Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 03:54 PM EDT

PDB ID	:	7TSN
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-(3,3-difluoroazetidin-1-yl)prop-1-yn-1-yl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-01-31
Resolution	:	2.08 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:

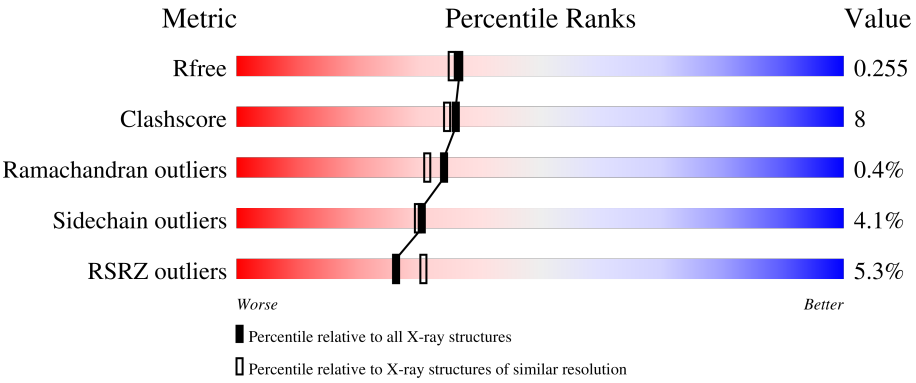
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	11% 70% 19% • 9%
1	B	440	% 75% 15% • 9%
1	C	440	8% 69% 21% • 9%
1	D	440	77% 14% 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13894 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.

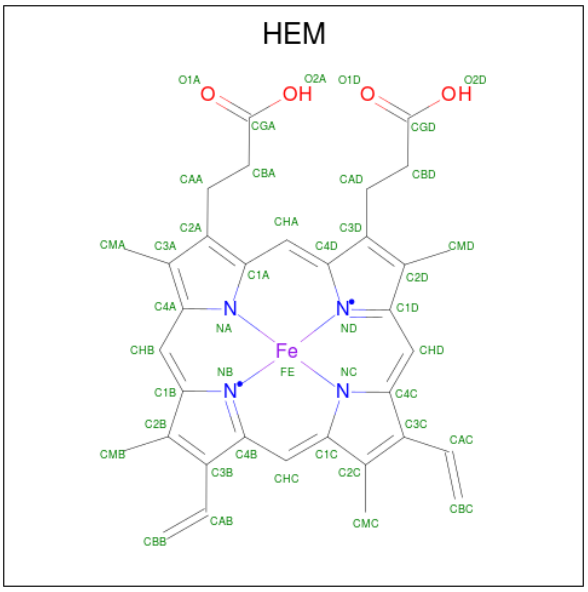
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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	0	0
			3211	2044	567	584	16			

There are 4 discrepancies between the modelled and reference sequences:

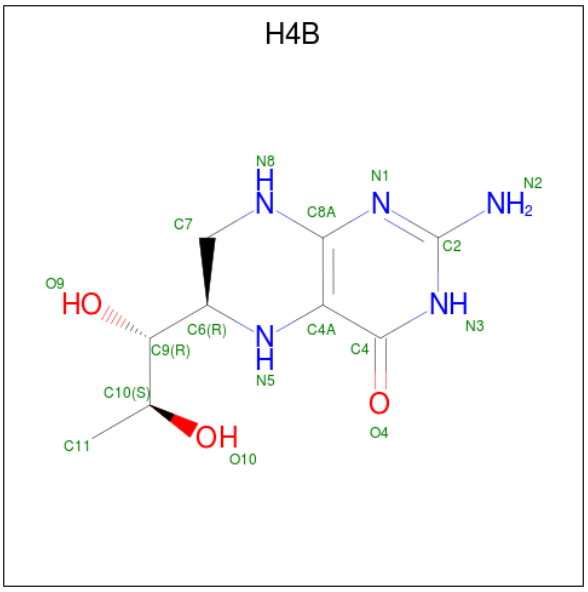
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



