Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2025 – 06:35 PM EDT

PDB ID	:	9CW2 / pdb_00009cw2
Title	:	Structure of human endothelial nitric oxide synthase heme domain bound with 4-methyl-6-(3-((methylamino)methyl)phenyl)pyridin-2-amine dihydrochloride
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2024-07-29
Resolution	:	2.10 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:

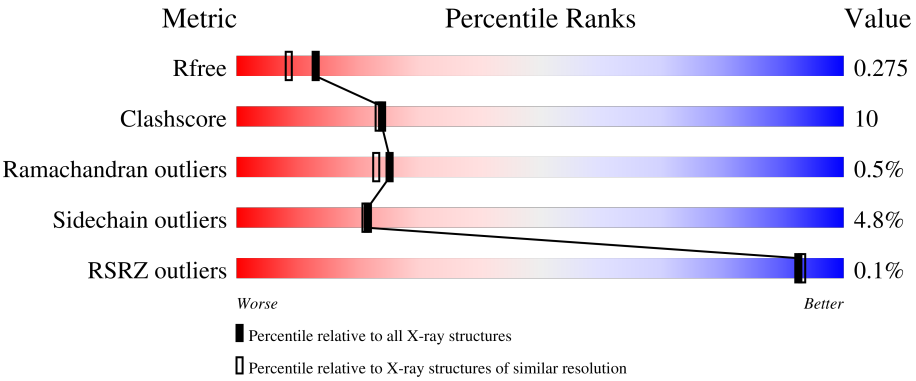
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 <=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	65% 23% • 9%
1	B	440	72% 18% • 9%
1	C	440	65% 25% • 9%
1	D	440	72% 18% • 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
6	GOL	C	508	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13853 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.

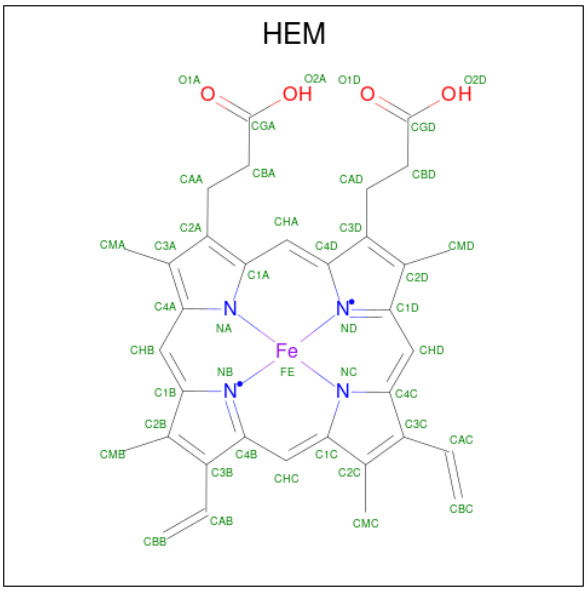
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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	2	0
			3208	2043	564	585	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:

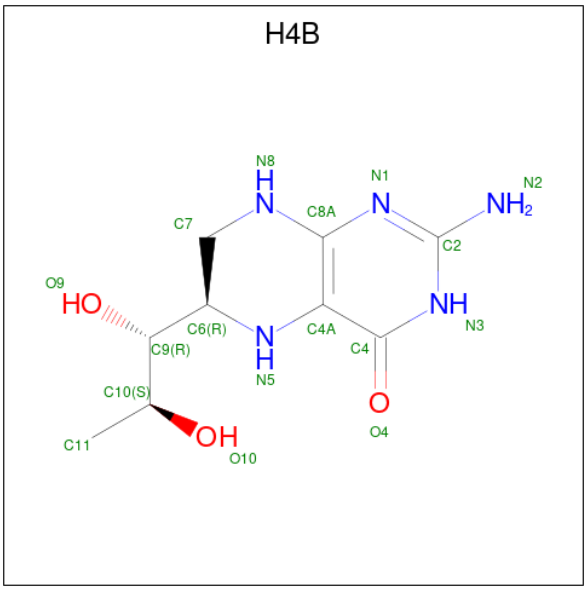
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



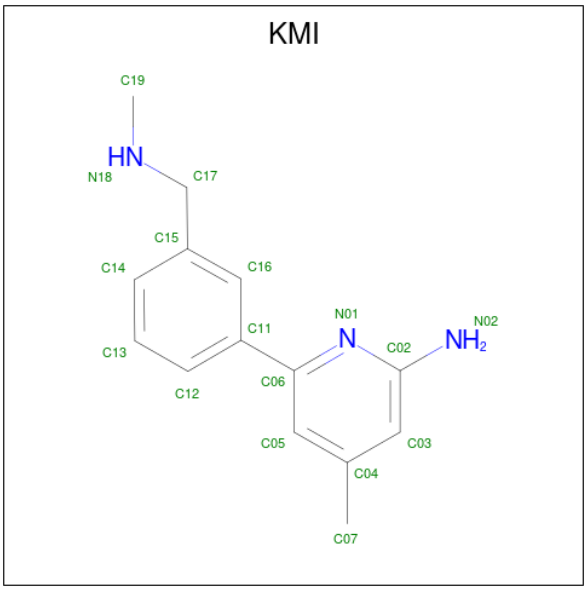
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



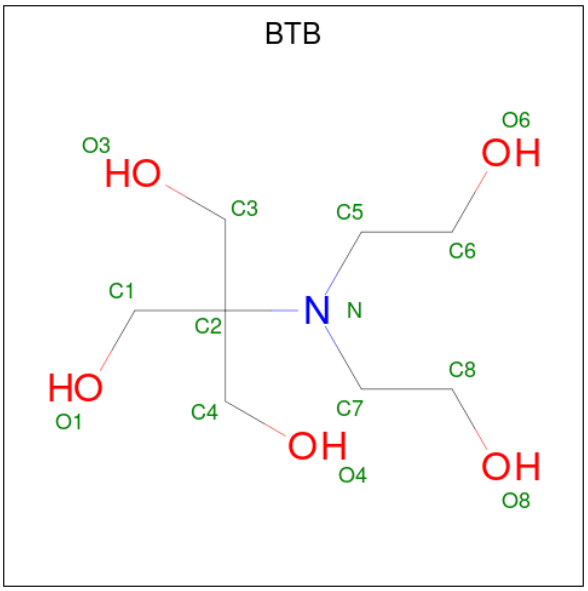
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 4-methyl-6-{3-[(methylamino)methyl]phenyl}pyridin-2-amine (CCD ID: KMI) (formula: $C_{14}H_{17}N_3$) (labeled as "Ligand of Interest" by depositor).



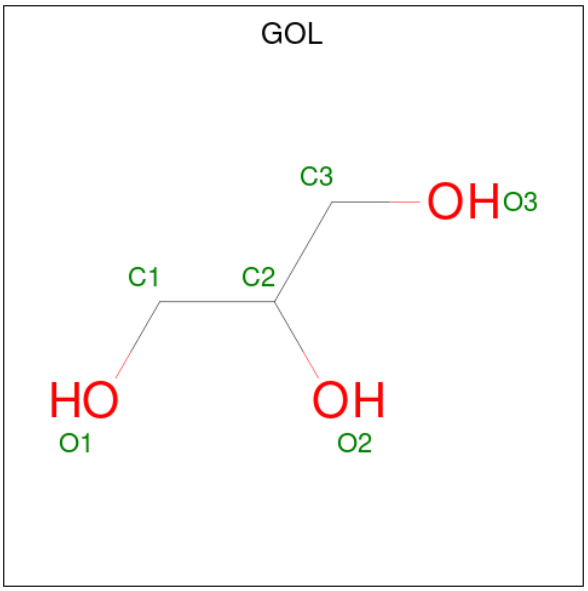
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 17 14 3	0	0
4	B	1	Total C N 17 14 3	0	0
4	C	1	Total C N 17 14 3	0	0
4	D	1	Total C N 17 14 3	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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

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

- Molecule 8 is GADOLINIUM ION (CCD ID: GD3) (formula: Gd).

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is water.

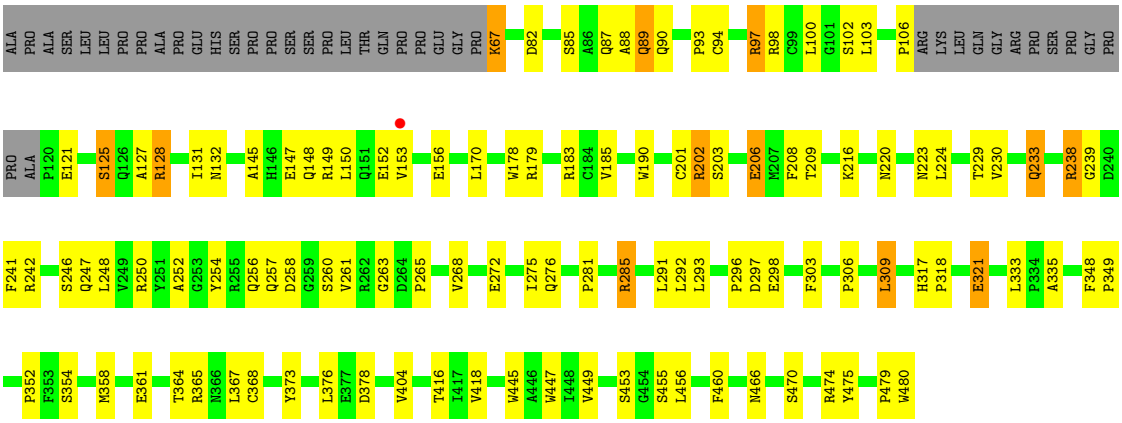
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	81	Total O 81 81	0	0
10	B	154	Total O 154 154	0	0
10	C	92	Total O 92 92	0	0
10	D	161	Total O 161 161	0	0

3 Residue-property plots (i)

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

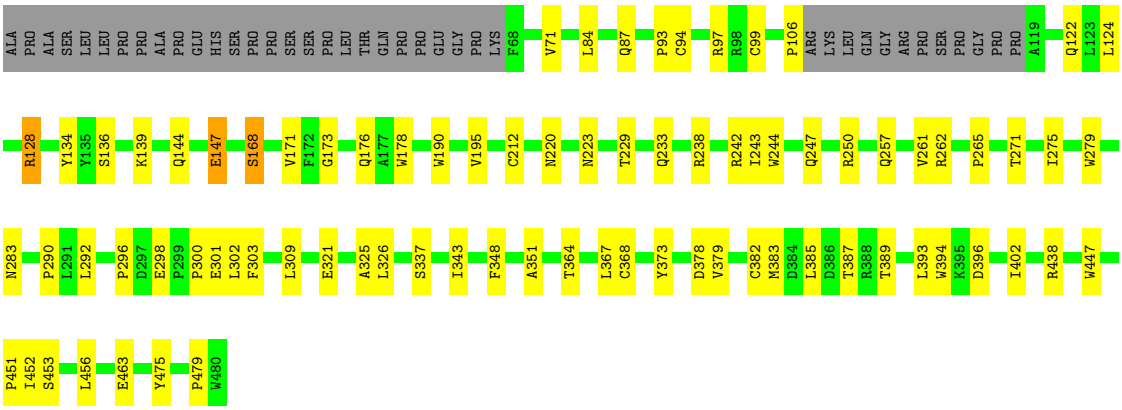
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



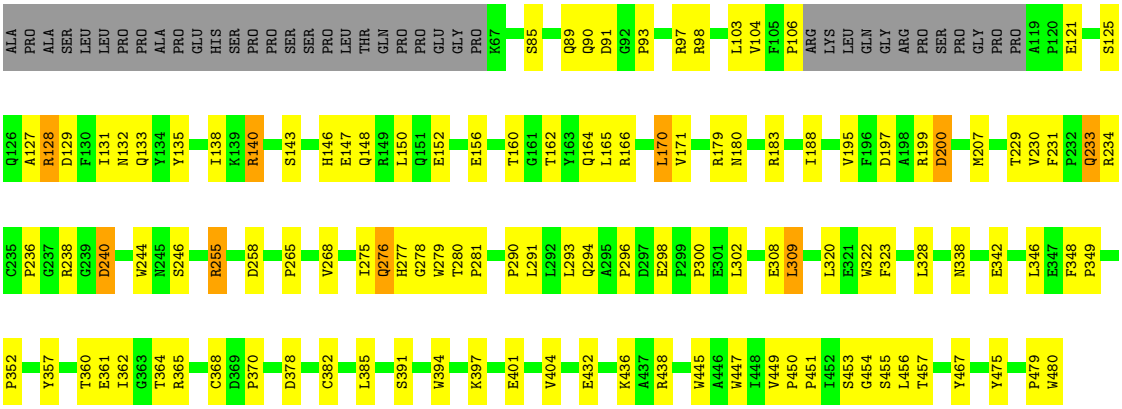
• Molecule 1: Nitric oxide synthase, endothelial

Chain B:



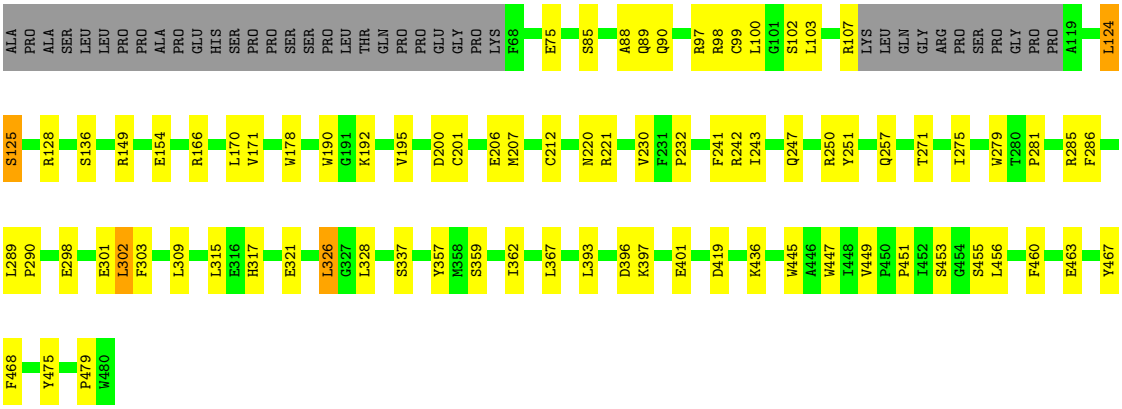
• Molecule 1: Nitric oxide synthase, endothelial

Chain C:



• Molecule 1: Nitric oxide synthase, endothelial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.92Å 151.39Å 107.48Å 90.00° 90.62° 90.00°	Depositor
Resolution (Å)	49.10 – 2.10 49.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.10-2.10) 95.7 (49.10-2.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.217 , 0.277 0.214 , 0.275	Depositor DCC
R_{free} test set	5403 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.872	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.239 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13853	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GD3, ZN, H4B, BTB, CL, GOL, KMI

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	0.38	0/3302	0.54	0/4498
1	B	0.43	0/3306	0.57	0/4506
1	C	0.37	0/3307	0.53	0/4506
1	D	0.45	0/3309	0.59	0/4509
All	All	0.41	0/13224	0.56	0/18019

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

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	73	1
1	B	3208	0	3109	56	0
1	C	3212	0	3116	76	0
1	D	3214	0	3116	52	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	1	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	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	17	0	0	1	0
4	B	17	0	0	0	0
4	C	17	0	0	1	0
4	D	17	0	0	1	0
5	A	42	0	57	5	0
5	B	28	0	37	7	0
5	C	42	0	55	6	0
5	D	28	0	36	6	1
6	A	18	0	24	0	0
6	B	12	0	16	0	0
6	C	24	0	32	1	0
6	D	12	0	16	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	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	81	0	0	3	0
10	B	154	0	0	5	0
10	C	92	0	0	6	0
10	D	161	0	0	5	0
All	All	13853	0	12906	261	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (261) 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:A:239:GLY:HA3	1:A:297:ASP:H	1.46	0.79
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.64	0.79
1:C:382:CYS:HA	5:C:504:BTB:H12	1.63	0.79
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASP:OD1	1:C:200:ASP:N	2.20	0.74
4:D:503:KMI:N18	7:D:508:CL:CL	2.59	0.73
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.71	0.72
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.74	0.70
1:A:378:ASP:OD1	10:A:601:HOH:O	2.08	0.70
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.74	0.69
1:A:263:GLY:H	1:A:285:ARG:HG3	1.58	0.69
1:C:160:THR:HG23	1:C:162:THR:H	1.58	0.69
1:C:129:ASP:HA	1:C:132:ASN:HD22	1.58	0.68
1:D:154:GLU:OE2	10:D:601:HOH:O	2.13	0.67
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.76	0.66
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.77	0.65
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.79	0.64
1:A:102:SER:O	3:A:502:H4B:O10	2.14	0.64
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.27	0.64
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.11	0.64
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.80	0.63
1:C:234:ARG:HA	1:C:238:ARG:HH21	1.64	0.63
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.11	0.63
1:C:276:GLN:O	1:C:278:GLY:N	2.29	0.62
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.34	0.62
1:C:133:GLN:NE2	10:C:602:HOH:O	2.14	0.62
1:C:179:ARG:NH2	1:C:438:ARG:HG3	2.15	0.61
1:A:291:LEU:HD23	1:A:293:LEU:HD21	1.80	0.61
1:B:124:LEU:HB3	1:B:128:ARG:HH22	1.66	0.61
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.83	0.61
5:B:505:BTB:O6	5:B:505:BTB:O8	2.18	0.61
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.14	0.60
1:A:455:SER:OG	1:B:451:PRO:HB2	2.01	0.59
1:C:97:ARG:NH2	10:C:606:HOH:O	2.26	0.59
1:B:243:ILE:HG21	1:B:337:SER:HB2	1.83	0.59
1:B:298:GLU:OE2	5:B:505:BTB:O8	2.20	0.58
1:A:466:ASN:HB3	1:B:99:CYS:HB3	1.86	0.58
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.83	0.58
1:C:451:PRO:HB2	1:D:455:SER:OG	2.04	0.58
5:A:505:BTB:O3	5:A:505:BTB:O4	2.20	0.57
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.39	0.57
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.40	0.57
1:B:271:THR:O	1:B:275:ILE:HG13	2.05	0.57
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.37	0.57
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:SER:HA	1:C:338:ASN:HB3	1.87	0.56
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.15	0.56
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.24	0.56
1:A:321:GLU:H	1:A:321:GLU:CD	2.07	0.56
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.88	0.55
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.89	0.54
1:A:128:ARG:O	1:A:132:ASN:ND2	2.41	0.54
1:B:382:CYS:SG	5:C:504:BTB:H42	2.48	0.54
1:C:165:LEU:HG	1:C:346:LEU:HD12	1.89	0.54
1:A:263:GLY:N	1:A:285:ARG:HG3	2.22	0.53
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.90	0.53
1:B:298:GLU:CD	5:B:505:BTB:H42	2.28	0.53
1:D:100:LEU:HB3	1:D:103:LEU:HD22	1.90	0.53
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.90	0.53
1:C:156:GLU:O	1:C:160:THR:HG22	2.09	0.53
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.43	0.53
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.09	0.53
1:B:326:LEU:HD11	5:C:504:BTB:H41	1.90	0.53
1:A:256:GLN:C	1:A:258:ASP:H	2.13	0.53
1:A:361:GLU:OE2	4:A:503:KMI:N02	2.42	0.53
1:D:170:LEU:HD11	1:D:230:VAL:HG11	1.91	0.53
1:C:291:LEU:HB3	1:C:293:LEU:HD21	1.90	0.52
1:C:401:GLU:OE2	1:D:397:LYS:NZ	2.42	0.52
1:A:94:CYS:HB3	1:B:94:CYS:HB3	1.91	0.52
1:A:127:ALA:O	1:A:131:ILE:HG12	2.09	0.52
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.45	0.52
1:B:238:ARG:NH2	10:B:617:HOH:O	2.42	0.52
1:C:240:ASP:OD1	1:C:349:PRO:HG2	2.09	0.52
1:A:152:GLU:O	1:A:156:GLU:HB2	2.10	0.52
1:A:453:SER:HA	1:B:452:ILE:HG22	1.92	0.52
1:C:432:GLU:HG2	1:C:436:LYS:HE3	1.92	0.52
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.91	0.52
1:C:197:ASP:OD2	1:C:199:ARG:NH2	2.31	0.52
1:C:229:THR:O	1:C:352:PRO:HD2	2.10	0.52
1:A:333:LEU:HD11	1:A:354:SER:HB2	1.92	0.52
1:B:447:TRP:HA	3:B:502:H4B:N1	2.25	0.52
1:C:90:GLN:NE2	10:C:612:HOH:O	2.43	0.51
1:A:224:LEU:HB2	1:A:416:THR:HB	1.92	0.51
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.93	0.51
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.46	0.51
1:D:124:LEU:HD22	1:D:128:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:TRP:HA	3:D:502:H4B:N1	2.26	0.50
1:C:378:ASP:OD1	10:C:603:HOH:O	2.19	0.50
1:A:367:LEU:HA	1:A:373:TYR:HB2	1.92	0.50
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.46	0.50
1:D:220:ASN:O	1:D:221:ARG:HG2	2.11	0.50
1:A:149:ARG:O	1:A:153:VAL:HG22	2.12	0.49
1:C:135:TYR:HA	1:C:138:ILE:HG12	1.94	0.49
1:C:171:VAL:HG22	1:C:195:VAL:HB	1.95	0.49
1:B:171:VAL:HG22	1:B:195:VAL:HB	1.94	0.49
1:A:89:GLN:HG3	1:A:90:GLN:N	2.27	0.49
1:C:97:ARG:HG2	1:D:88:ALA:HB3	1.95	0.49
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.93	0.49
1:C:370:PRO:HB2	1:D:75:GLU:HG3	1.94	0.49
1:B:212:CYS:HA	1:B:309:LEU:HD21	1.94	0.49
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.53	0.49
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.47	0.49
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.48	0.48
1:B:244:TRP:CD1	1:B:479:PRO:HG2	2.47	0.48
1:B:173:GLY:HA3	1:B:343:ILE:HD13	1.94	0.48
1:B:326:LEU:CD1	5:C:504:BTB:H41	2.44	0.48
1:C:85:SER:HB3	1:C:467:TYR:CE1	2.49	0.48
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.79	0.48
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.96	0.48
1:B:262:ARG:NE	1:B:283:ASN:O	2.41	0.48
1:C:361:GLU:OE2	4:C:503:KMI:N02	2.47	0.48
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.49	0.48
1:A:238:ARG:HD3	1:A:296:PRO:HB3	1.96	0.47
1:A:252:ALA:HB1	1:A:254:TYR:CE1	2.49	0.47
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.50	0.47
1:A:404:VAL:HG23	1:B:393:LEU:HD12	1.96	0.47
1:A:229:THR:O	1:A:352:PRO:HD2	2.14	0.47
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.96	0.47
1:B:229:THR:O	1:B:351:ALA:HA	2.14	0.47
1:B:244:TRP:CH2	1:B:300:PRO:HG3	2.50	0.47
5:B:504:BTB:H61	10:B:718:HOH:O	2.15	0.47
1:C:128:ARG:O	1:C:132:ASN:ND2	2.47	0.47
1:D:397:LYS:NZ	10:D:613:HOH:O	2.47	0.47
1:C:180:ASN:OD1	1:C:438:ARG:NH2	2.34	0.47
1:D:279:TRP:HB2	1:D:302:LEU:HD11	1.97	0.47
1:A:248:LEU:HD12	1:A:335:ALA:HB1	1.96	0.46
1:A:298:GLU:OE1	5:A:506:BTB:O4	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.83	0.46
1:C:143:SER:O	1:C:147:GLU:HG2	2.14	0.46
1:C:244:TRP:CZ2	1:C:300:PRO:HG3	2.50	0.46
5:C:506:BTB:H42	5:C:506:BTB:H51	1.64	0.46
5:A:505:BTB:H51	5:A:505:BTB:H11	1.51	0.46
1:D:359:SER:OG	1:D:419:ASP:HA	2.15	0.46
1:A:82:ASP:O	1:A:85:SER:OG	2.33	0.46
1:C:103:LEU:HA	1:D:463:GLU:HG2	1.97	0.46
1:C:104:VAL:HG13	1:C:447:TRP:HZ2	1.81	0.46
1:B:301:GLU:HB3	1:B:303:PHE:CE1	2.51	0.46
1:A:306:PRO:HB2	1:A:309:LEU:HB2	1.96	0.46
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.50	0.46
1:A:455:SER:HA	1:A:460:PHE:CG	2.51	0.46
1:C:296:PRO:O	1:C:298:GLU:HG2	2.16	0.46
1:D:171:VAL:HA	1:D:195:VAL:HG21	1.98	0.45
1:A:220:ASN:ND2	1:A:223:ASN:HB3	2.31	0.45
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.51	0.45
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.99	0.45
1:C:148:GLN:O	1:C:152:GLU:HB2	2.16	0.45
1:C:255:ARG:HH12	1:C:268:VAL:HG11	1.80	0.45
1:C:275:ILE:HA	1:C:279:TRP:O	2.16	0.45
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.99	0.45
1:C:236:PRO:C	1:C:238:ARG:H	2.20	0.45
1:D:201:CYS:SG	1:D:206:GLU:HB3	2.57	0.45
1:A:93:PRO:HB3	1:A:106:PRO:HB3	1.98	0.45
1:C:397:LYS:NZ	10:C:614:HOH:O	2.48	0.45
1:D:85:SER:HB3	1:D:467:TYR:CE1	2.52	0.45
1:D:271:THR:O	1:D:275:ILE:HG12	2.17	0.45
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.52	0.45
1:B:321:GLU:OE1	5:B:504:BTB:H82	2.16	0.45
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.46	0.45
1:B:106:PRO:HG3	10:B:656:HOH:O	2.17	0.44
1:B:238:ARG:HD3	10:B:752:HOH:O	2.16	0.44
1:A:179:ARG:O	10:A:602:HOH:O	2.21	0.44
1:A:125:SER:HA	1:A:128:ARG:NH1	2.32	0.44
1:B:367:LEU:HA	1:B:373:TYR:HB2	1.98	0.44
1:D:171:VAL:HG22	1:D:195:VAL:HB	1.99	0.44
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.99	0.44
1:A:246:SER:OG	1:A:250:ARG:HD2	2.18	0.44
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.61	0.44
1:D:247:GLN:HB2	1:D:250:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:TYR:CD1	1:C:138:ILE:HD11	2.53	0.44
1:C:404:VAL:HG23	1:D:393:LEU:HD12	2.00	0.44
1:C:127:ALA:O	1:C:131:ILE:HG12	2.18	0.44
5:C:504:BTB:H32	5:C:504:BTB:O6	2.18	0.44
5:B:505:BTB:H51	5:B:505:BTB:H11	1.60	0.44
1:C:445:TRP:CE2	1:C:449:VAL:HG21	2.53	0.44
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.52	0.44
1:A:358:MET:HA	1:A:418:VAL:O	2.18	0.44
5:D:504:BTB:H11	5:D:504:BTB:H72	1.68	0.44
1:A:67:LYS:HB3	1:A:67:LYS:HE2	1.70	0.44
1:A:94:CYS:SG	1:A:100:LEU:N	2.87	0.44
1:A:254:TYR:O	1:A:261:VAL:HA	2.18	0.44
1:B:325:ALA:HB1	1:C:322:TRP:HB2	1.99	0.44
1:B:451:PRO:HG3	10:B:668:HOH:O	2.17	0.44
1:D:243:ILE:HG21	1:D:337:SER:HB2	2.00	0.44
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.32	0.43
1:D:455:SER:HA	1:D:460:PHE:CG	2.53	0.43
1:C:323:PHE:CE1	1:C:328:LEU:HD12	2.54	0.43
1:B:134:TYR:OH	1:B:168[A]:SER:HB3	2.18	0.43
1:C:148:GLN:OE1	1:C:166:ARG:NH2	2.51	0.43
1:D:275:ILE:HD12	1:D:281:PRO:HB3	2.01	0.43
1:D:298:GLU:OE1	5:D:505:BTB:H51	2.19	0.43
1:B:387:THR:HA	1:B:394:TRP:CD1	2.54	0.43
1:A:239:GLY:O	10:A:603:HOH:O	2.21	0.43
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.34	0.43
1:D:285:ARG:HD3	10:D:698:HOH:O	2.18	0.43
1:D:301:GLU:HB3	1:D:303:PHE:HE1	1.83	0.43
1:A:88:ALA:O	1:B:97:ARG:NH2	2.52	0.43
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.58	0.43
1:C:385:LEU:HD13	1:C:394:TRP:HA	2.00	0.43
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.87	0.43
1:B:97:ARG:HH11	1:B:97:ARG:HB3	1.84	0.42
1:B:242:ARG:CZ	1:B:479:PRO:HG3	2.49	0.42
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.54	0.42
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.53	0.42
1:A:202:ARG:NH1	1:A:202:ARG:HB2	2.34	0.42
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.55	0.42
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.22	0.42
1:C:156:GLU:OE2	1:C:164:GLN:N	2.51	0.42
1:D:251:TYR:CE1	1:D:286:PHE:HB3	2.54	0.42
1:D:75:GLU:OE2	10:D:602:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ARG:HB2	1:C:255:ARG:NH1	2.35	0.42
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.55	0.42
1:A:364:THR:O	1:A:368:CYS:HB2	2.19	0.42
1:C:146:HIS:O	1:C:150:LEU:HG	2.20	0.42
1:C:342:GLU:HA	1:C:346:LEU:O	2.20	0.42
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.54	0.42
1:B:84:LEU:HB2	1:B:438:ARG:O	2.20	0.42
1:C:450:PRO:HG3	1:C:457:THR:HG21	2.02	0.42
1:D:315:LEU:HD12	1:D:328:LEU:HB3	2.02	0.42
1:B:134:TYR:OH	1:B:168[B]:SER:HB2	2.19	0.42
5:D:505:BTB:H52	5:D:505:BTB:HO3	1.85	0.42
1:A:247:GLN:HB2	1:A:250:ARG:HG2	2.01	0.41
1:B:364:THR:O	1:B:368:CYS:HB2	2.19	0.41
5:D:505:BTB:H11	5:D:505:BTB:H72	1.84	0.41
1:A:145:ALA:HA	1:A:148:GLN:HB2	2.02	0.41
1:C:455:SER:OG	1:D:451:PRO:HB2	2.20	0.41
1:A:242:ARG:HG3	1:A:479:PRO:HB3	2.02	0.41
1:D:232:PRO:HD2	1:D:241:PHE:CD1	2.55	0.41
1:A:238:ARG:HH12	1:A:241:PHE:HD1	1.69	0.41
1:C:364:THR:O	1:C:368:CYS:HB2	2.20	0.41
1:D:125:SER:HB2	10:D:629:HOH:O	2.20	0.41
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.83	0.41
1:D:367:LEU:HD23	1:D:367:LEU:HA	1.95	0.41
1:B:379:VAL:HG21	1:B:402:ILE:HD11	2.02	0.41
1:C:188:ILE:HD12	1:C:188:ILE:HA	1.85	0.41
1:A:238:ARG:HG2	1:A:296:PRO:HB3	2.03	0.41
1:B:220:ASN:HB3	1:B:223:ASN:O	2.21	0.41
1:B:238:ARG:HG2	1:B:296:PRO:CB	2.51	0.41
5:D:504:BTB:H32	5:D:504:BTB:H51	1.70	0.41
1:C:255:ARG:HB2	1:C:255:ARG:HH11	1.86	0.41
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.36	0.41
1:C:265:PRO:O	1:C:268:VAL:HG23	2.20	0.40
6:C:507:GOL:H11	10:C:673:HOH:O	2.21	0.40
1:A:247:GLN:HA	1:A:335:ALA:O	2.21	0.40
5:A:506:BTB:H51	5:A:506:BTB:H11	1.60	0.40
1:C:138:ILE:HG13	1:C:140:ARG:HB2	2.03	0.40
1:C:360:THR:O	1:C:364:THR:HB	2.20	0.40
1:A:103:LEU:HD12	1:B:463:GLU:HB3	2.04	0.40
1:A:185:VAL:HG22	1:A:185:VAL:O	2.21	0.40
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.91	0.40
1:B:147:GLU:H	1:B:147:GLU:HG2	1.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.93	0.40
1:B:383:MET:HE2	1:B:385:LEU:HD11	2.04	0.40
1:D:212:CYS:HA	1:D:309:LEU:HD21	2.03	0.40
1:A:479:PRO:HD2	1:A:480:TRP:CZ3	2.56	0.40
5:A:506:BTB:H41	5:A:506:BTB:H72	1.72	0.40
1:D:445:TRP:CZ2	1:D:449:VAL:HG21	2.56	0.40
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.56	0.40
1:C:170:LEU:HD11	1:C:230:VAL:HG21	2.04	0.40
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.57	0.40
1:C:275:ILE:HD11	1:C:281:PRO:HB3	2.03	0.40
1:D:279:TRP:HB2	1:D:302:LEU:HD21	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:OE2	5:D:505:BTB:O4[2_851]	1.94	0.26

