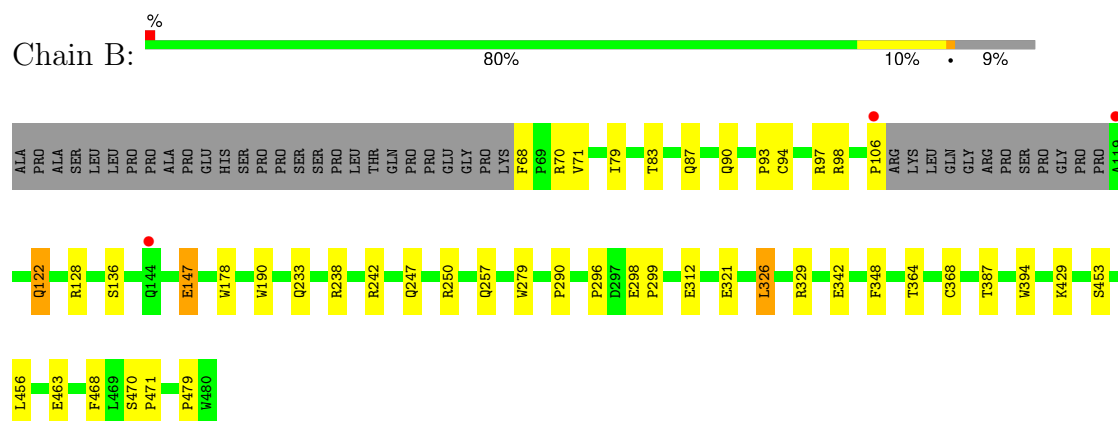
3 Residue-property plots

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.

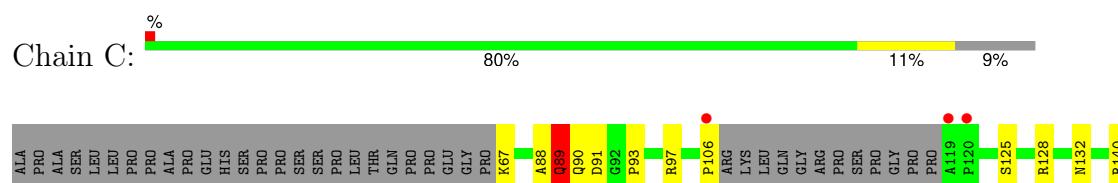
- Molecule 1: Nitric oxide synthase, endothelial

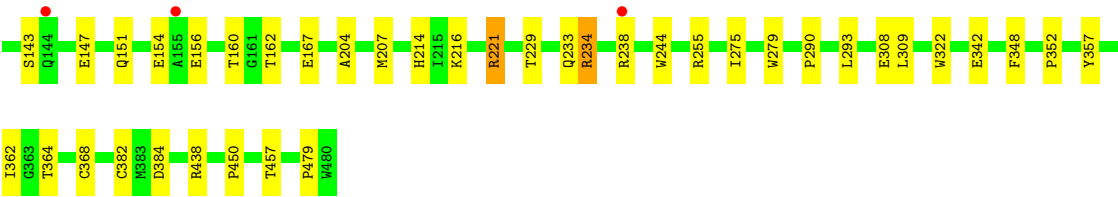


- Molecule 1: Nitric oxide synthase, endothelial

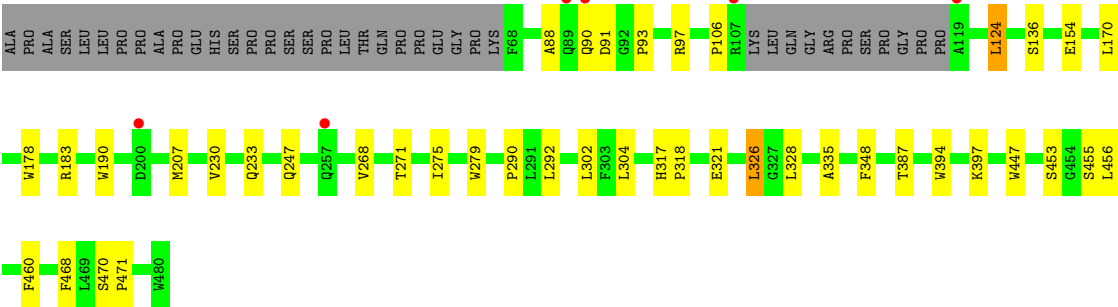
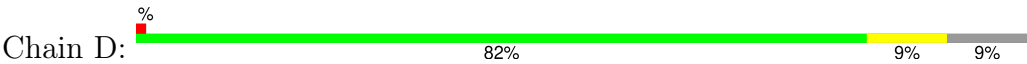


- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.71Å 152.96Å 108.49Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	49.73 – 2.00 49.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.73-2.00) 98.7 (49.73-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.199 , 0.245 0.193 , 0.238	Depositor DCC
R_{free} test set	6625 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14169	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, CL, GOL, HEM, GD, ZN, V5D

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	0.29	0/3302	0.50	0/4498
1	B	0.33	0/3312	0.52	0/4514
1	C	0.29	0/3307	0.49	0/4506
1	D	0.36	0/3309	0.55	0/4509
All	All	0.32	0/13230	0.51	0/18027