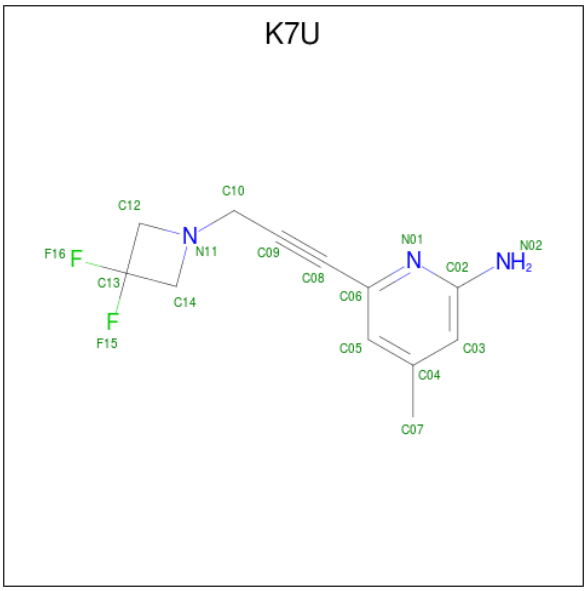
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



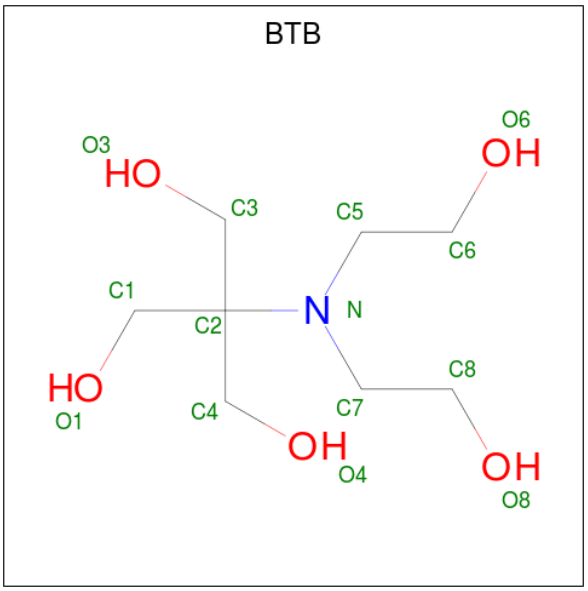
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 6-[3-(3,3-difluoroazetidin-1-yl)prop-1-yn-1-yl]-4-methylpyridin-2-amine (three-letter code: K7U) (formula: $C_{12}H_{13}F_2N_3$) (labeled as "Ligand of Interest" by depositor).



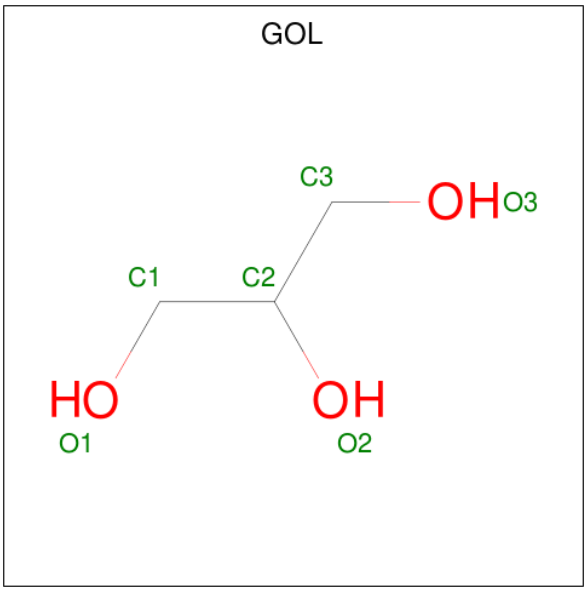
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 17 12 2 3	0	0
4	B	1	Total C F N 17 12 2 3	0	0
4	C	1	Total C F N 17 12 2 3	0	0
4	D	1	Total C F N 17 12 2 3	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: 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 (three-letter code: 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	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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
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 ATOM (three-letter code: GD) (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 (three-letter code: 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.