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%)	366 (92%)	29 (7%)	3 (1%)	16 13
1	B	399/440 (91%)	377 (94%)	22 (6%)	0	100 100
1	C	399/440 (91%)	378 (95%)	17 (4%)	4 (1%)	13 9
1	D	399/440 (91%)	389 (98%)	9 (2%)	1 (0%)	37 37
All	All	1595/1760 (91%)	1510 (95%)	77 (5%)	8 (0%)	25 23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	277	HIS
1	C	89	GLN
1	A	203	SER
1	A	257	GLN
1	C	276	GLN
1	D	89	GLN
1	A	233	GLN
1	C	454	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%)	322 (94%)	20 (6%)	17	15
1	B	342/373 (92%)	327 (96%)	15 (4%)	24	24
1	C	342/373 (92%)	326 (95%)	16 (5%)	22	22
1	D	342/373 (92%)	327 (96%)	15 (4%)	24	24
All	All	1368/1492 (92%)	1302 (95%)	66 (5%)	21	21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	87	GLN
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	125	SER
1	A	128	ARG
1	A	202	ARG
1	A	206	GLU
1	A	209	THR
1	A	216	LYS
1	A	238	ARG
1	A	260	SER
1	A	272	GLU

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Mol	Chain	Res	Type
1	A	276	GLN
1	A	285	ARG
1	A	309	LEU
1	A	321	GLU
1	A	470	SER
1	A	474	ARG
1	B	71	VAL
1	B	87	GLN
1	B	122	GLN
1	B	128	ARG
1	B	136	SER
1	B	139	LYS
1	B	144	GLN
1	B	147	GLU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	176	GLN
1	B	257	GLN
1	B	378	ASP
1	B	389	THR
1	B	396	ASP
1	C	98	ARG
1	C	121	GLU
1	C	125	SER
1	C	128	ARG
1	C	140	ARG
1	C	170	LEU
1	C	200	ASP
1	C	233	GLN
1	C	240	ASP
1	C	255	ARG
1	C	258	ASP
1	C	280	THR
1	C	294	GLN
1	C	308	GLU
1	C	309	LEU
1	C	391	SER
1	D	98	ARG
1	D	99	CYS
1	D	102	SER
1	D	107	ARG
1	D	124	LEU

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Mol	Chain	Res	Type
1	D	125	SER
1	D	136	SER
1	D	192	LYS
1	D	200	ASP
1	D	207	MET
1	D	257	GLN
1	D	302	LEU
1	D	326	LEU
1	D	396	ASP
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 10 are monoatomic - leaving 33 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	$\#\|Z\|>2$
4	KMI	A	503	-	18,18,18	0.40	0	23,24,24	1.66	3 (13%)
3	H4B	B	502	-	16,18,18	0.86	0	14,26,26	2.57	6 (42%)
4	KMI	B	503	-	18,18,18	0.65	1 (5%)	23,24,24	1.18	3 (13%)
5	BTB	D	505	-	13,13,13	0.68	0	7,16,16	1.08	0
6	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.41	0
3	H4B	A	502	-	16,18,18	0.94	0	14,26,26	2.44	6 (42%)
4	KMI	D	503	-	18,18,18	0.57	0	23,24,24	1.42	4 (17%)
5	BTB	B	505	-	13,13,13	0.58	0	7,16,16	1.22	1 (14%)
6	GOL	C	508	-	5,5,5	0.79	0	5,5,5	1.93	2 (40%)
3	H4B	D	502	-	16,18,18	0.72	0	14,26,26	2.41	4 (28%)
6	GOL	C	510	-	5,5,5	0.35	0	5,5,5	0.26	0
6	GOL	A	509	-	5,5,5	0.41	0	5,5,5	0.34	0
5	BTB	C	504	8	13,13,13	0.51	0	7,16,16	1.36	1 (14%)
2	HEM	B	501	1	42,50,50	1.52	6 (14%)	46,82,82	1.93	16 (34%)
5	BTB	C	505	-	13,13,13	0.65	0	7,16,16	1.04	1 (14%)
6	GOL	B	507	-	5,5,5	0.36	0	5,5,5	0.36	0
2	HEM	D	501	1	42,50,50	1.59	7 (16%)	46,82,82	1.79	12 (26%)
6	GOL	C	507	-	5,5,5	0.42	0	5,5,5	0.18	0
2	HEM	C	501	1	42,50,50	1.53	8 (19%)	46,82,82	1.77	9 (19%)
6	GOL	D	507	-	5,5,5	0.37	0	5,5,5	0.34	0
2	HEM	A	501	1	42,50,50	1.56	5 (11%)	46,82,82	1.55	9 (19%)
6	GOL	A	508	-	5,5,5	0.62	0	5,5,5	1.27	1 (20%)
5	BTB	A	505	-	13,13,13	0.79	1 (7%)	7,16,16	1.33	1 (14%)
5	BTB	D	504	8	13,13,13	0.56	0	7,16,16	0.74	0
4	KMI	C	503	-	18,18,18	0.50	0	23,24,24	1.88	4 (17%)
6	GOL	D	506	-	5,5,5	0.48	0	5,5,5	0.46	0
5	BTB	B	504	8	13,13,13	0.44	0	7,16,16	0.60	0
5	BTB	A	504	8	13,13,13	0.35	0	7,16,16	0.78	0
6	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.48	0
6	GOL	C	509	-	5,5,5	0.37	0	5,5,5	0.29	0
5	BTB	A	506	-	13,13,13	0.43	0	7,16,16	0.65	0
5	BTB	C	506	-	13,13,13	0.44	0	7,16,16	0.45	0
3	H4B	C	502	-	16,18,18	0.88	0	14,26,26	2.52	5 (35%)