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	48	0
1	B	3211	0	3114	29	0
1	C	3212	0	3116	29	0
1	D	3214	0	3116	23	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	0	0
3	C	32	0	0	0	0
3	D	32	0	0	1	0
4	A	42	0	56	9	0
4	B	42	0	54	14	0
4	C	28	0	38	6	0
4	D	28	0	37	7	0
5	A	18	0	24	1	0
5	C	12	0	16	1	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	2	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	148	0	0	3	0
9	B	243	0	0	3	0
9	C	185	0	0	2	0
9	D	269	0	0	3	0
All	All	14169	0	12803	156	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 6.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:507:BTB:O3	9:B:601:HOH:O	1.98	0.81
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.68	0.75
3:D:502:V5D:N28	9:D:602:HOH:O	2.21	0.72
4:B:507:BTB:O4	4:B:507:BTB:H72	1.89	0.72
1:D:321:GLU:OE2	4:D:503:BTB:O4	2.09	0.70
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.76	0.68
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.76	0.67
4:B:507:BTB:H12	1:C:382:CYS:HA	1.77	0.67
1:A:89:GLN:HG3	1:A:90:GLN:H	1.60	0.66
1:D:397:LYS:NZ	9:D:603:HOH:O	2.25	0.65
1:A:93:PRO:HB3	1:A:106:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:OD1	9:A:601:HOH:O	2.13	0.64
4:C:503:BTB:O1	4:C:503:BTB:O6	2.16	0.64
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.79	0.63
1:A:70:ARG:NH2	9:A:604:HOH:O	2.28	0.62
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.82	0.62
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.81	0.62
1:C:160:THR:HG23	1:C:162:THR:H	1.63	0.62
1:A:384:ASP:OD1	4:A:503:BTB:O3	2.18	0.61
1:C:128:ARG:O	1:C:132:ASN:ND2	2.34	0.61
1:A:89:GLN:HG3	1:A:90:GLN:N	2.16	0.61
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.83	0.59
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.85	0.59
1:A:94:CYS:HB3	1:B:94:CYS:HB3	1.85	0.58
1:C:204:ALA:HA	1:C:207:MET:HE2	1.84	0.58
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.86	0.57
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.87	0.57
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.86	0.57
1:B:298:GLU:CD	4:B:504:BTB:H42	2.30	0.57
1:C:97:ARG:HG3	1:D:88:ALA:HB3	1.86	0.57
1:C:88:ALA:HB3	1:D:97:ARG:HD3	1.85	0.56
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.86	0.56
4:A:504:BTB:O3	4:A:504:BTB:O4	2.22	0.56
1:C:156:GLU:O	1:C:160:THR:HG22	2.06	0.56
1:A:147:GLU:O	1:A:151:GLN:NE2	2.39	0.55
4:D:504:BTB:H52	4:D:504:BTB:O4	2.07	0.55
1:D:170:LEU:HD11	1:D:230:VAL:HG11	1.89	0.55
1:A:321:GLU:H	1:A:321:GLU:CD	2.15	0.54
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.90	0.54
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.74	0.53
1:C:234:ARG:HA	1:C:238:ARG:HH21	1.74	0.53
1:C:143:SER:O	1:C:147:GLU:HG2	2.09	0.53
4:D:504:BTB:H32	4:D:504:BTB:H62	1.91	0.53
4:B:504:BTB:O8	4:B:504:BTB:O6	2.16	0.52
1:B:90:GLN:HB3	1:B:468:PHE:CD2	2.45	0.52
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.91	0.52
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.92	0.52
1:A:364:THR:O	1:A:368:CYS:HB2	2.10	0.51
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.45	0.51
1:A:257:GLN:OE1	9:A:602:HOH:O	2.19	0.51
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.46	0.51
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:OE2	5:A:506:GOL:H2	2.11	0.50
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.94	0.50
1:A:377:GLU:OE1	4:A:504:BTB:O3	2.20	0.50
1:B:122:GLN:CD	1:B:122:GLN:H	2.19	0.50
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.49
4:B:507:BTB:O4	4:B:507:BTB:C7	2.61	0.48
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.94	0.48
4:C:504:BTB:H31	4:C:504:BTB:H72	1.62	0.48
2:B:501:HEM:HH2	2:B:501:HEM:HBB2	1.95	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.95	0.48
1:A:125:SER:HA	1:A:128:ARG:NH1	2.28	0.48
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.49	0.48
1:C:167:GLU:OE2	5:C:505:GOL:O2	2.27	0.48
1:B:298:GLU:HG2	9:B:751:HOH:O	2.14	0.47
1:C:128:ARG:NH2	1:C:154:GLU:OE1	2.46	0.47
4:C:503:BTB:H31	4:C:503:BTB:H71	1.39	0.47
1:D:91:ASP:OD1	9:D:601:HOH:O	2.20	0.47
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.50	0.47
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.50	0.47
1:A:216:LYS:HG3	1:A:217:TYR:N	2.28	0.47
1:C:229:THR:O	1:C:352:PRO:HD2	2.15	0.47
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.50	0.47
4:D:504:BTB:H32	4:D:504:BTB:C6	2.45	0.47
1:A:267:ASN:O	1:A:269:GLU:N	2.47	0.47
1:D:271:THR:O	1:D:275:ILE:HG12	2.15	0.47
4:B:507:BTB:H62	1:C:322:TRP:CD1	2.50	0.47
4:D:503:BTB:H32	4:D:503:BTB:H51	1.72	0.46
4:D:503:BTB:H72	4:D:503:BTB:H11	1.67	0.46
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.50	0.46
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.24	0.46
4:A:505:BTB:H11	4:A:505:BTB:H51	1.82	0.46
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.80	0.46
1:C:128:ARG:HH21	1:C:154:GLU:CD	2.23	0.46
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.50	0.46
1:B:364:THR:O	1:B:368:CYS:HB2	2.16	0.46
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.56	0.46
4:B:504:BTB:O1	9:B:602:HOH:O	2.21	0.46
1:A:202:ARG:O	1:A:203:SER:HB3	2.17	0.45
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.50	0.45
1:C:91:ASP:OD1	9:C:601:HOH:O	2.20	0.45
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:503:BTB:HO6	4:C:503:BTB:HO1	1.56	0.45
4:A:504:BTB:H11	4:A:504:BTB:H51	1.51	0.45
1:A:90:GLN:HB3	1:A:468:PHE:CD2	2.51	0.45
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.32	0.45
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.98	0.45
1:B:429:LYS:HA	1:B:429:LYS:HD2	1.79	0.45
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.99	0.45
4:A:503:BTB:H12	4:A:503:BTB:H72	1.48	0.45
4:C:504:BTB:H41	4:C:504:BTB:H51	1.91	0.44
4:B:507:BTB:O3	1:C:384:ASP:OD1	2.35	0.44
1:A:256:GLN:C	1:A:258:ASP:H	2.26	0.44
4:B:507:BTB:O8	4:B:507:BTB:O6	2.33	0.44
1:D:124:LEU:HD11	1:D:154:GLU:HG3	2.00	0.44
1:B:298:GLU:HG3	1:B:299:PRO:HD2	2.00	0.44
4:C:503:BTB:H42	4:C:503:BTB:H51	1.52	0.44
1:C:89:GLN:HB2	1:C:90:GLN:H	1.65	0.44
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.53	0.44
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	2.00	0.44
1:A:88:ALA:O	1:B:97:ARG:NH2	2.50	0.44
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.53	0.44
1:A:238:ARG:NH2	1:A:240:ASP:OD1	2.51	0.44
1:A:465:VAL:HG12	1:A:467:TYR:HD1	1.83	0.44
1:A:139:LYS:HE3	1:A:139:LYS:HB2	1.82	0.43
1:C:221:ARG:HG2	1:C:221:ARG:HH11	1.83	0.43
1:A:67:LYS:HE3	1:A:67:LYS:HB2	1.88	0.43
1:B:326:LEU:HD12	4:B:507:BTB:H72	2.00	0.43
1:D:387:THR:HA	1:D:394:TRP:CD1	2.53	0.43
4:D:504:BTB:H11	4:D:504:BTB:H72	1.75	0.43
1:B:122:GLN:CD	1:B:122:GLN:N	2.76	0.43
4:B:503:BTB:H12	9:C:676:HOH:O	2.18	0.43
1:B:298:GLU:OE1	4:B:504:BTB:H42	2.19	0.43
4:A:505:BTB:H72	4:A:505:BTB:H41	1.39	0.43
1:B:321:GLU:OE2	4:B:503:BTB:O4	2.36	0.43
1:A:393:LEU:O	1:A:397:LYS:HG3	2.19	0.43
1:A:149:ARG:O	1:A:153:VAL:HG22	2.19	0.42
1:A:103:LEU:HD12	1:B:463:GLU:HB3	2.01	0.42
1:A:263:GLY:H	1:A:285:ARG:HG3	1.84	0.42
1:A:387:THR:HA	1:A:394:TRP:CD1	2.54	0.42
1:B:387:THR:HA	1:B:394:TRP:CD1	2.54	0.42
1:C:275:ILE:HA	1:C:279:TRP:O	2.19	0.42
1:D:292:LEU:HD23	1:D:292:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.59	0.42
1:D:455:SER:HA	1:D:460:PHE:CG	2.55	0.42
1:B:147:GLU:H	1:B:147:GLU:HG2	1.59	0.42
1:A:239:GLY:O	1:A:296:PRO:HB3	2.19	0.42
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.54	0.42
1:B:470:SER:HA	1:B:471:PRO:C	2.45	0.42
1:D:326:LEU:HB3	1:D:328:LEU:HG	2.02	0.42
4:A:503:BTB:H51	4:A:503:BTB:H32	1.56	0.41
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.56	0.41
1:A:367:LEU:HA	1:A:373:TYR:HB2	2.02	0.41
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.94	0.41
1:D:247:GLN:HA	1:D:335:ALA:O	2.19	0.41
1:D:470:SER:HA	1:D:471:PRO:C	2.45	0.41
1:D:279:TRP:HB2	1:D:302:LEU:HD21	2.01	0.41
1:A:156:GLU:O	1:A:160:THR:OG1	2.31	0.41
1:A:145:ALA:HA	1:A:148:GLN:HB2	2.04	0.40
1:C:233:GLN:O	1:C:238:ARG:NH2	2.55	0.40
1:A:298:GLU:OE2	4:A:505:BTB:H32	2.21	0.40
1:A:202:ARG:HA	1:A:241:PHE:HZ	1.87	0.40
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.56	0.40
1:C:214:HIS:CD2	1:C:214:HIS:C	2.99	0.40
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

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%)	379 (95%)	17 (4%)	2 (0%)	25	21
1	B	400/440 (91%)	389 (97%)	11 (3%)	0	100	100
1	C	399/440 (91%)	385 (96%)	13 (3%)	1 (0%)	37	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	399/440 (91%)	392 (98%)	7 (2%)	0	100	100
All	All	1596/1760 (91%)	1545 (97%)	48 (3%)	3 (0%)	44	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	C	89	GLN
1	A	203	SER

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%)	319 (93%)	23 (7%)	13	10
1	B	343/373 (92%)	333 (97%)	10 (3%)	37	39
1	C	342/373 (92%)	329 (96%)	13 (4%)	28	28
1	D	342/373 (92%)	337 (98%)	5 (2%)	60	66
All	All	1369/1492 (92%)	1318 (96%)	51 (4%)	29	29

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	122	GLN
1	A	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	129	ASP
1	A	136	SER
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	206	GLU
1	A	209	THR
1	A	238	ARG
1	A	256	GLN
1	A	272	GLU
1	A	276	GLN
1	A	285	ARG
1	A	304	LEU
1	A	321	GLU
1	A	329	ARG
1	A	375	ILE
1	A	474	ARG
1	B	71	VAL
1	B	87	GLN
1	B	98	ARG
1	B	122	GLN
1	B	128	ARG
1	B	136	SER
1	B	147	GLU
1	B	257	GLN
1	B	326	LEU
1	B	342	GLU
1	C	67	LYS
1	C	89	GLN
1	C	125	SER
1	C	140	ARG
1	C	151	GLN
1	C	216	LYS
1	C	221	ARG
1	C	234	ARG
1	C	255	ARG
1	C	308	GLU
1	C	309	LEU
1	C	342	GLU
1	C	438	ARG
1	D	124	LEU
1	D	136	SER
1	D	207	MET
1	D	268	VAL
1	D	326	LEU

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

Mol	Chain	Res	Type
1	A	256	GLN
1	A	276	GLN
1	A	277	HIS
1	A	476	GLN
1	B	256	GLN
1	C	133	GLN
1	C	144	GLN
1	C	164	GLN
1	D	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	501	1	42,50,50	1.56	7 (16%)	46,82,82	1.75	10 (21%)
3	V5D	B	502	-	35,35,35	1.40	2 (5%)	45,46,46	1.41	6 (13%)
5	GOL	A	511	-	5,5,5	0.61	0	5,5,5	1.62	2 (40%)
4	BTB	B	503	7	13,13,13	0.53	0	7,16,16	0.52	0
5	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BTB	A	503	7	13,13,13	0.71	0	7,16,16	1.46	1 (14%)
3	V5D	A	502	-	35,35,35	1.45	2 (5%)	45,46,46	1.16	4 (8%)
4	BTB	B	507	7	13,13,13	0.59	0	7,16,16	1.07	1 (14%)
3	V5D	C	502	-	35,35,35	1.36	2 (5%)	45,46,46	1.67	8 (17%)
2	HEM	D	501	1	42,50,50	1.57	6 (14%)	46,82,82	1.67	12 (26%)
4	BTB	A	504	-	13,13,13	0.54	0	7,16,16	0.94	0
5	GOL	C	506	-	5,5,5	0.37	0	5,5,5	0.32	0
4	BTB	D	503	7	13,13,13	0.55	0	7,16,16	0.45	0
3	V5D	D	502	-	35,35,35	1.32	2 (5%)	45,46,46	1.45	6 (13%)
2	HEM	A	501	1	42,50,50	1.53	5 (11%)	46,82,82	1.79	13 (28%)
4	BTB	D	504	-	13,13,13	0.66	0	7,16,16	0.72	0
4	BTB	C	503	-	13,13,13	0.63	0	7,16,16	1.04	0
4	BTB	B	504	-	13,13,13	0.46	0	7,16,16	1.22	0
5	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.63	0
4	BTB	C	504	-	13,13,13	0.38	0	7,16,16	0.37	0
5	GOL	C	505	-	5,5,5	0.34	0	5,5,5	0.47	0
4	BTB	A	505	-	13,13,13	0.54	0	7,16,16	0.42	0
2	HEM	B	501	1	42,50,50	1.56	7 (16%)	46,82,82	1.57	10 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	1/12/54/54	-
3	V5D	B	502	-	-	3/14/14/14	0/4/4/4
5	GOL	A	511	-	-	2/4/4/4	-
4	BTB	B	503	7	-	3/21/21/21	-
5	GOL	A	507	-	-	4/4/4/4	-
4	BTB	A	503	7	-	5/21/21/21	-
3	V5D	A	502	-	-	2/14/14/14	0/4/4/4
4	BTB	B	507	7	-	6/21/21/21	-
3	V5D	C	502	-	-	4/14/14/14	0/4/4/4
2	HEM	D	501	1	-	0/12/54/54	-
4	BTB	A	504	-	-	11/21/21/21	-
5	GOL	C	506	-	-	2/4/4/4	-
4	BTB	D	503	7	-	7/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	V5D	D	502	-	-	2/14/14/14	0/4/4/4
2	HEM	A	501	1	-	2/12/54/54	-
4	BTB	D	504	-	-	6/21/21/21	-
4	BTB	C	503	-	-	16/21/21/21	-
4	BTB	B	504	-	-	11/21/21/21	-
5	GOL	A	506	-	-	0/4/4/4	-
4	BTB	C	504	-	-	3/21/21/21	-
5	GOL	C	505	-	-	4/4/4/4	-
4	BTB	A	505	-	-	13/21/21/21	-
2	HEM	B	501	1	-	1/12/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	V5D	O18-C17	6.45	1.52	1.37
3	C	502	V5D	O18-C17	6.15	1.51	1.37
3	D	502	V5D	O18-C17	5.96	1.51	1.37
3	B	502	V5D	O18-C17	5.78	1.50	1.37
2	B	501	HEM	C3C-CAC	3.92	1.56	1.47
2	C	501	HEM	C3C-C2C	-3.87	1.35	1.40
2	D	501	HEM	C3C-C4C	3.80	1.47	1.41
2	A	501	HEM	C3C-C2C	-3.45	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.45	1.35	1.40
2	D	501	HEM	C3C-CAC	3.43	1.55	1.47
2	A	501	HEM	C3C-CAC	3.42	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.38	1.35	1.40
2	C	501	HEM	C3C-CAC	3.38	1.55	1.47
2	D	501	HEM	CAB-C3B	3.37	1.56	1.47
2	C	501	HEM	CAB-C3B	3.28	1.56	1.47
2	A	501	HEM	CAB-C3B	3.21	1.56	1.47
2	B	501	HEM	CAB-C3B	3.19	1.55	1.47
3	A	502	V5D	O18-C19	3.08	1.53	1.43
2	A	501	HEM	C3C-C4C	3.05	1.45	1.41
2	C	501	HEM	C3C-C4C	3.03	1.45	1.41
3	B	502	V5D	O18-C19	2.85	1.52	1.43
2	D	501	HEM	CMD-C2D	2.81	1.56	1.50
3	C	502	V5D	O18-C19	2.75	1.52	1.43
2	A	501	HEM	FE-NB	2.72	2.13	1.98
2	B	501	HEM	C3C-C4C	2.71	1.45	1.41
3	D	502	V5D	O18-C19	2.71	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CMD-C2D	2.55	1.56	1.50
2	B	501	HEM	CMB-C2B	2.38	1.55	1.50
2	C	501	HEM	CMD-C2D	2.24	1.55	1.50
2	D	501	HEM	FE-NB	2.23	2.10	1.98
2	C	501	HEM	FE-NB	2.21	2.10	1.98
2	C	501	HEM	CMB-C2B	2.05	1.55	1.50
2	B	501	HEM	FE-NB	2.01	2.09	1.98