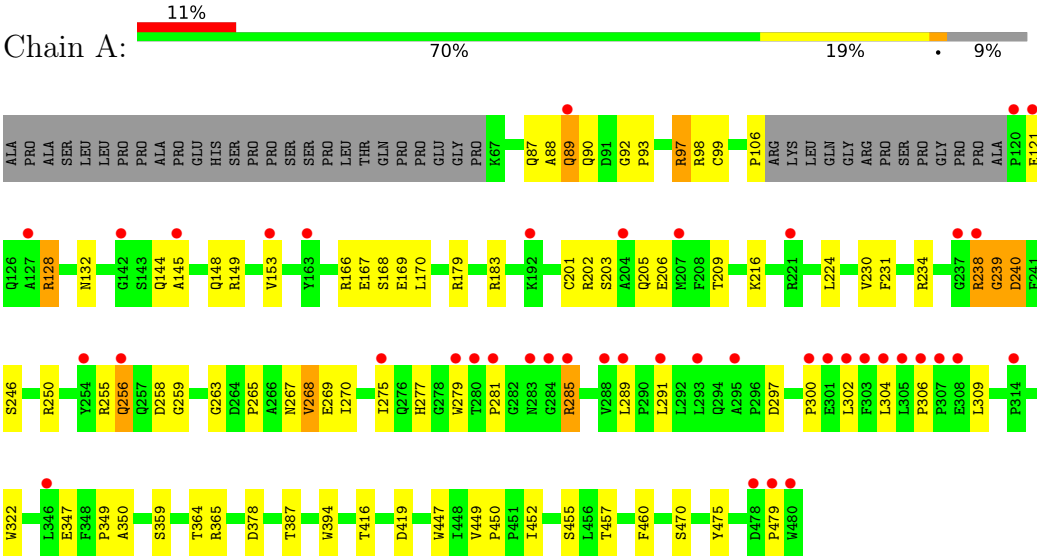
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	84	Total O 84 84	0	0
10	B	166	Total O 166 166	0	0
10	C	116	Total O 116 116	0	0
10	D	181	Total O 181 181	0	0

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.

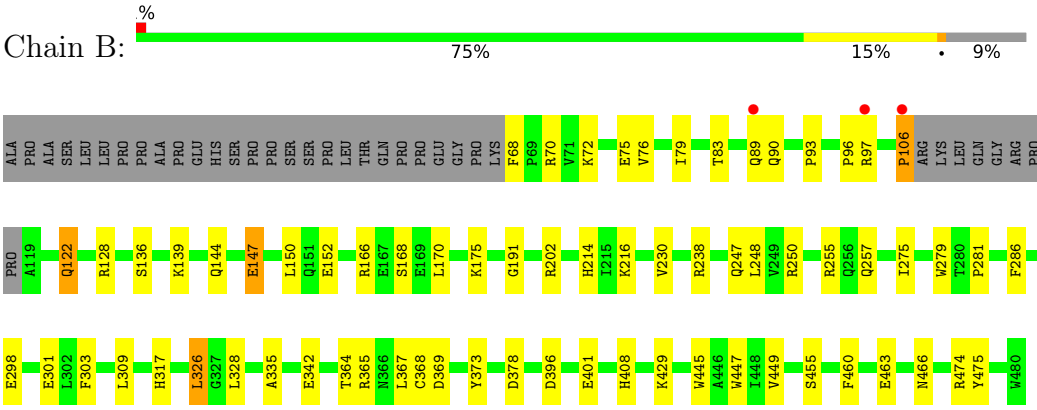
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



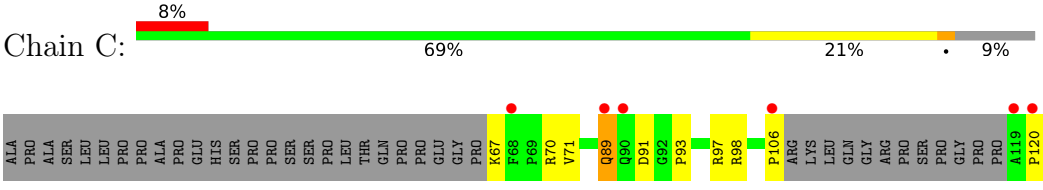
• Molecule 1: Nitric oxide synthase, endothelial