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
4	KMI	A	503	-	-	0/7/7/7	0/2/2/2
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	KMI	B	503	-	-	1/7/7/7	0/2/2/2
5	BTB	D	505	-	-	6/21/21/21	-
6	GOL	B	506	-	-	2/4/4/4	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
4	KMI	D	503	-	-	5/7/7/7	0/2/2/2
5	BTB	B	505	-	-	11/21/21/21	-
6	GOL	C	508	-	-	4/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	510	-	-	0/4/4/4	-
6	GOL	A	509	-	-	2/4/4/4	-
5	BTB	C	504	8	-	7/21/21/21	-
2	HEM	B	501	1	-	2/12/54/54	-
5	BTB	C	505	-	-	11/21/21/21	-
6	GOL	B	507	-	-	2/4/4/4	-
2	HEM	D	501	1	-	0/12/54/54	-
6	GOL	C	507	-	-	4/4/4/4	-
2	HEM	C	501	1	-	2/12/54/54	-
6	GOL	D	507	-	-	2/4/4/4	-
2	HEM	A	501	1	-	3/12/54/54	-
6	GOL	A	508	-	-	4/4/4/4	-
5	BTB	A	505	-	-	13/21/21/21	-
5	BTB	D	504	8	-	7/21/21/21	-
4	KMI	C	503	-	-	0/7/7/7	0/2/2/2
6	GOL	D	506	-	-	3/4/4/4	-
5	BTB	B	504	8	-	3/21/21/21	-
5	BTB	A	504	8	-	8/21/21/21	-
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	C	509	-	-	2/4/4/4	-
5	BTB	A	506	-	-	3/21/21/21	-
5	BTB	C	506	-	-	15/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-4.50	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-4.30	1.34	1.40
2	B	501	HEM	C3C-C4C	4.24	1.47	1.41
2	D	501	HEM	C3C-C4C	3.73	1.46	1.41
2	C	501	HEM	C3C-C2C	-3.50	1.35	1.40
2	C	501	HEM	C3C-CAC	3.45	1.55	1.47
2	A	501	HEM	CAB-C3B	3.44	1.56	1.47
2	B	501	HEM	CAB-C3B	3.40	1.56	1.47
2	A	501	HEM	C3C-CAC	3.37	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.26	1.36	1.40
2	B	501	HEM	C3C-CAC	3.19	1.54	1.47
2	D	501	HEM	C3C-CAC	3.13	1.54	1.47
2	C	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	C3C-C4C	2.98	1.45	1.41
2	D	501	HEM	CAB-C3B	2.97	1.55	1.47
2	A	501	HEM	FE-NB	2.80	2.13	1.98
2	B	501	HEM	FE-ND	2.76	2.13	1.98
5	A	505	BTB	C3-C2	-2.57	1.50	1.53
2	A	501	HEM	C3C-C4C	2.56	1.45	1.41
2	D	501	HEM	CMD-C2D	2.50	1.55	1.50
2	D	501	HEM	FE-NB	2.38	2.11	1.98
2	C	501	HEM	CMB-C2B	2.11	1.55	1.50
2	B	501	HEM	CMB-C2B	2.09	1.55	1.50
2	C	501	HEM	CHA-C4D	2.09	1.39	1.34
4	B	503	KMI	C17-N18	2.08	1.49	1.46
2	C	501	HEM	FE-NB	2.05	2.09	1.98
2	C	501	HEM	CMD-C2D	2.03	1.54	1.50
2	D	501	HEM	FE-ND	2.02	2.09	1.98

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	KMI	C06-N01-C02	6.83	122.76	118.52
4	A	503	KMI	C06-N01-C02	6.14	122.33	118.52
3	C	502	H4B	C8A-C4A-C4	5.94	119.90	114.50
3	D	502	H4B	C8A-C4A-C4	5.83	119.81	114.50
3	A	502	H4B	C8A-C4A-C4	5.80	119.78	114.50
3	B	502	H4B	C8A-C4A-C4	5.70	119.68	114.50
2	C	501	HEM	C4B-CHC-C1C	4.55	128.57	122.56
2	B	501	HEM	C4B-CHC-C1C	4.29	128.22	122.56
3	D	502	H4B	C2-N3-C4	3.96	121.46	115.96
2	C	501	HEM	C3B-C4B-NB	-3.84	106.71	109.47
2	A	501	HEM	C3B-C2B-C1B	3.79	109.25	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	CBA-CAA-C2A	-3.70	106.31	112.54
2	D	501	HEM	C3B-C2B-C1B	3.70	109.19	106.41
2	C	501	HEM	CBA-CAA-C2A	-3.54	106.58	112.54
2	A	501	HEM	C4B-CHC-C1C	3.51	127.19	122.56
3	B	502	H4B	C11-C10-C9	-3.50	107.82	112.11
2	D	501	HEM	CMA-C3A-C4A	-3.49	123.35	128.46
2	B	501	HEM	C3B-C4B-NB	-3.48	106.97	109.47
3	B	502	H4B	N1-C2-N3	-3.46	120.17	125.48
6	C	508	GOL	O1-C1-C2	-3.42	94.97	110.38
2	C	501	HEM	C1B-NB-C4B	3.41	109.25	105.21
3	A	502	H4B	N1-C2-N3	-3.41	120.26	125.48
3	D	502	H4B	N1-C2-N3	-3.40	120.27	125.48
3	C	502	H4B	C2-N3-C4	3.39	120.68	115.96
2	B	501	HEM	C1B-NB-C4B	3.34	109.17	105.21
2	B	501	HEM	C4D-ND-C1D	3.34	109.16	105.21
3	C	502	H4B	N1-C2-N3	-3.30	120.42	125.48
3	A	502	H4B	C2-N3-C4	3.27	120.51	115.96
3	B	502	H4B	C2-N3-C4	3.24	120.47	115.96
3	C	502	H4B	C11-C10-C9	-3.24	108.15	112.11
2	D	501	HEM	CMC-C2C-C3C	3.16	131.00	124.68
4	D	503	KMI	C06-N01-C02	3.11	120.45	118.52
2	B	501	HEM	CHD-C1D-ND	3.11	127.78	124.44
4	C	503	KMI	N02-C02-N01	2.99	121.40	116.59
3	B	502	H4B	C2-N1-C8A	2.95	121.60	114.59
2	C	501	HEM	C3D-C4D-ND	-2.95	106.94	110.17
4	D	503	KMI	C11-C06-N01	2.91	120.25	116.04
5	A	505	BTB	O3-C3-C2	-2.85	104.69	111.40
2	C	501	HEM	C4D-ND-C1D	2.85	108.59	105.21
2	B	501	HEM	C3D-C4D-ND	-2.83	107.07	110.17
2	B	501	HEM	CAD-CBD-CGD	-2.78	106.30	113.67
2	D	501	HEM	C4C-CHD-C1D	2.75	126.19	122.56
2	B	501	HEM	C2D-C1D-ND	-2.75	106.72	109.90
2	A	501	HEM	C4C-CHD-C1D	2.72	126.14	122.56
2	D	501	HEM	C3D-C4D-ND	-2.71	107.19	110.17
2	B	501	HEM	C3B-C2B-C1B	2.60	108.36	106.41
5	C	504	BTB	O4-C4-C2	2.60	117.51	111.40
3	A	502	H4B	C2-N1-C8A	2.60	120.76	114.59
2	C	501	HEM	C3B-C2B-C1B	2.59	108.36	106.41
2	D	501	HEM	C4D-ND-C1D	2.58	108.26	105.21
2	A	501	HEM	C4A-C3A-C2A	2.57	108.78	107.00
2	A	501	HEM	C1B-NB-C4B	2.56	108.24	105.21
3	C	502	H4B	C2-N1-C8A	2.55	120.65	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CBD-CAD-C3D	-2.52	105.56	112.53
2	D	501	HEM	C1B-NB-C4B	2.47	108.13	105.21
4	C	503	KMI	C05-C06-N01	-2.44	119.51	122.34
3	A	502	H4B	C11-C10-C9	-2.41	109.16	112.11
2	A	501	HEM	CMA-C3A-C4A	-2.40	124.94	128.46
3	D	502	H4B	C2-N1-C8A	2.37	120.21	114.59
4	B	503	KMI	C06-N01-C02	2.36	119.99	118.52
4	B	503	KMI	C11-C06-N01	2.34	119.43	116.04
2	B	501	HEM	C1D-C2D-C3D	2.34	109.44	106.98
4	C	503	KMI	C11-C06-N01	2.33	119.40	116.04
4	B	503	KMI	C15-C17-N18	-2.31	107.11	112.67
2	A	501	HEM	CBA-CAA-C2A	-2.31	108.66	112.54
4	A	503	KMI	C05-C06-N01	-2.29	119.69	122.34
3	B	502	H4B	N2-C2-N3	2.28	120.64	117.22
2	C	501	HEM	C2B-C1B-NB	-2.25	107.25	109.84
2	B	501	HEM	C2B-C1B-NB	-2.24	107.26	109.84
2	B	501	HEM	C4A-C3A-C2A	2.24	108.56	107.00
6	C	508	GOL	O2-C2-C1	-2.23	99.95	109.18
2	B	501	HEM	O1D-CGD-CBD	-2.22	116.04	123.09
2	B	501	HEM	CMA-C3A-C4A	-2.21	125.21	128.46
2	C	501	HEM	CHC-C4B-C3B	2.20	127.94	124.57
2	B	501	HEM	CMC-C2C-C3C	2.20	129.07	124.68
2	D	501	HEM	C4A-C3A-C2A	2.19	108.52	107.00
2	A	501	HEM	C3B-C4B-NB	-2.18	107.90	109.47
2	D	501	HEM	C2B-C1B-NB	-2.15	107.37	109.84
2	D	501	HEM	C4B-CHC-C1C	2.15	125.39	122.56
4	D	503	KMI	C05-C06-C11	-2.10	118.97	121.82
6	A	508	GOL	O2-C2-C3	-2.09	100.54	109.18
3	A	502	H4B	N2-C2-N3	2.08	120.35	117.22
2	B	501	HEM	CBD-CAD-C3D	-2.05	106.86	112.53
4	A	503	KMI	C11-C06-N01	2.04	118.99	116.04
4	D	503	KMI	C15-C17-N18	-2.04	107.77	112.67
2	D	501	HEM	CAD-C3D-C2D	-2.03	124.07	127.87
5	C	505	BTB	C6-C5-N	-2.03	103.67	111.59
5	B	505	BTB	O3-C3-C2	-2.02	106.64	111.40

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	KMI	C15-C17-N18-C19
4	D	503	KMI	C15-C17-N18-C19

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	A	506	BTB	O1-C1-C2-N
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	O1-C1-C2-C4
5	C	504	BTB	C1-C2-C3-O3
5	C	504	BTB	C3-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	C	505	BTB	C8-C7-N-C5
5	C	506	BTB	O1-C1-C2-C3
5	C	506	BTB	O1-C1-C2-C4
5	C	506	BTB	O1-C1-C2-N
5	C	506	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	506	BTB	C3-C2-C4-O4
5	C	506	BTB	N-C2-C4-O4
5	C	506	BTB	C1-C2-N-C5
5	C	506	BTB	C1-C2-N-C7
5	C	506	BTB	C3-C2-N-C5
5	C	506	BTB	C3-C2-N-C7
5	C	506	BTB	C4-C2-N-C5
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C6-C5-N-C7
6	A	507	GOL	O1-C1-C2-C3
6	A	508	GOL	O1-C1-C2-C3
6	A	509	GOL	O1-C1-C2-O2
6	A	509	GOL	O1-C1-C2-C3
6	B	506	GOL	O1-C1-C2-C3
6	B	507	GOL	O1-C1-C2-O2
6	B	507	GOL	O1-C1-C2-C3
6	C	507	GOL	C1-C2-C3-O3
6	C	508	GOL	O1-C1-C2-C3
6	C	508	GOL	C1-C2-C3-O3
6	C	509	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-C3
6	D	507	GOL	C1-C2-C3-O3
5	D	505	BTB	N-C7-C8-O8
5	B	505	BTB	N-C5-C6-O6
5	C	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
6	D	506	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
6	C	507	GOL	O1-C1-C2-C3
5	A	504	BTB	N-C5-C6-O6
5	C	506	BTB	N-C5-C6-O6
5	C	505	BTB	C3-C2-C4-O4
6	A	507	GOL	O1-C1-C2-O2
6	A	508	GOL	O1-C1-C2-O2
6	C	507	GOL	O2-C2-C3-O3
6	C	508	GOL	O2-C2-C3-O3
6	C	509	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	D	507	GOL	O2-C2-C3-O3
5	B	505	BTB	N-C7-C8-O8
2	B	501	HEM	C2A-CAA-CBA-CGA
6	B	506	GOL	O1-C1-C2-O2
6	C	507	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-O2
3	A	502	H4B	C7-C6-C9-C10
5	C	505	BTB	N-C7-C8-O8
5	D	505	BTB	O1-C1-C2-C3
6	A	508	GOL	O2-C2-C3-O3
5	D	504	BTB	N-C7-C8-O8
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
3	A	502	H4B	C7-C6-C9-O9
5	A	506	BTB	O1-C1-C2-C4
5	B	505	BTB	C4-C2-N-C5
5	C	506	BTB	C4-C2-N-C7
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C3-C2-N-C5
5	C	506	BTB	C1-C2-C4-O4
2	C	501	HEM	CAA-CBA-CGA-O2A
5	C	504	BTB	N-C7-C8-O8
6	A	508	GOL	C1-C2-C3-O3
2	C	501	HEM	CAA-CBA-CGA-O1A
4	D	503	KMI	C05-C06-C11-C16
4	D	503	KMI	N01-C06-C11-C16
6	D	506	GOL	O2-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C3
5	A	506	BTB	C4-C2-C3-O3
5	C	506	BTB	C1-C2-C3-O3
5	A	504	BTB	N-C7-C8-O8
4	D	503	KMI	N01-C06-C11-C12
3	A	502	H4B	N5-C6-C9-O9
4	D	503	KMI	C05-C06-C11-C12
5	A	505	BTB	O1-C1-C2-N
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	N-C2-C3-O3
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	D	504	BTB	C4-C2-N-C5

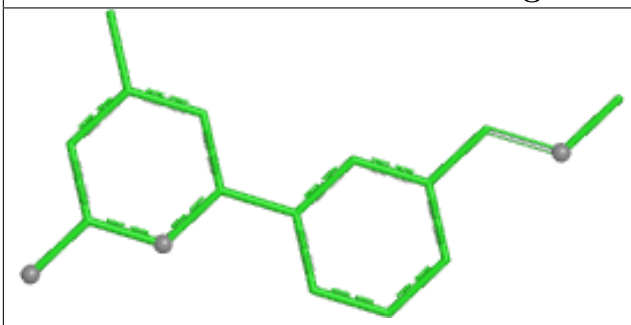
There are no ring outliers.