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	V5D	C02-N32-C06	6.09	122.62	118.07
2	C	501	HEM	CBA-CAA-C2A	-4.76	104.54	112.54
2	C	501	HEM	C4B-CHC-C1C	4.59	128.61	122.56
2	A	501	HEM	CBD-CAD-C3D	-4.01	101.45	112.53
2	D	501	HEM	CMA-C3A-C4A	-3.97	122.64	128.46
3	B	502	V5D	C02-N32-C06	3.86	120.96	118.07
2	B	501	HEM	CBA-CAA-C2A	-3.82	106.12	112.54
2	D	501	HEM	C4B-CHC-C1C	3.82	127.59	122.56
2	A	501	HEM	C3B-C2B-C1B	3.69	109.18	106.41
2	A	501	HEM	C4B-CHC-C1C	3.68	127.41	122.56
4	A	503	BTB	O3-C3-C2	3.68	120.05	111.40
3	B	502	V5D	C09-C08-C07	-3.52	99.04	113.74
3	C	502	V5D	C12-N11-C10	-3.47	101.00	113.20
2	C	501	HEM	CMA-C3A-C4A	-3.46	123.38	128.46
3	A	502	V5D	C02-N32-C06	3.41	120.62	118.07
3	D	502	V5D	C02-N32-C06	3.41	120.62	118.07
3	D	502	V5D	C09-C08-C07	-3.34	99.80	113.74
3	D	502	V5D	C19-O18-C17	-3.33	109.69	117.62
2	B	501	HEM	C3B-C2B-C1B	3.23	108.84	106.41
2	B	501	HEM	CMC-C2C-C3C	3.19	131.06	124.68
2	A	501	HEM	C4D-ND-C1D	3.17	108.96	105.21
3	B	502	V5D	C19-O18-C17	-3.17	110.06	117.62
2	D	501	HEM	CMC-C2C-C3C	3.09	130.87	124.68
3	A	502	V5D	C07-C06-N32	3.08	120.72	116.06
3	D	502	V5D	C07-C06-N32	3.04	120.67	116.06
2	C	501	HEM	CBD-CAD-C3D	-2.96	104.35	112.53
3	C	502	V5D	C12-C13-C31	-2.78	114.70	120.63
2	D	501	HEM	CHD-C1D-ND	2.76	127.41	124.44
2	C	501	HEM	C3D-C4D-ND	-2.76	107.14	110.17
2	A	501	HEM	C3D-C4D-ND	-2.76	107.15	110.17
3	C	502	V5D	N27-C26-N28	2.74	120.51	118.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3D-C4D-ND	-2.73	107.18	110.17
2	A	501	HEM	CMA-C3A-C4A	-2.69	124.51	128.46
2	D	501	HEM	C4A-C3A-C2A	2.69	108.87	107.00
2	A	501	HEM	C1B-NB-C4B	2.68	108.38	105.21
5	A	511	GOL	O2-C2-C1	-2.61	98.39	109.18
2	D	501	HEM	CHC-C4B-C3B	2.56	128.48	124.57
2	A	501	HEM	C2D-C1D-ND	-2.54	106.97	109.90
2	A	501	HEM	C4A-C3A-C2A	2.54	108.76	107.00
3	D	502	V5D	C09-C10-N11	-2.49	105.37	112.07
2	C	501	HEM	C4D-ND-C1D	2.48	108.15	105.21
2	C	501	HEM	C3B-C2B-C1B	2.47	108.27	106.41
2	D	501	HEM	CBD-CAD-C3D	-2.43	105.81	112.53
2	C	501	HEM	C1B-NB-C4B	2.42	108.07	105.21
3	B	502	V5D	C20-C30-C29	-2.41	119.19	121.11
2	B	501	HEM	C1B-NB-C4B	2.39	108.03	105.21
5	A	511	GOL	O1-C1-C2	-2.38	99.66	110.38
2	D	501	HEM	C1B-NB-C4B	2.37	108.01	105.21
3	D	502	V5D	C20-C30-C29	-2.35	119.24	121.11
2	D	501	HEM	CBA-CAA-C2A	-2.33	108.62	112.54
4	B	507	BTB	O3-C3-C2	2.33	116.88	111.40
2	B	501	HEM	C4D-ND-C1D	2.31	107.95	105.21
3	B	502	V5D	C12-N11-C10	-2.31	105.06	113.20
3	A	502	V5D	C19-O18-C17	-2.29	112.17	117.62
3	C	502	V5D	C03-C02-N32	-2.25	119.12	121.83
2	C	501	HEM	CHC-C4B-C3B	2.23	127.99	124.57
2	C	501	HEM	C3B-C4B-NB	-2.23	107.87	109.47
3	C	502	V5D	C07-C06-N32	2.22	119.42	116.06
2	A	501	HEM	C3B-C4B-NB	-2.21	107.88	109.47
2	D	501	HEM	C4D-ND-C1D	2.21	107.82	105.21
3	C	502	V5D	C20-C30-C29	-2.19	119.37	121.11
3	B	502	V5D	C03-C02-N32	-2.17	119.21	121.83
2	D	501	HEM	C3B-C2B-C1B	2.17	108.04	106.41
2	B	501	HEM	C4C-CHD-C1D	2.14	125.38	122.56
2	A	501	HEM	CHB-C1B-NB	2.11	126.98	124.37
2	B	501	HEM	CMB-C2B-C3B	-2.10	123.34	128.43
2	B	501	HEM	C3B-C4B-NB	-2.10	107.96	109.47
3	C	502	V5D	C22-C23-C29	2.08	121.24	118.43
2	B	501	HEM	CMA-C3A-C4A	-2.05	125.46	128.46
2	B	501	HEM	C3D-C4D-ND	-2.04	107.93	110.17
3	A	502	V5D	N01-C02-N32	2.02	119.83	116.59
2	A	501	HEM	C2B-C1B-NB	-2.02	107.52	109.84
2	A	501	HEM	CBA-CAA-C2A	-2.02	109.15	112.54

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	BTB	C1-C2-C4-O4
4	A	503	BTB	C3-C2-C4-O4
4	A	503	BTB	N-C2-C4-O4
4	A	504	BTB	C1-C2-C4-O4
4	A	504	BTB	C3-C2-C4-O4
4	A	504	BTB	N-C2-C4-O4
4	A	504	BTB	C1-C2-N-C5
4	A	504	BTB	C1-C2-N-C7
4	A	504	BTB	C3-C2-N-C5
4	A	504	BTB	C3-C2-N-C7
4	A	504	BTB	C4-C2-N-C5
4	A	504	BTB	C4-C2-N-C7
4	A	505	BTB	O1-C1-C2-C3
4	A	505	BTB	O1-C1-C2-N
4	A	505	BTB	C1-C2-C4-O4
4	A	505	BTB	C3-C2-C4-O4
4	A	505	BTB	N-C2-C4-O4
4	A	505	BTB	C4-C2-N-C7
4	B	503	BTB	O1-C1-C2-C3
4	B	503	BTB	O1-C1-C2-C4
4	B	503	BTB	O1-C1-C2-N
4	B	504	BTB	C1-C2-C3-O3
4	B	504	BTB	C4-C2-C3-O3
4	B	504	BTB	N-C2-C3-O3
4	B	504	BTB	C1-C2-N-C5
4	B	504	BTB	C1-C2-N-C7
4	B	504	BTB	C3-C2-N-C5
4	B	504	BTB	C3-C2-N-C7
4	B	504	BTB	C4-C2-N-C7
4	B	507	BTB	C1-C2-C4-O4
4	B	507	BTB	C3-C2-C4-O4
4	B	507	BTB	N-C2-C4-O4
4	C	503	BTB	O1-C1-C2-C4
4	C	503	BTB	O1-C1-C2-N
4	C	503	BTB	C1-C2-C3-O3
4	C	503	BTB	C4-C2-C3-O3
4	C	503	BTB	N-C2-C3-O3
4	C	503	BTB	C3-C2-C4-O4
4	C	503	BTB	C1-C2-N-C5
4	C	503	BTB	C1-C2-N-C7