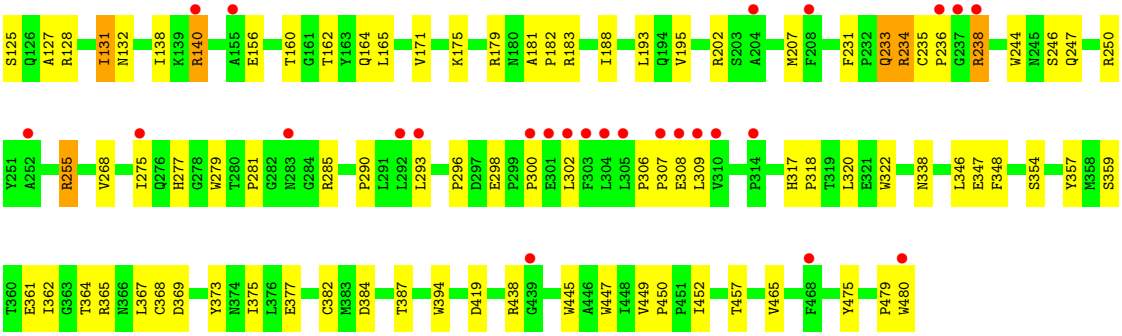
Chain B:



• Molecule 1: Nitric oxide synthase, endothelial

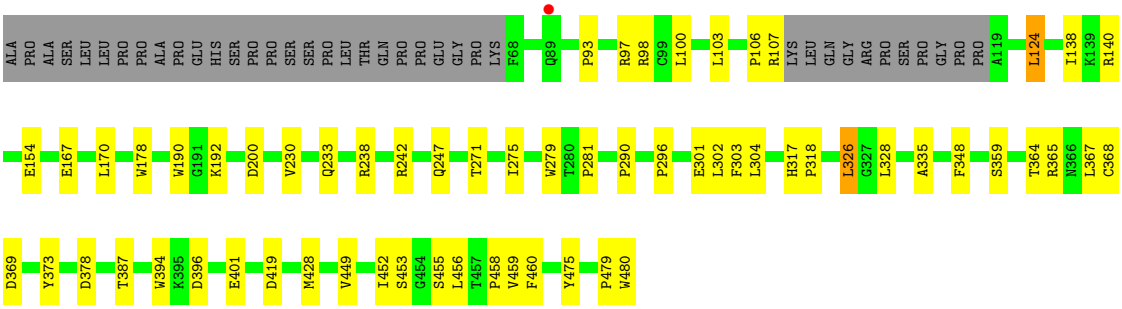
Chain C:





• 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	58.78Å 151.03Å 107.41Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	49.02 – 2.08 49.01 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.02-2.08) 99.4 (49.01-2.08)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.262 0.203 , 0.255	Depositor DCC
R_{free} test set	5582 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.995	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.096 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13894	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ZN, BTB, GD, H4B, HEM, GOL, CL, K7U