20 monomers are involved in 43 short contacts:

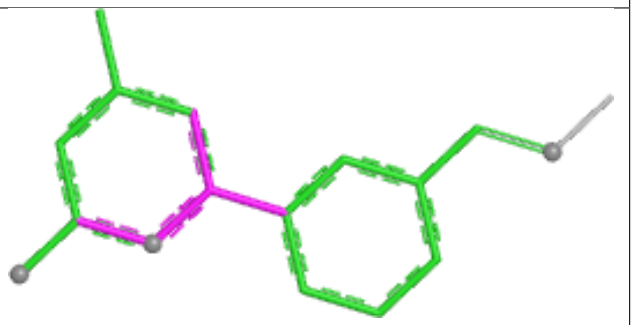
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	KMI	1	0
3	B	502	H4B	1	0
5	D	505	BTB	3	1
3	A	502	H4B	2	0
4	D	503	KMI	1	0
5	B	505	BTB	5	0
3	D	502	H4B	1	0
5	C	504	BTB	5	0
2	B	501	HEM	3	0
2	D	501	HEM	1	0
6	C	507	GOL	1	0
2	C	501	HEM	2	0
2	A	501	HEM	3	0
5	A	505	BTB	2	0
5	D	504	BTB	3	0
4	C	503	KMI	1	0
5	B	504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