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Mol	Chain	Res	Type	Atoms
4	C	503	BTB	C3-C2-N-C5
4	C	503	BTB	C3-C2-N-C7
4	C	503	BTB	C4-C2-N-C5
4	C	503	BTB	C4-C2-N-C7
4	C	503	BTB	C8-C7-N-C5
4	C	504	BTB	C3-C2-C4-O4
4	C	504	BTB	N-C2-C4-O4
4	D	503	BTB	C1-C2-C4-O4
4	D	503	BTB	C3-C2-C4-O4
4	D	503	BTB	N-C2-C4-O4
4	D	504	BTB	C1-C2-C3-O3
4	D	504	BTB	C4-C2-C3-O3
4	D	504	BTB	N-C2-C3-O3
4	D	504	BTB	C6-C5-N-C7
5	A	507	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	511	GOL	O1-C1-C2-C3
5	C	505	GOL	O1-C1-C2-C3
5	C	506	GOL	O1-C1-C2-O2
5	C	506	GOL	O1-C1-C2-C3
3	A	502	V5D	C08-C09-C10-N11
3	C	502	V5D	C06-C07-C08-C09
4	A	503	BTB	N-C7-C8-O8
4	C	503	BTB	N-C5-C6-O6
5	C	505	GOL	O1-C1-C2-O2
4	B	504	BTB	N-C7-C8-O8
4	D	504	BTB	N-C5-C6-O6
3	D	502	V5D	C08-C09-C10-N11
5	A	507	GOL	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
3	B	502	V5D	C20-C19-O18-C17
3	C	502	V5D	C08-C09-C10-N11
3	C	502	V5D	C07-C08-C09-C10
4	D	504	BTB	N-C7-C8-O8
3	A	502	V5D	C20-C19-O18-C17
2	A	501	HEM	C2A-CAA-CBA-CGA
4	B	504	BTB	N-C5-C6-O6
5	A	511	GOL	O1-C1-C2-O2
3	D	502	V5D	C20-C19-O18-C17
3	C	502	V5D	C20-C19-O18-C17
4	A	505	BTB	N-C5-C6-O6
3	B	502	V5D	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
5	C	505	GOL	O2-C2-C3-O3
4	B	507	BTB	N-C5-C6-O6
4	C	504	BTB	N-C5-C6-O6
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
4	A	505	BTB	N-C2-C3-O3
4	A	505	BTB	C1-C2-N-C5
4	A	505	BTB	C1-C2-N-C7
4	A	505	BTB	C3-C2-N-C5
4	B	504	BTB	C4-C2-N-C5
4	D	503	BTB	C1-C2-N-C5
4	D	503	BTB	C3-C2-N-C5
4	A	504	BTB	N-C7-C8-O8
5	C	505	GOL	C1-C2-C3-O3
4	A	504	BTB	N-C5-C6-O6
4	B	507	BTB	C1-C2-C3-O3
4	C	503	BTB	O1-C1-C2-C3
4	D	503	BTB	N-C7-C8-O8
2	B	501	HEM	C4B-C3B-CAB-CBB
4	A	503	BTB	N-C2-C3-O3
4	A	505	BTB	C3-C2-N-C7
4	A	505	BTB	C4-C2-N-C5
4	B	507	BTB	N-C2-C3-O3
4	C	503	BTB	N-C2-C4-O4
4	D	503	BTB	C4-C2-N-C5
3	B	502	V5D	C08-C09-C10-N11

There are no ring outliers.

17 monomers are involved in 45 short contacts:

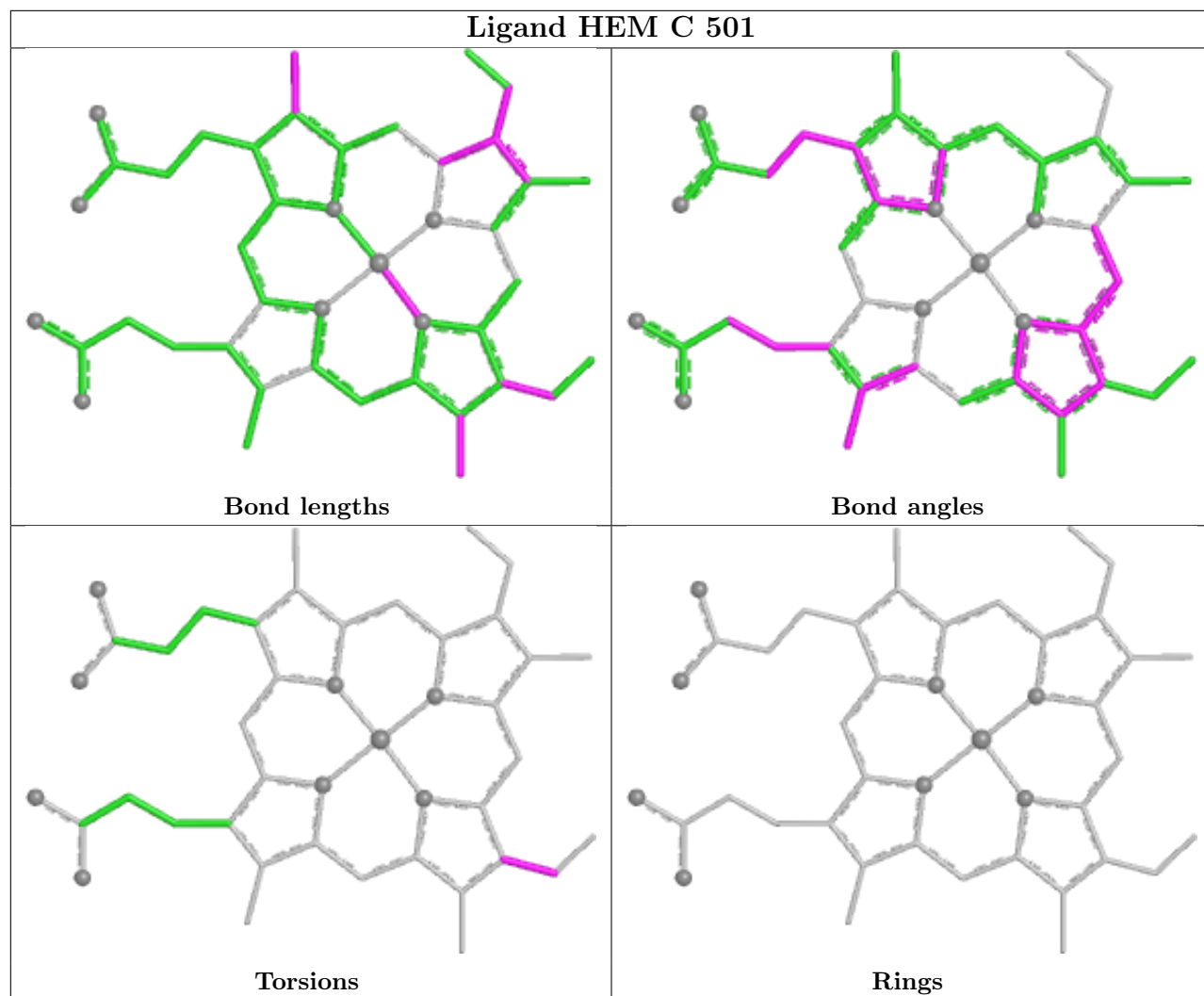
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	1	0
4	B	503	BTB	2	0
4	A	503	BTB	3	0
4	B	507	BTB	8	0
2	D	501	HEM	2	0
4	A	504	BTB	3	0
4	D	503	BTB	3	0
3	D	502	V5D	1	0
2	A	501	HEM	1	0
4	D	504	BTB	4	0
4	C	503	BTB	4	0

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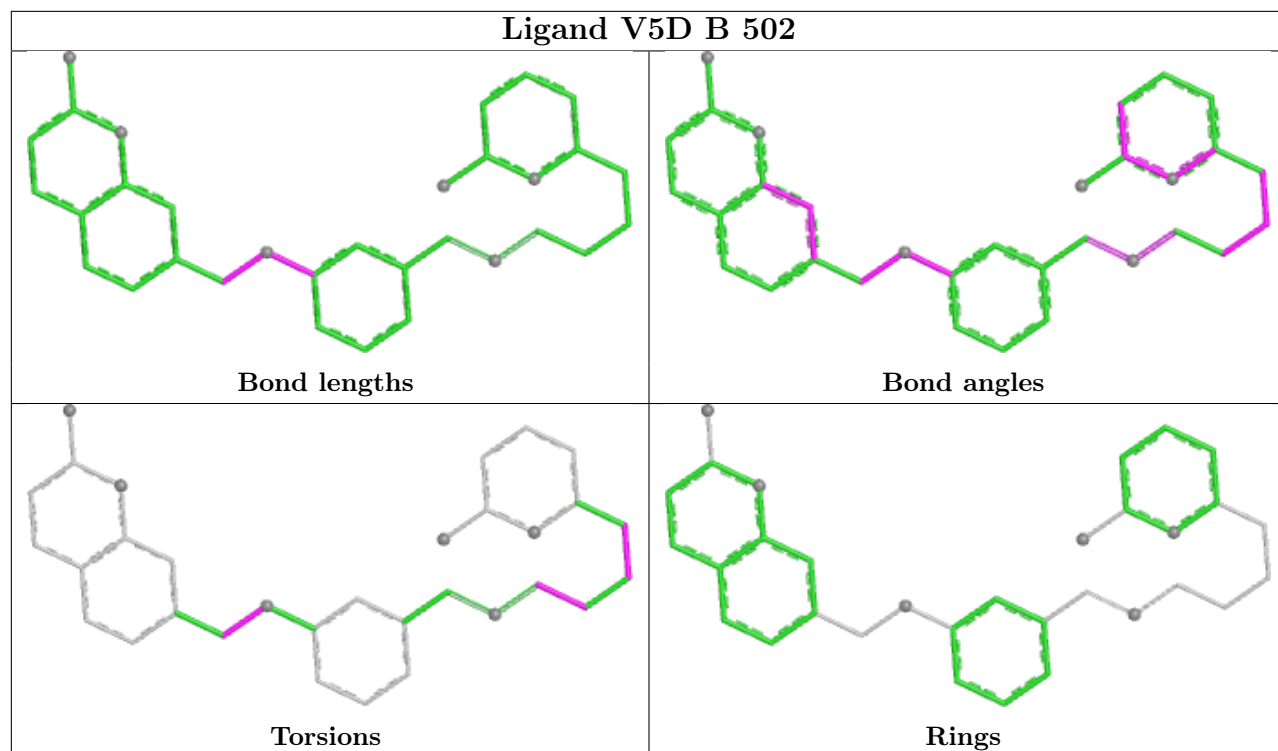
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	BTB	4	0
5	A	506	GOL	1	0
4	C	504	BTB	2	0
5	C	505	GOL	1	0
4	A	505	BTB	3	0
2	B	501	HEM	2	0