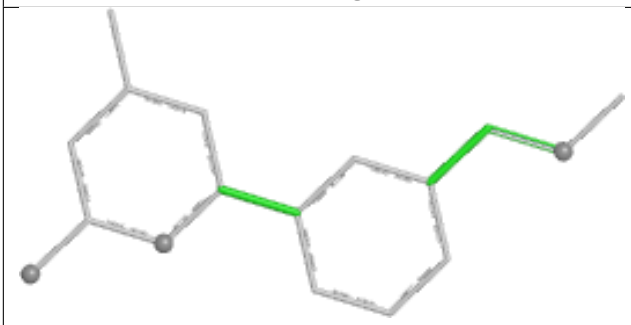
Ligand KMI A 503



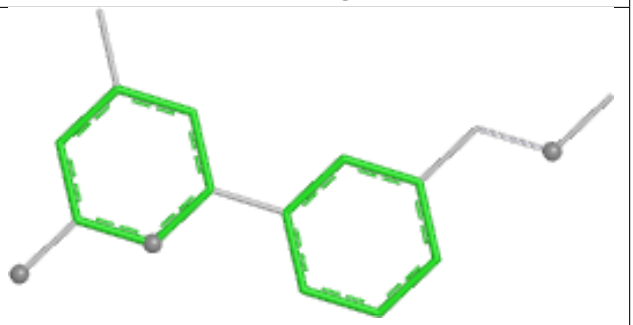
Bond lengths



Bond angles

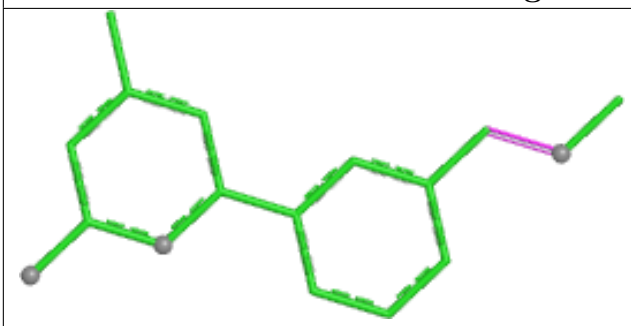


Torsions

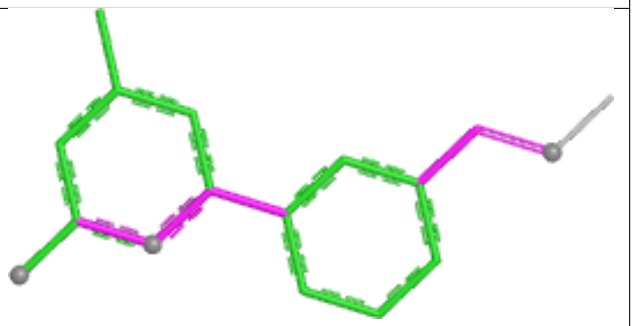


Rings

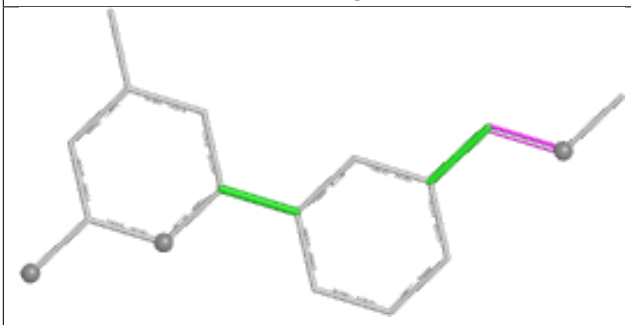
Ligand KMI B 503



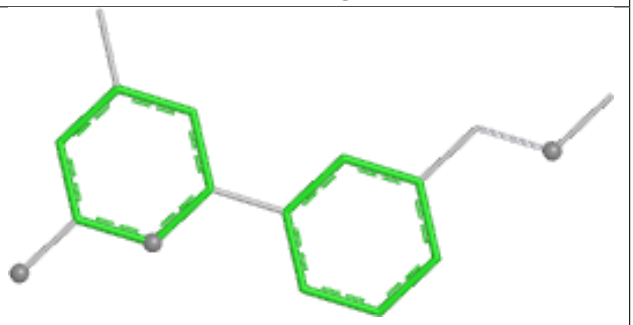
Bond lengths



Bond angles

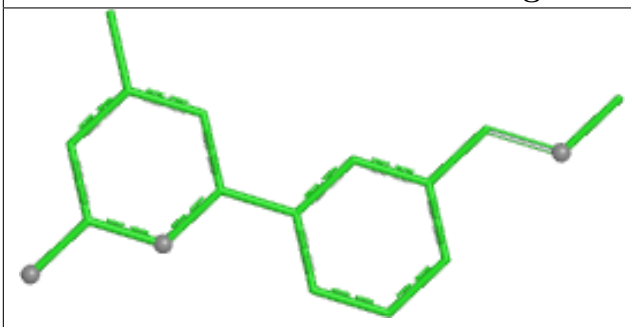


Torsions

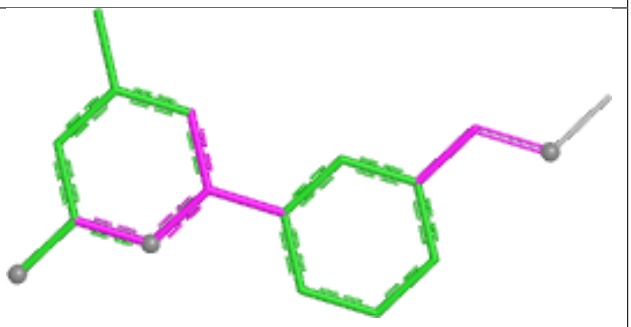


Rings

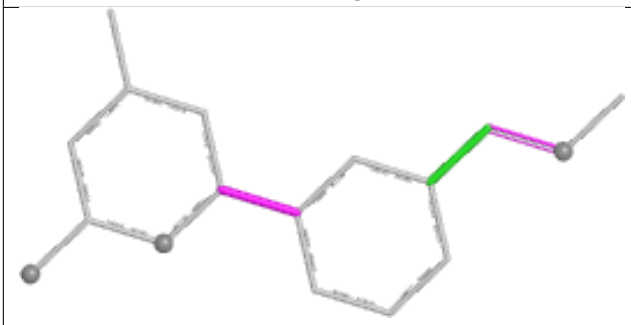
Ligand KMI D 503



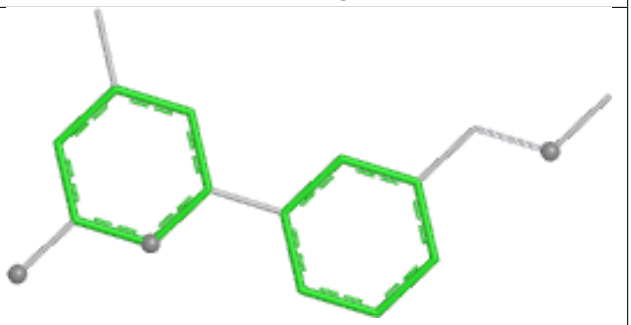
Bond lengths



Bond angles

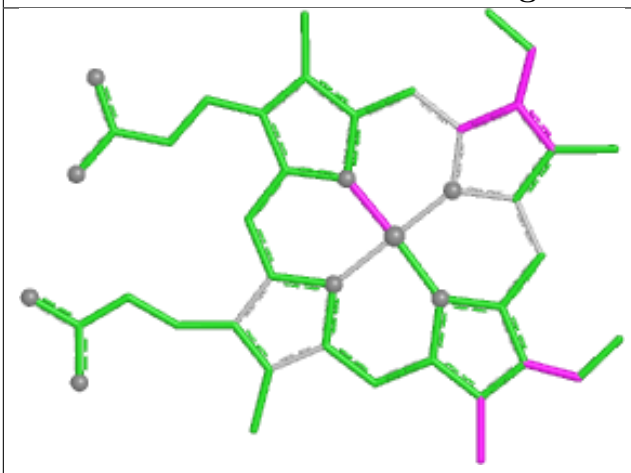


Torsions

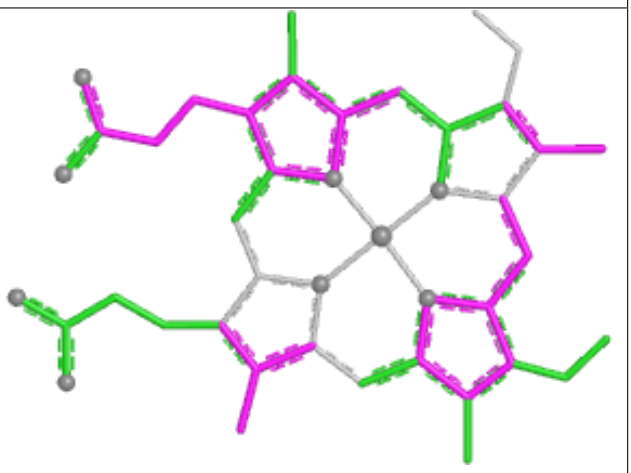


Rings

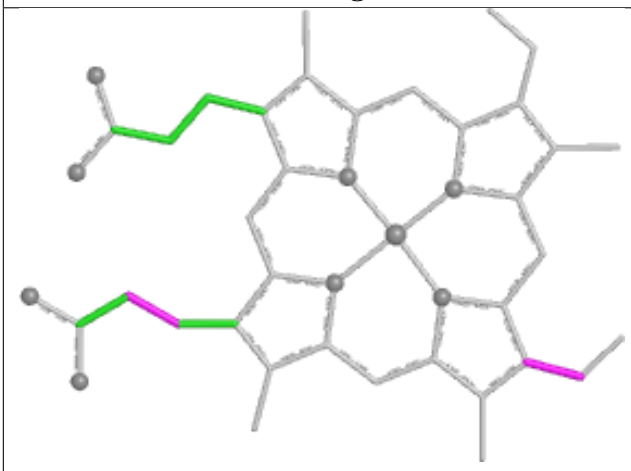
Ligand HEM B 501



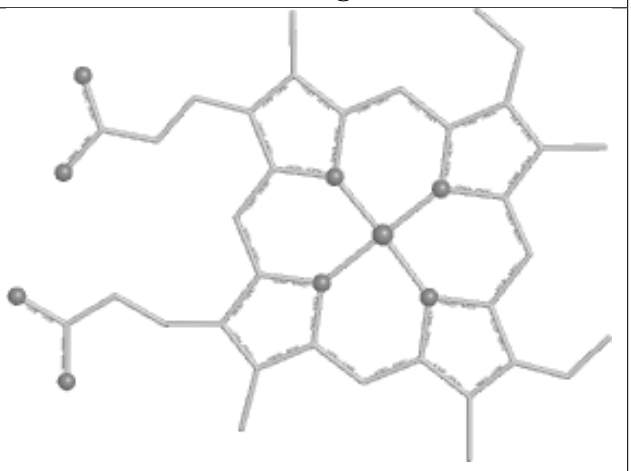
Bond lengths



Bond angles

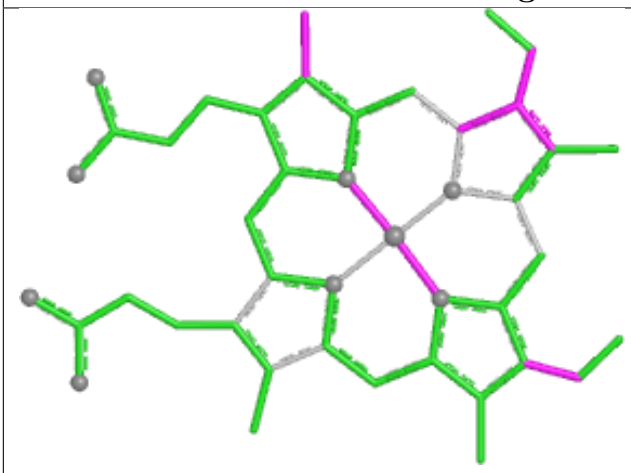


Torsions

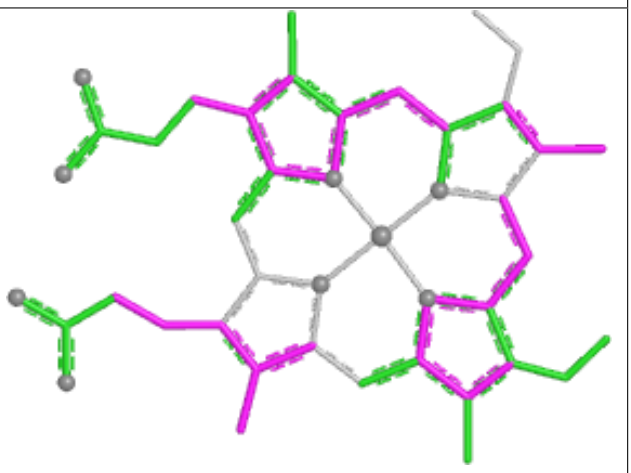


Rings

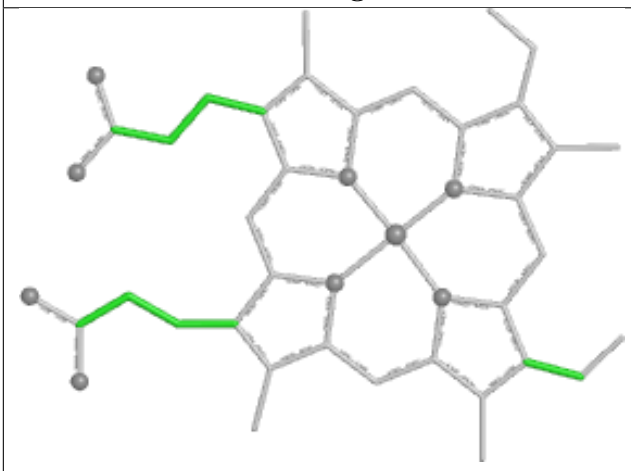
Ligand HEM D 501



Bond lengths



Bond angles



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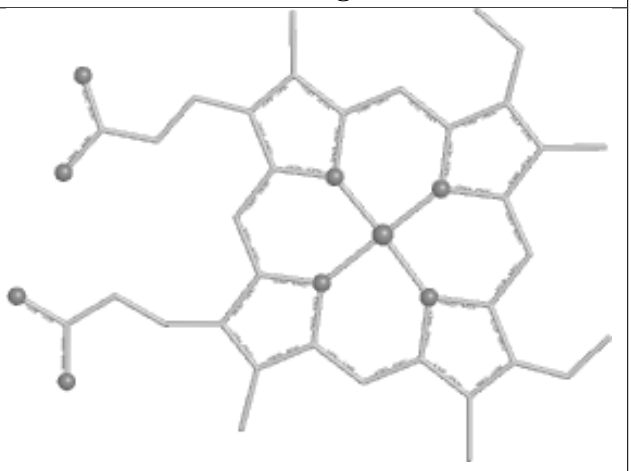
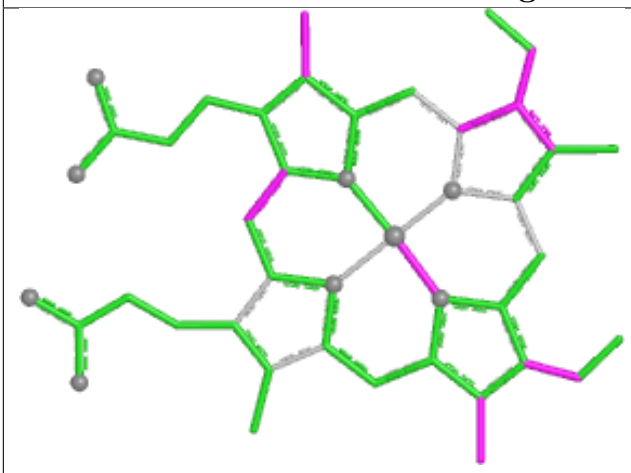


Rings

Ligand HEM C 501



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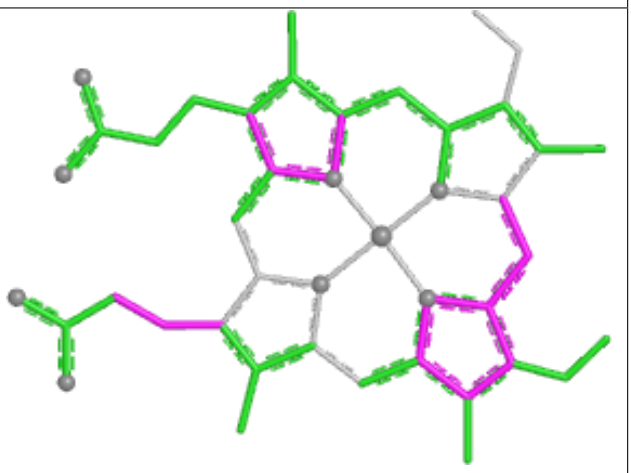
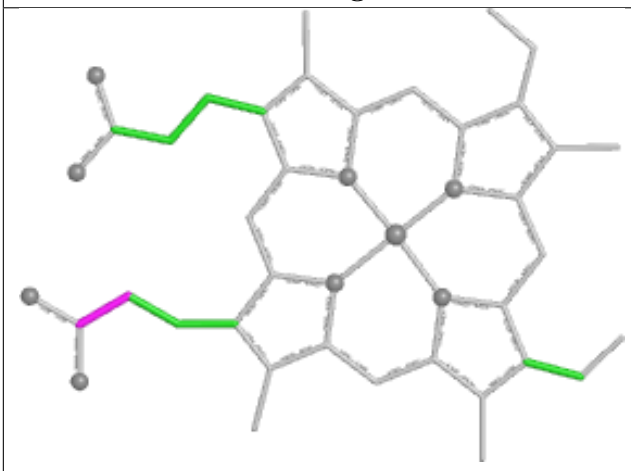
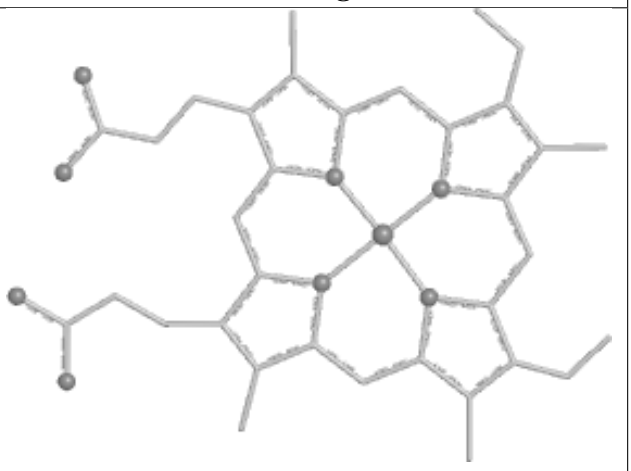


Bond angles

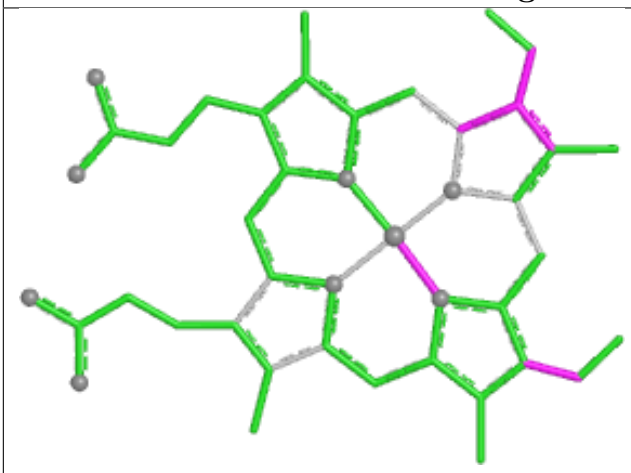


Torsions

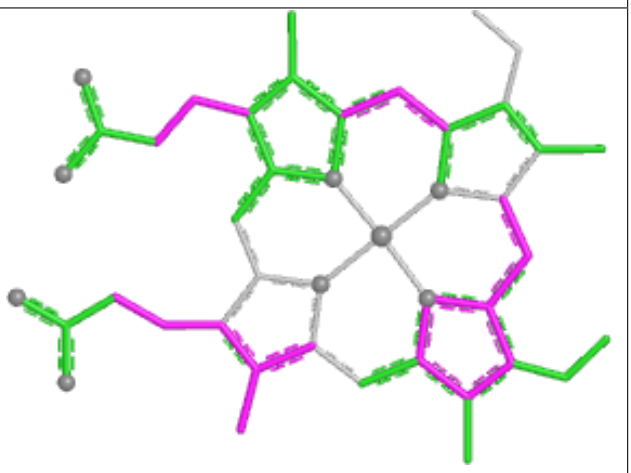


Rings

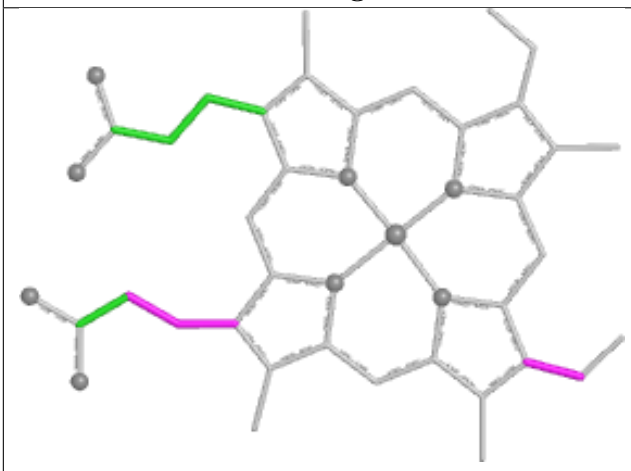
Ligand HEM A 501



Bond lengths



Bond angles



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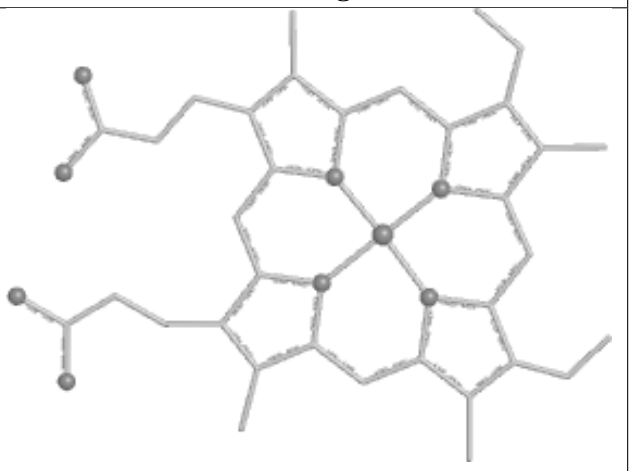
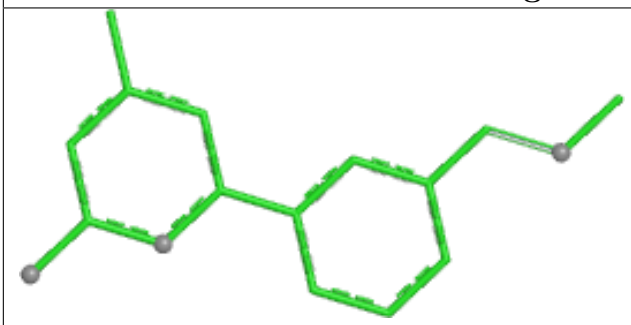
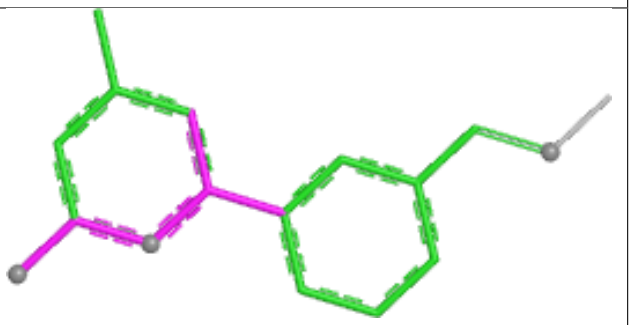