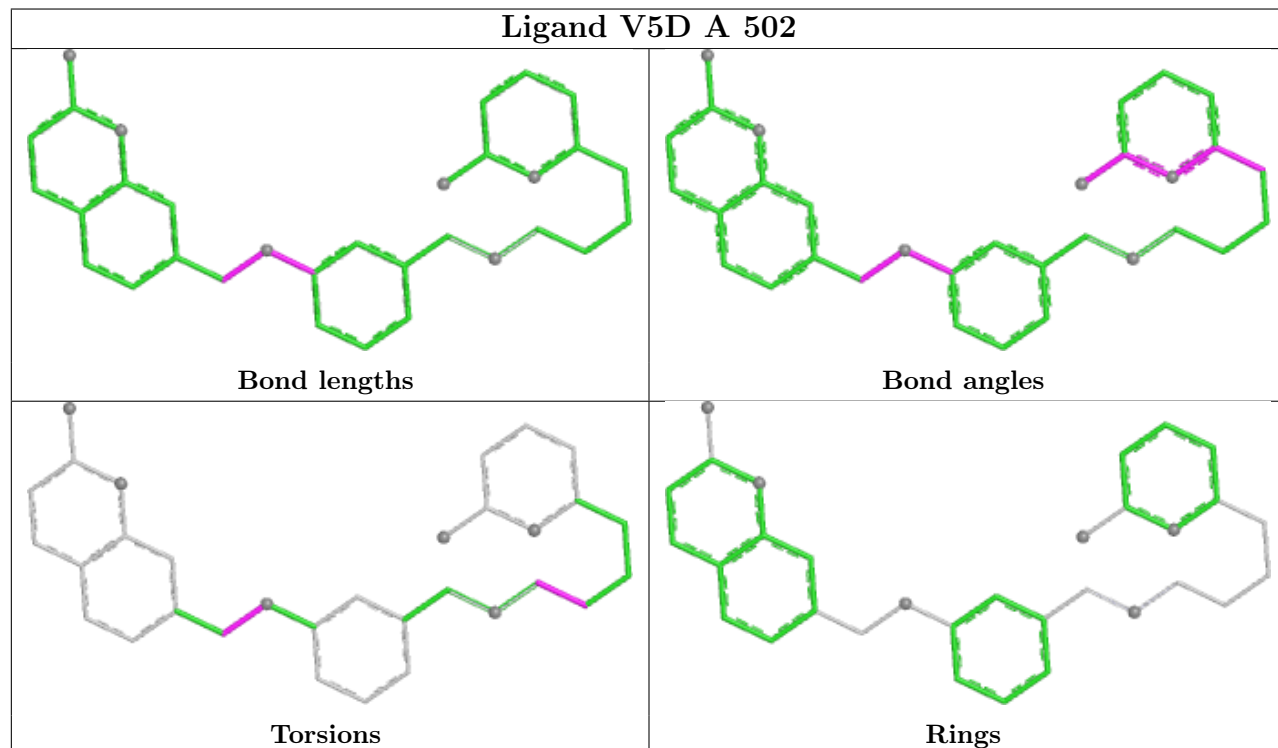
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