Rings

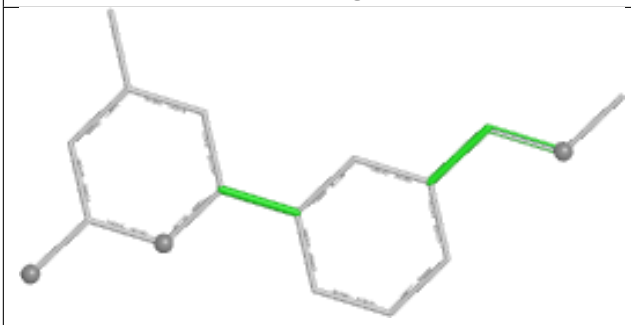
Ligand KMI C 503



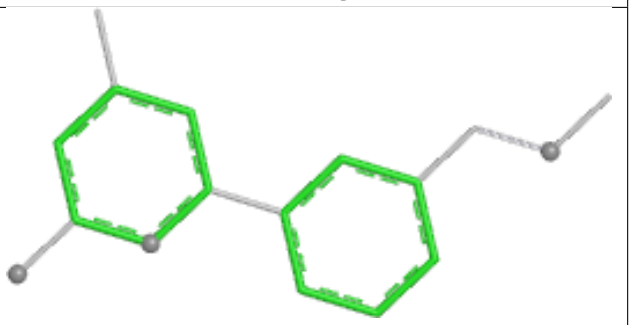
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.92	1 (0%) 92 92	27, 59, 107, 156	1 (0%)
1	B	401/440 (91%)	-1.20	0 100 100	19, 41, 81, 115	2 (0%)
1	C	402/440 (91%)	-1.02	0 100 100	28, 56, 99, 129	1 (0%)
1	D	402/440 (91%)	-1.26	0 100 100	25, 40, 66, 118	1 (0%)
All	All	1606/1760 (91%)	-1.10	1 (0%) 92 93	19, 48, 96, 156	5 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	BTB	C	506	14/14	0.94	0.06	71,83,87,88	0

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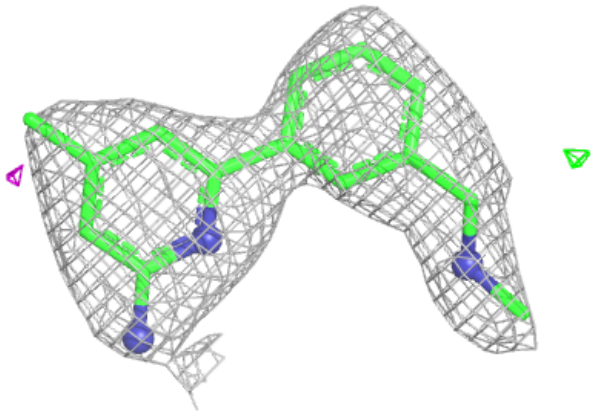
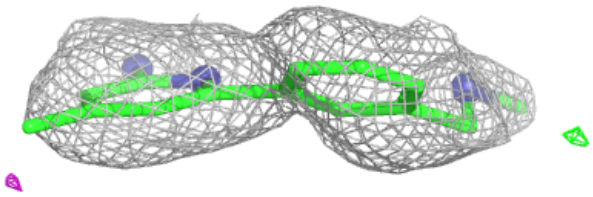
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	D	507	6/6	0.94	0.05	65,71,78,79	0
6	GOL	C	510	6/6	0.96	0.05	60,68,69,72	0
6	GOL	B	507	6/6	0.96	0.05	64,69,73,73	0
6	GOL	D	506	6/6	0.97	0.07	54,67,76,88	0
5	BTB	A	506	14/14	0.97	0.05	73,88,94,95	0
3	H4B	A	502	17/17	0.98	0.06	49,62,76,76	0
5	BTB	B	505	14/14	0.98	0.04	40,69,72,77	0
5	BTB	C	505	14/14	0.98	0.04	25,58,68,72	0
3	H4B	D	502	17/17	0.98	0.05	41,56,66,69	0
5	BTB	D	505	14/14	0.98	0.04	47,65,79,82	0
6	GOL	A	507	6/6	0.98	0.04	57,59,69,70	0
6	GOL	A	509	6/6	0.98	0.06	56,62,63,66	0
6	GOL	B	506	6/6	0.98	0.06	53,61,67,69	0
4	KMI	A	503	17/17	0.98	0.05	35,47,68,72	0
6	GOL	C	507	6/6	0.98	0.03	47,50,56,67	0
6	GOL	C	509	6/6	0.98	0.05	51,53,58,61	0
4	KMI	B	503	17/17	0.98	0.05	22,33,57,57	0
4	KMI	C	503	17/17	0.98	0.06	35,50,76,77	0
5	BTB	A	505	14/14	0.98	0.04	45,64,73,77	0
2	HEM	C	501	43/43	0.99	0.04	26,45,61,73	0
6	GOL	A	508	6/6	0.99	0.03	31,51,68,70	0
2	HEM	A	501	43/43	0.99	0.04	38,57,74,78	0
5	BTB	B	504	14/14	0.99	0.05	20,51,65,66	0
3	H4B	B	502	17/17	0.99	0.04	41,48,59,61	0
5	BTB	C	504	14/14	0.99	0.04	48,62,73,74	0
6	GOL	C	508	6/6	0.99	0.07	25,29,51,56	0
3	H4B	C	502	17/17	0.99	0.05	59,66,70,70	0
4	KMI	D	503	17/17	0.99	0.04	17,32,61,64	0
5	BTB	D	504	14/14	0.99	0.05	38,64,73,78	0
5	BTB	A	504	14/14	0.99	0.04	55,77,92,96	0
7	CL	A	510	1/1	0.99	0.03	46,46,46,46	0
2	HEM	B	501	43/43	1.00	0.03	16,33,50,61	0
2	HEM	D	501	43/43	1.00	0.03	19,35,49,59	0
7	CL	B	508	1/1	1.00	0.01	35,35,35,35	0
7	CL	C	511	1/1	1.00	0.02	44,44,44,44	0
7	CL	D	508	1/1	1.00	0.02	40,40,40,40	0
8	GD3	A	511	1/1	1.00	0.02	138,138,138,138	0
8	GD3	B	509	1/1	1.00	0.01	43,43,43,43	0
8	GD3	C	512	1/1	1.00	0.02	80,80,80,80	1
8	GD3	D	509	1/1	1.00	0.01	48,48,48,48	0
9	ZN	A	512	1/1	1.00	0.02	52,52,52,52	0
9	ZN	C	513	1/1	1.00	0.01	51,51,51,51	0

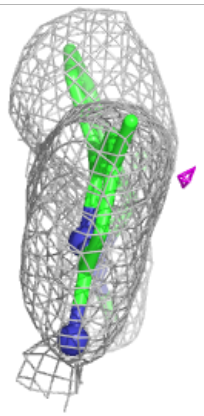
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KMI A 503:

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

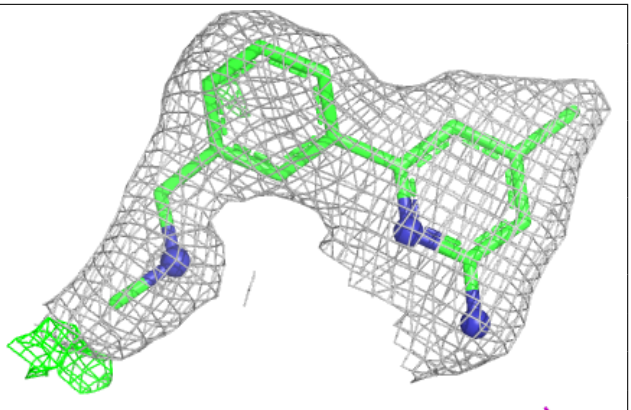


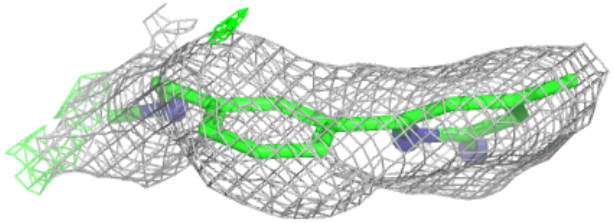


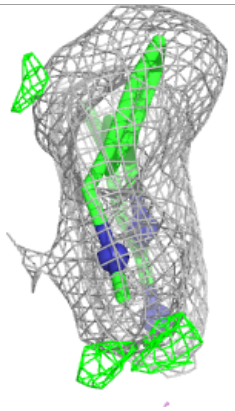


Electron density around KMI B 503:

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

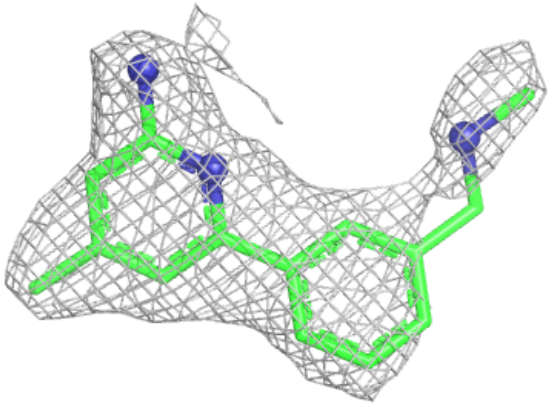


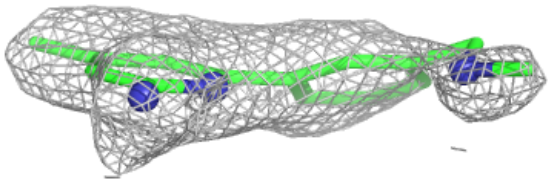


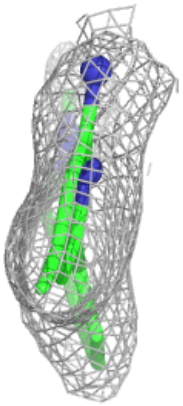


Electron density around KMI C 503:

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

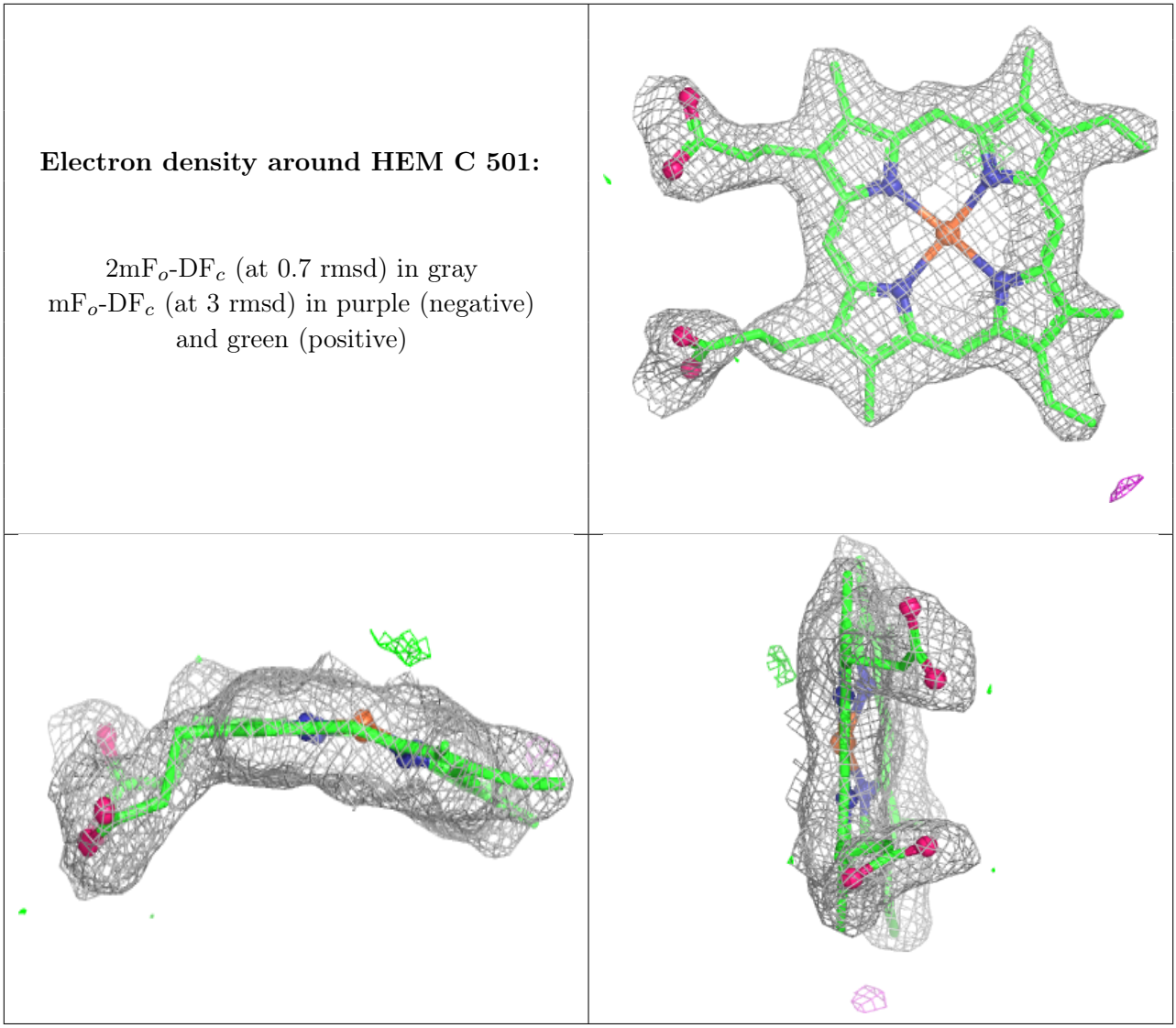






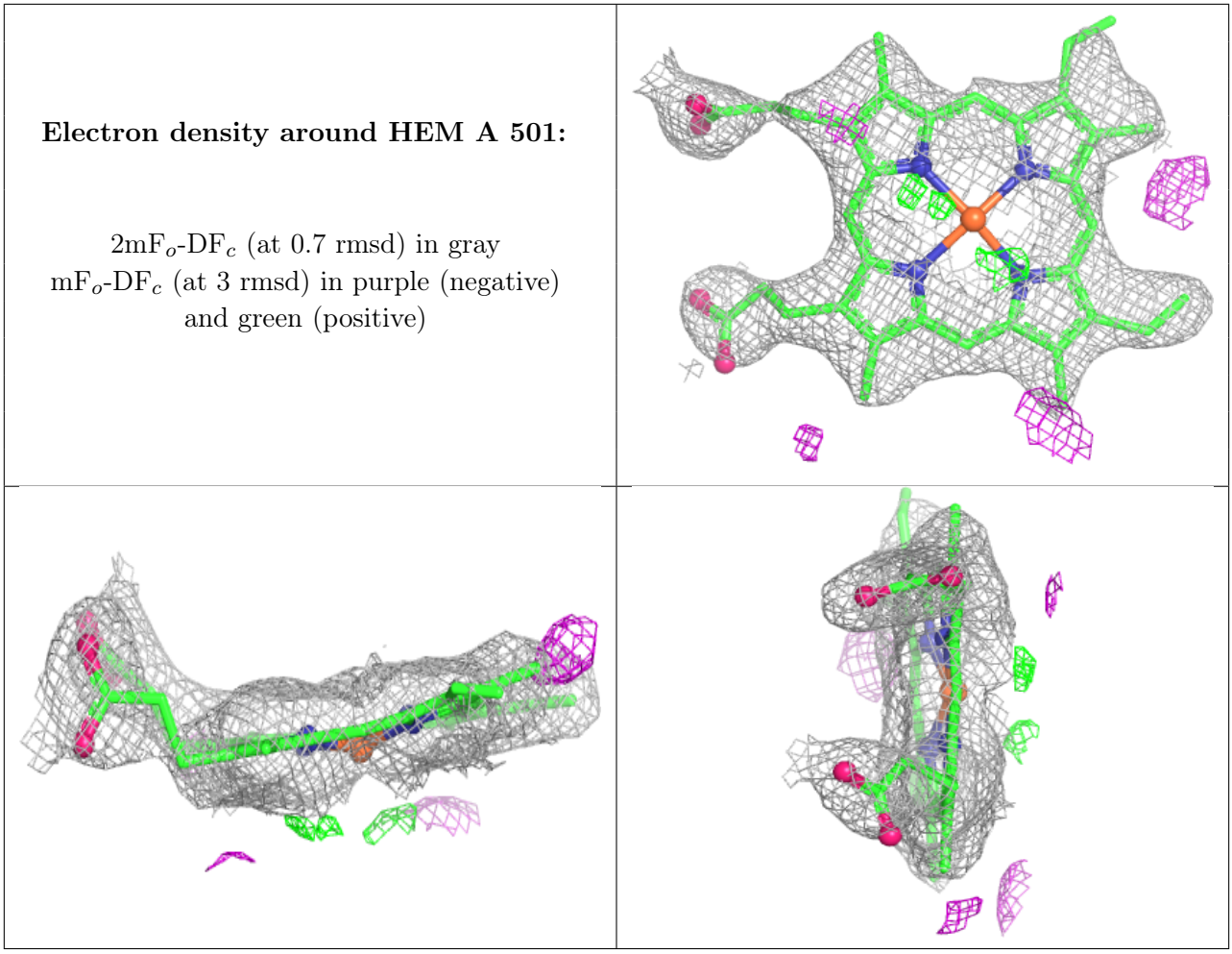
Electron density around HEM C 501:

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



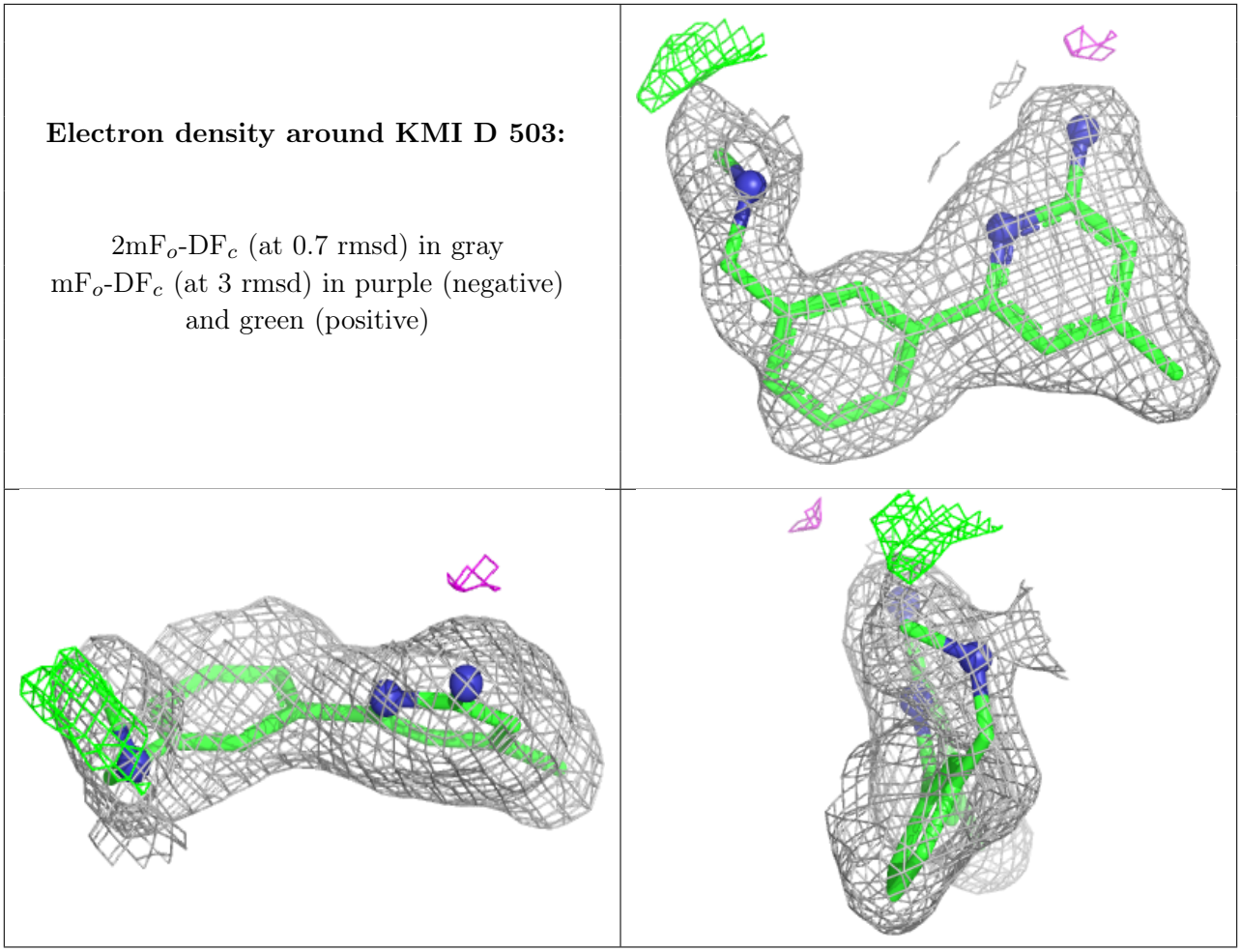
Electron density around HEM A 501:

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



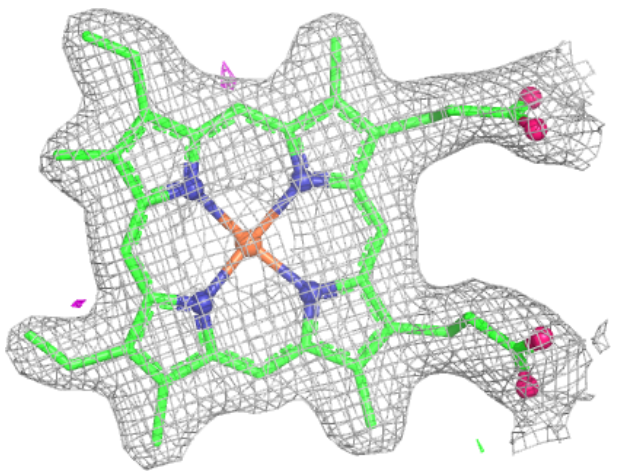
Electron density around KMI D 503:

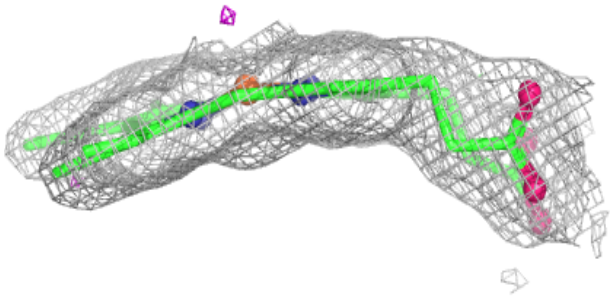
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

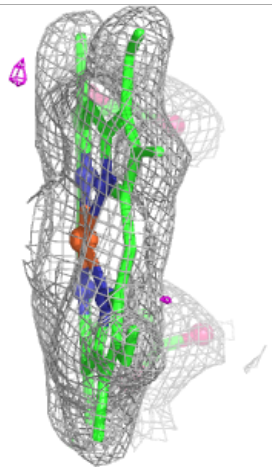


Electron density around HEM B 501:

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

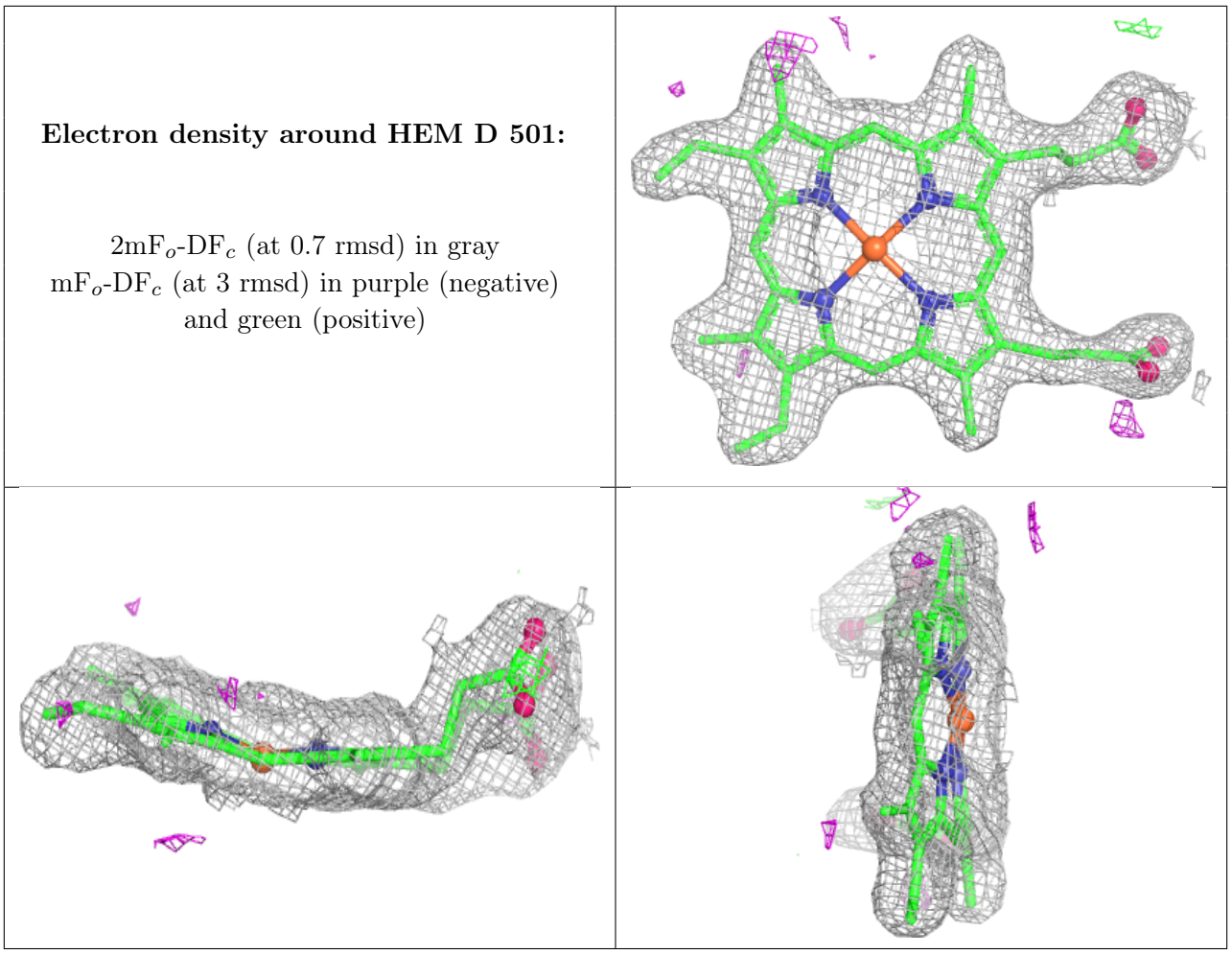






Electron density around HEM D 501:

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



6.5 Other polymers

There are no such residues in this entry.