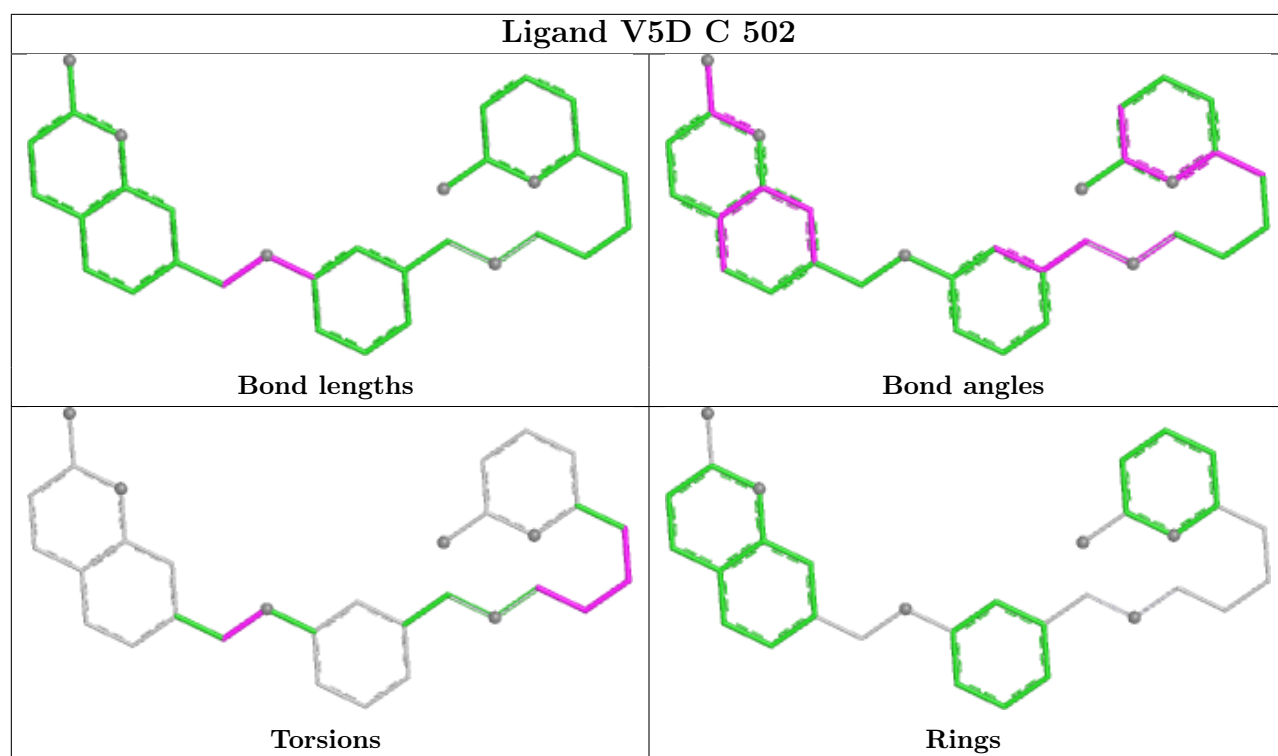


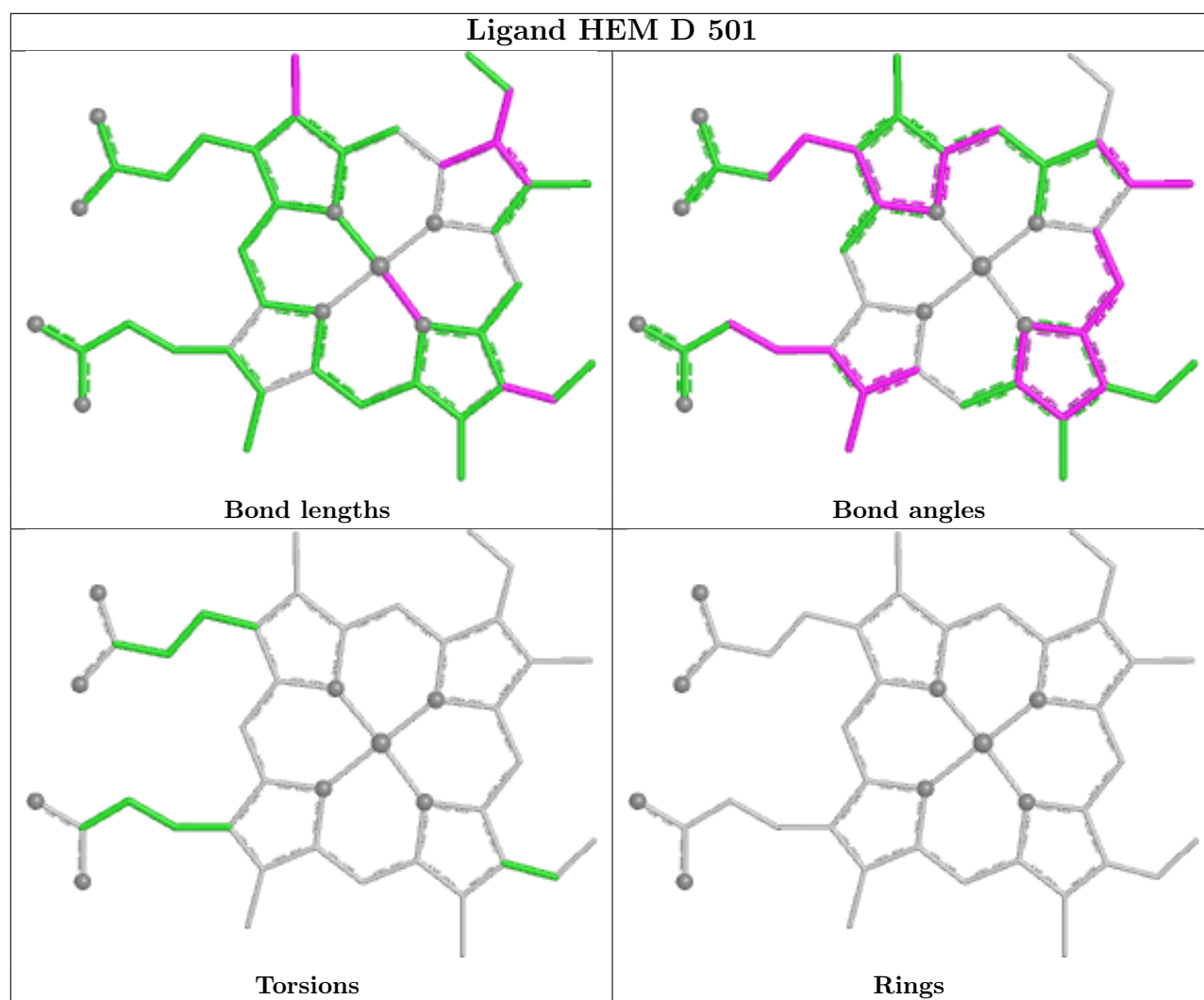
Ligand V5D B 502

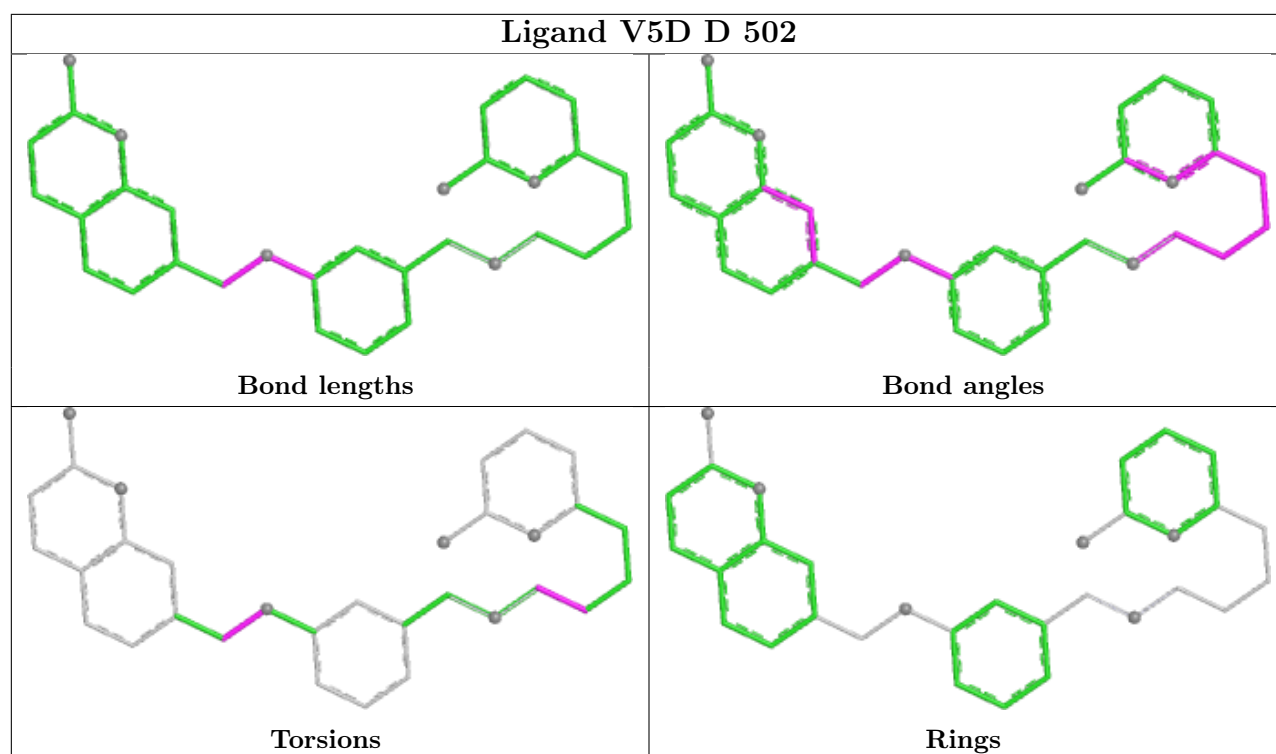


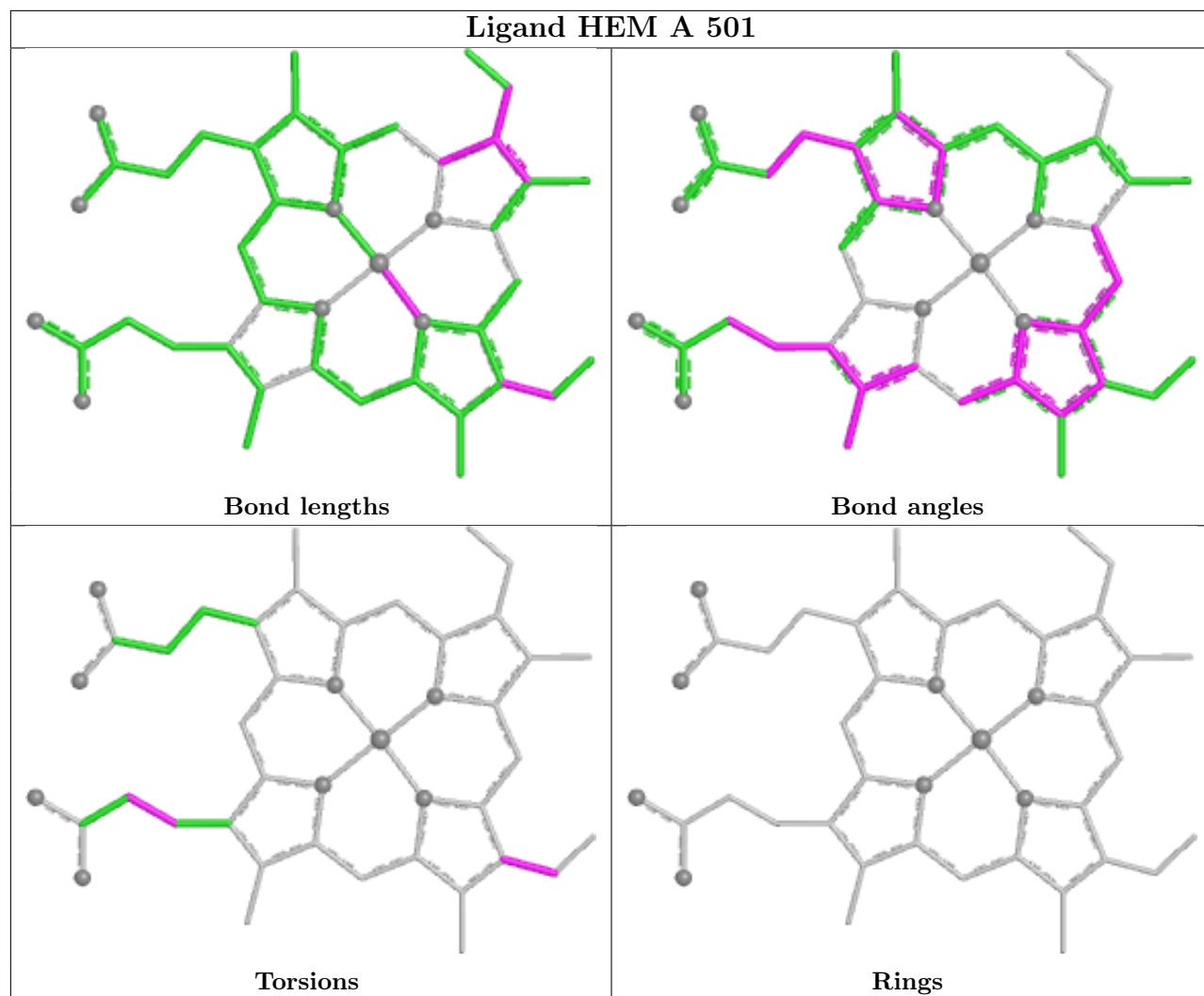
Ligand V5D A 502

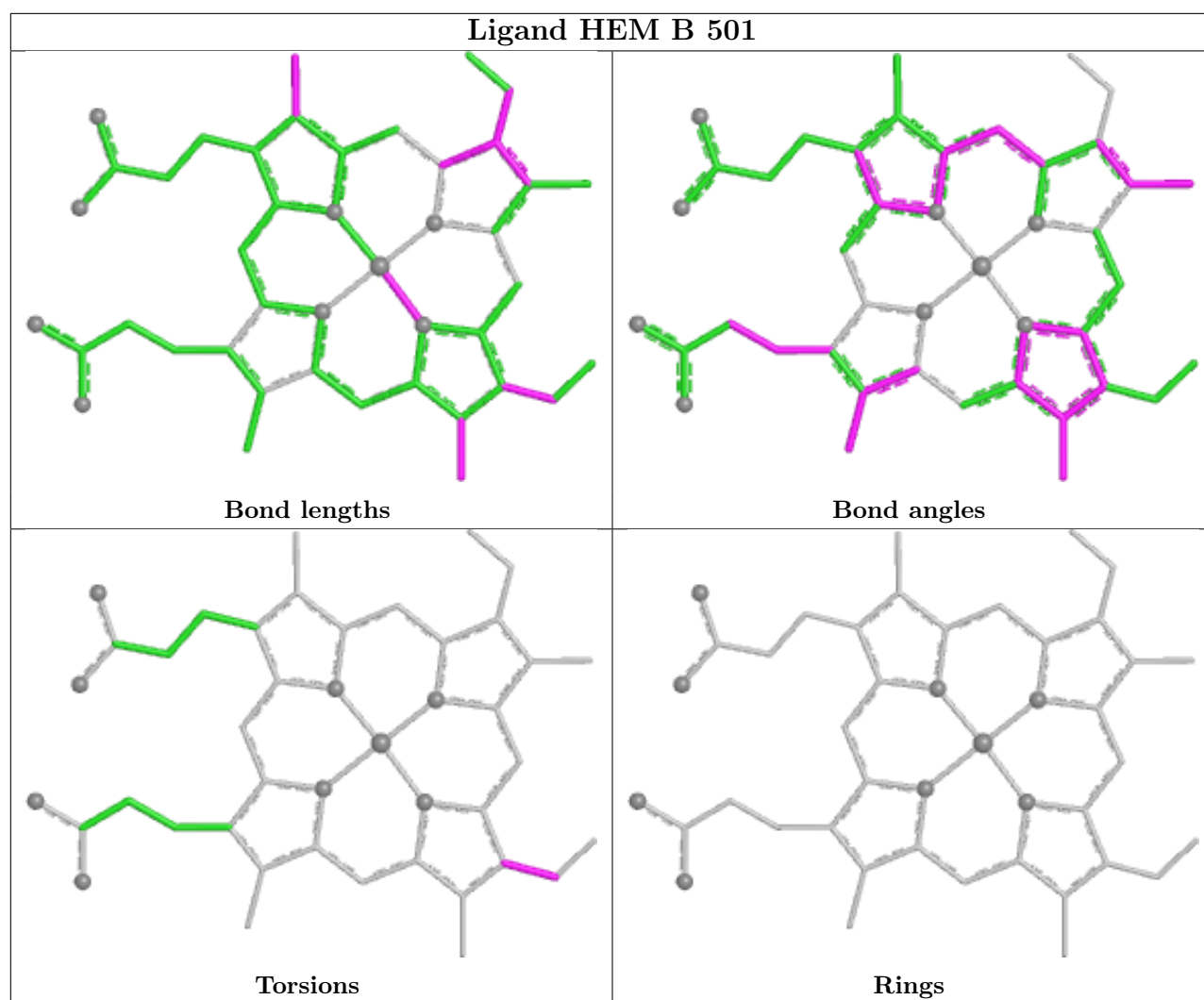












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/440 (91%)	0.30	15 (3%) 45 43	22, 55, 101, 132	1 (0%)
1	B	401/440 (91%)	-0.27	3 (0%) 84 83	18, 37, 70, 110	3 (0%)
1	C	402/440 (91%)	0.03	6 (1%) 71 70	24, 49, 88, 111	1 (0%)
1	D	402/440 (91%)	-0.37	6 (1%) 71 70	21, 36, 64, 129	1 (0%)
All	All	1606/1760 (91%)	-0.07	30 (1%) 66 65	18, 43, 89, 132	6 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PRO	4.2
1	A	204	ALA	4.2
1	C	106	PRO	4.1
1	D	107	ARG	3.6
1	B	106	PRO	3.5
1	A	120	PRO	3.0
1	A	153	VAL	3.0
1	A	235	CYS	2.7
1	D	90	GLN	2.7
1	A	145	ALA	2.7
1	D	119	ALA	2.7
1	B	144	GLN	2.6
1	C	120	PRO	2.6
1	A	268	VAL	2.5
1	A	292	LEU	2.4
1	C	119	ALA	2.4
1	A	299	PRO	2.3
1	A	244	TRP	2.3
1	D	200	ASP	2.3
1	A	343	ILE	2.2
1	D	89	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	143	SER	2.2
1	D	257	GLN	2.1
1	A	152	GLU	2.1
1	A	238	ARG	2.1
1	C	144	GLN	2.1
1	A	300	PRO	2.0
1	C	155	ALA	2.0
1	C	238	ARG	2.0
1	B	119	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BTB	A	505	14/14	0.68	0.16	75,85,92,92	0
5	GOL	C	506	6/6	0.68	0.12	67,74,76,81	0
4	BTB	C	504	14/14	0.70	0.14	97,111,119,119	0
4	BTB	D	504	14/14	0.76	0.17	46,72,83,91	0
5	GOL	A	507	6/6	0.81	0.17	59,70,81,84	0
5	GOL	A	506	6/6	0.83	0.11	52,71,78,82	0
4	BTB	A	504	14/14	0.84	0.15	49,68,76,78	0
5	GOL	C	505	6/6	0.85	0.10	57,60,73,74	0
4	BTB	B	504	14/14	0.88	0.12	33,74,88,88	0
5	GOL	A	511	6/6	0.89	0.14	30,36,62,64	0
4	BTB	D	503	14/14	0.89	0.12	39,62,72,72	0
3	V5D	C	502	32/32	0.89	0.13	29,49,68,72	0
4	BTB	B	503	14/14	0.90	0.12	29,47,59,60	0
4	BTB	C	503	14/14	0.90	0.15	15,62,73,81	0

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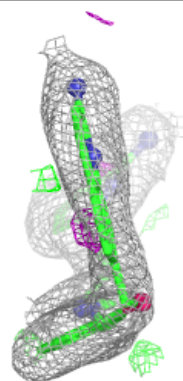
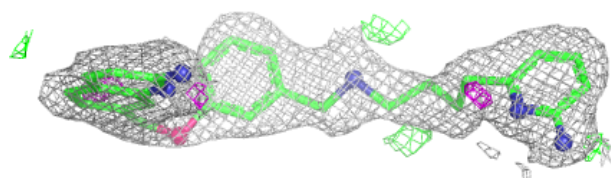
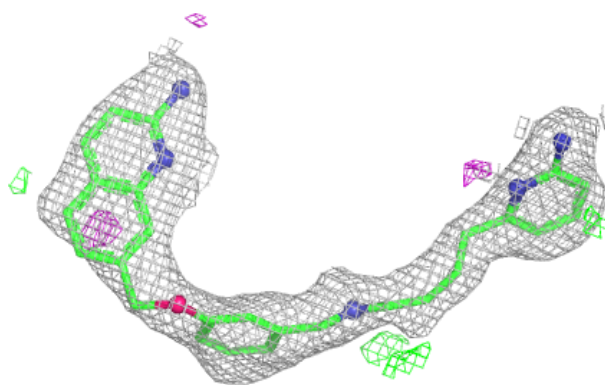
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	V5D	B	502	32/32	0.91	0.11	27,39,55,58	0
3	V5D	A	502	32/32	0.92	0.11	35,63,82,84	0
4	BTB	A	503	14/14	0.93	0.12	35,77,86,88	0
3	V5D	D	502	32/32	0.93	0.11	19,44,60,63	0
4	BTB	B	507	14/14	0.96	0.09	22,62,66,67	0
2	HEM	A	501	43/43	0.96	0.09	29,44,54,69	0
2	HEM	C	501	43/43	0.97	0.07	27,39,48,54	0
6	CL	A	508	1/1	0.97	0.07	48,48,48,48	0
2	HEM	B	501	43/43	0.98	0.05	20,29,46,52	0
2	HEM	D	501	43/43	0.98	0.06	20,27,41,49	0
6	CL	C	507	1/1	0.98	0.06	41,41,41,41	0
7	GD	A	509	1/1	0.98	0.04	80,80,80,80	1
7	GD	D	506	1/1	0.98	0.04	46,46,46,46	0
6	CL	B	505	1/1	0.99	0.05	33,33,33,33	0
7	GD	B	506	1/1	0.99	0.03	42,42,42,42	0
7	GD	B	508	1/1	0.99	0.02	59,59,59,59	1
6	CL	D	505	1/1	0.99	0.03	38,38,38,38	0
8	ZN	A	510	1/1	0.99	0.02	38,38,38,38	0
8	ZN	C	508	1/1	1.00	0.01	33,33,33,33	0

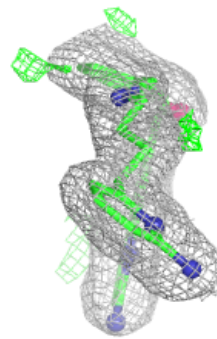
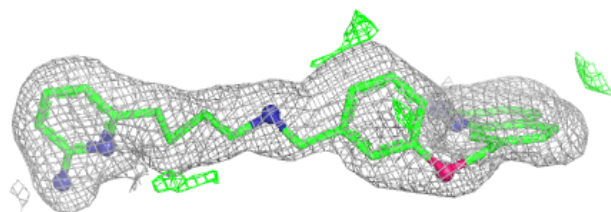
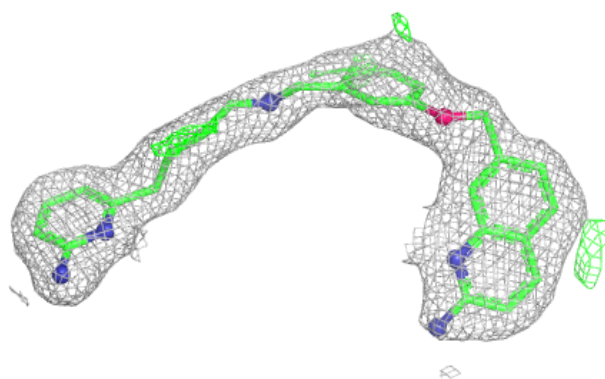
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V5D C 502:

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

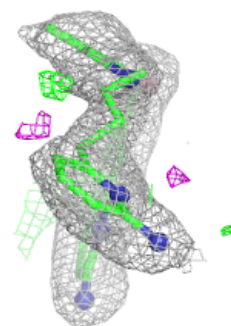
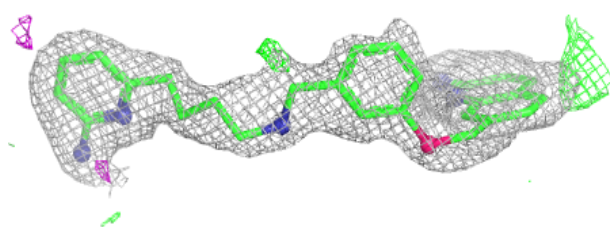
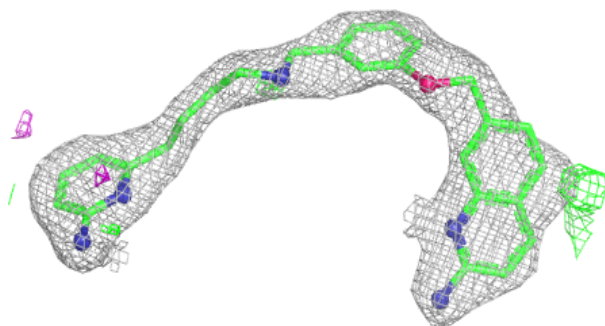
**Electron density around V5D B 502:**

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

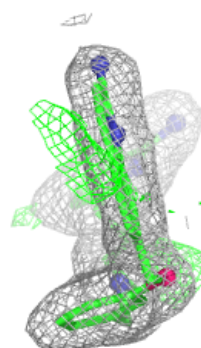
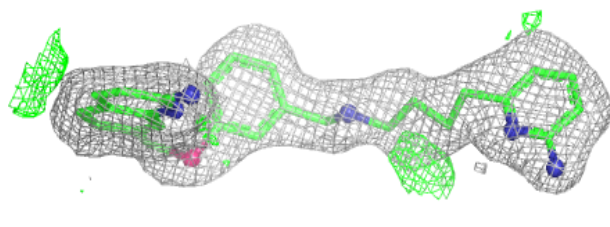
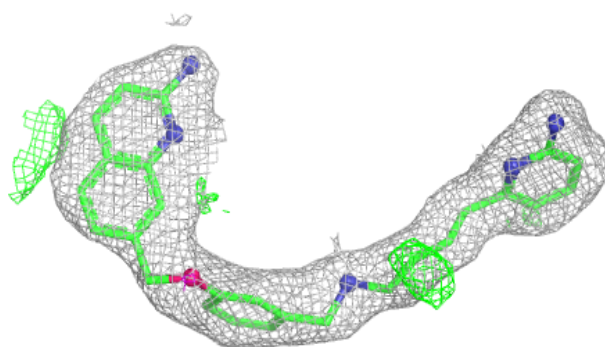


Electron density around V5D A 502:

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

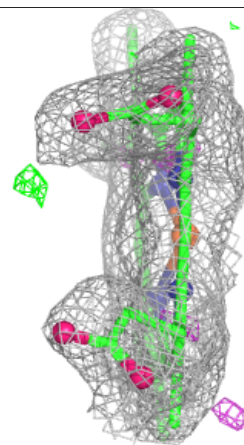
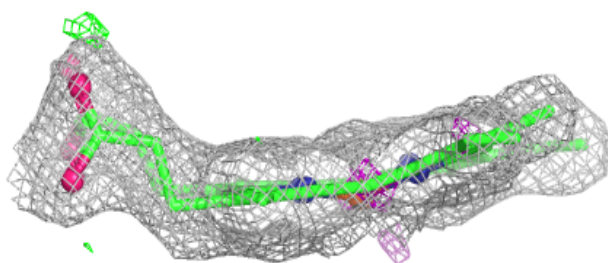
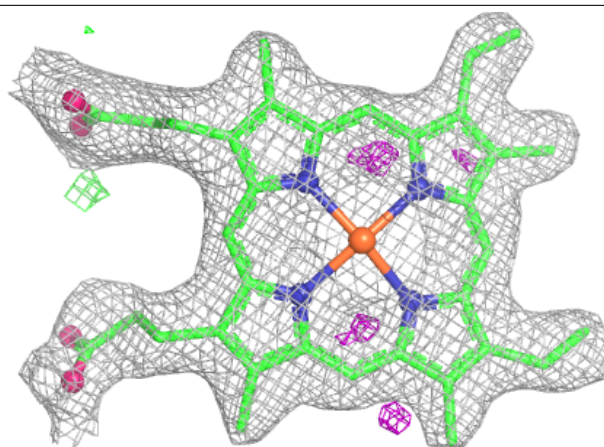
**Electron density around V5D D 502:**

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



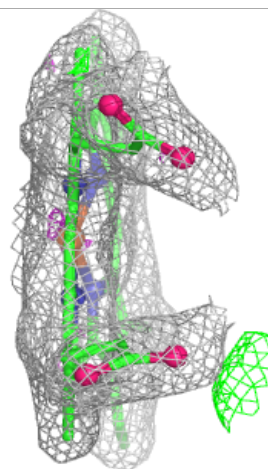
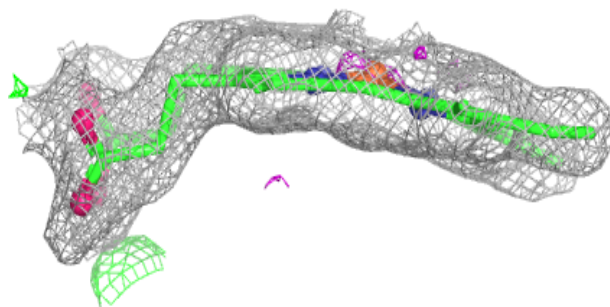
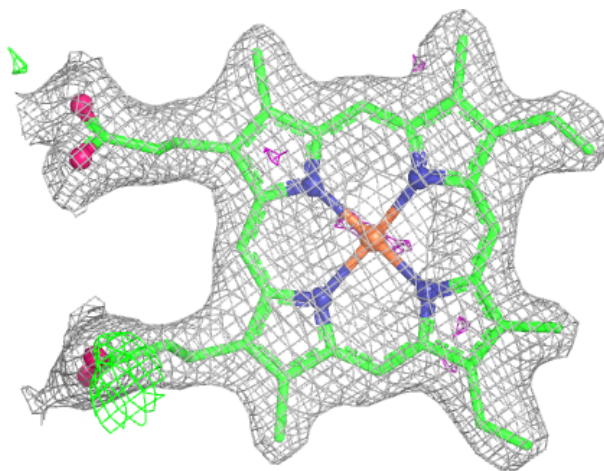
Electron density around HEM A 501:

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



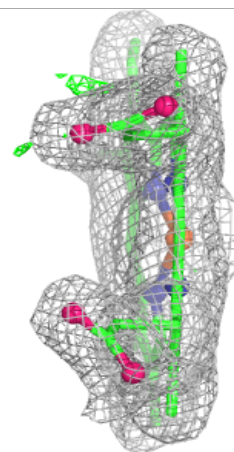
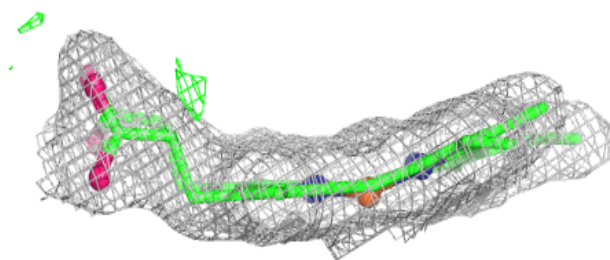
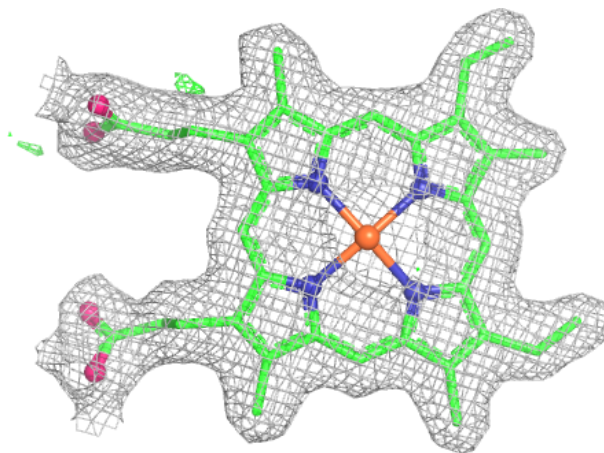
Electron density around HEM C 501:

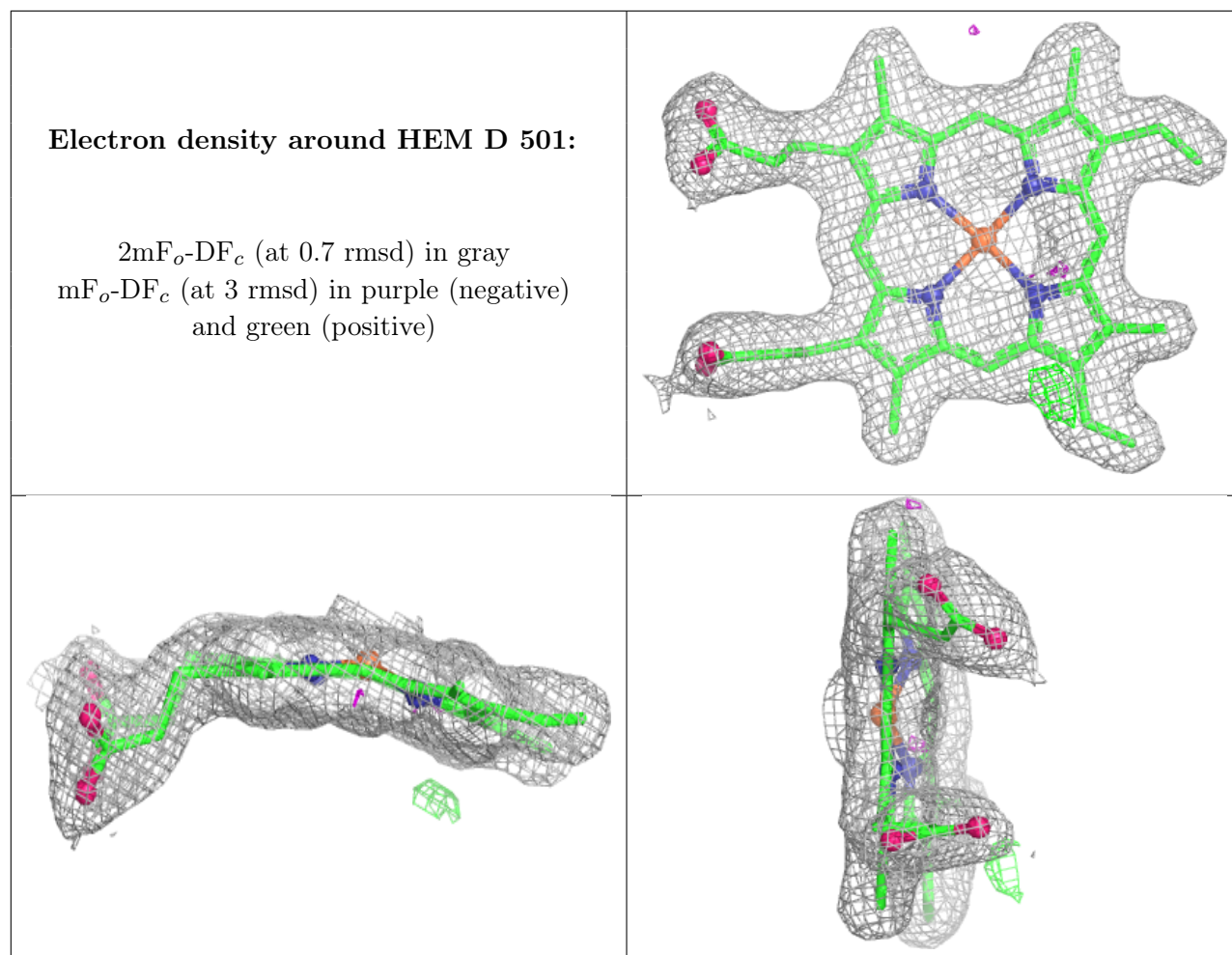
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.