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3302	0.51	0/4498
1	B	0.42	0/3312	0.55	0/4514
1	C	0.37	0/3307	0.51	0/4506
1	D	0.43	0/3303	0.57	0/4501
All	All	0.39	0/13224	0.53	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	57	0
1	B	3211	0	3114	44	0
1	C	3212	0	3116	55	0
1	D	3211	0	3111	37	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	17	0	15	1	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	0	0
3	D	17	0	15	0	0
4	A	17	0	0	0	0
4	B	17	0	0	0	0
4	C	17	0	0	2	0
4	D	17	0	0	0	0
5	A	42	0	56	5	0
5	B	28	0	37	6	0
5	C	42	0	55	8	0
5	D	28	0	37	3	0
6	A	12	0	16	1	0
6	B	6	0	8	0	0
6	C	24	0	31	0	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	84	0	0	3	0
10	B	166	0	0	4	0
10	C	116	0	0	1	0
10	D	181	0	0	2	0
All	All	13894	0	12881	211	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 8.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.63	0.80
1:C:128:ARG:O	1:C:132:ASN:ND2	2.15	0.79
1:A:263:GLY:H	1:A:285:ARG:HG3	1.51	0.75
1:C:382:CYS:HA	5:C:504:BTB:H12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.21	0.74
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.69	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.72	0.71
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.73	0.69
1:B:365:ARG:NH2	1:B:369:ASP:OD2	2.26	0.69
5:B:505:BTB:O8	5:B:505:BTB:O3	2.07	0.69
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.75	0.68
1:B:216:LYS:HB2	1:B:309:LEU:HD11	1.76	0.66
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.78	0.65
1:D:378:ASP:OD2	10:D:601:HOH:O	2.14	0.65
1:A:168:SER:OG	10:A:601:HOH:O	2.14	0.64
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.79	0.64
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.80	0.64
1:A:378:ASP:OD1	10:A:602:HOH:O	2.15	0.63
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.81	0.61
1:D:100:LEU:HB3	1:D:103:LEU:HD22	1.82	0.61
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.82	0.60
1:A:321:GLU:H	1:A:321:GLU:CD	2.06	0.59
1:C:377:GLU:OE1	5:C:505:BTB:O1	2.20	0.58
1:D:170:LEU:HD11	1:D:230:VAL:HG11	1.85	0.58
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.37	0.58
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.18	0.57
1:C:246:SER:HA	1:C:338:ASN:HB3	1.85	0.57
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.86	0.57
1:A:179:ARG:O	10:A:603:HOH:O	2.17	0.57
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.87	0.57
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.16	0.56
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.31	0.56
1:B:301:GLU:HB3	1:B:303:PHE:CE1	2.41	0.56
1:B:275:ILE:HG12	1:B:281:PRO:HG3	1.88	0.56
1:A:263:GLY:N	1:A:285:ARG:HG3	2.21	0.56
1:C:171:VAL:HG22	1:C:195:VAL:HB	1.88	0.55
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.87	0.55
1:A:128:ARG:O	1:A:132:ASN:ND2	2.40	0.55
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.89	0.55
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.08	0.54
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.40	0.54
1:C:175:LYS:HG2	1:C:193:LEU:HD23	1.89	0.54
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.88	0.54
1:A:267:ASN:O	1:A:269:GLU:N	2.41	0.53
1:A:89:GLN:HG3	1:A:90:GLN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.73	0.53
1:C:361:GLU:OE2	4:C:503:K7U:N02	2.41	0.53
1:C:285:ARG:HD3	10:C:704:HOH:O	2.08	0.53
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.53
1:D:364:THR:O	1:D:368:CYS:HB2	2.09	0.53
1:A:306:PRO:HB2	1:A:309:LEU:HB2	1.90	0.52
1:C:255:ARG:HH12	1:C:268:VAL:HG11	1.75	0.52
1:B:147:GLU:HA	1:B:150:LEU:HD12	1.91	0.52
1:C:359:SER:OG	1:C:419:ASP:HA	2.10	0.52
1:D:449:VAL:HG22	1:D:459:VAL:HG23	1.90	0.52
1:D:271:THR:O	1:D:275:ILE:HG12	2.10	0.51
1:B:342:GLU:HG3	1:B:474:ARG:NH1	2.25	0.51
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.46	0.51
1:C:160:THR:HG23	1:C:162:THR:H	1.76	0.51
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.46	0.51
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.77	0.50
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.42	0.50
1:D:238:ARG:HG3	1:D:296:PRO:HB3	1.93	0.50
1:C:235:CYS:HB2	1:C:236:PRO:HD2	1.94	0.50
1:D:154:GLU:OE2	10:D:602:HOH:O	2.19	0.50
1:D:455:SER:HA	1:D:460:PHE:CG	2.47	0.50
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.46	0.50
1:B:367:LEU:HA	1:B:373:TYR:HB2	1.92	0.49
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.94	0.49
1:C:120:PRO:O	1:C:124:LEU:HG	2.12	0.49
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.47	0.49
1:A:92:GLY:N	1:B:96:PRO:O	2.44	0.49
1:A:166:ARG:HB2	1:A:169:GLU:CD	2.32	0.49
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.28	0.48
1:C:445:TRP:CE2	1:C:449:VAL:HG21	2.48	0.48
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.27	0.48
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.96	0.48
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.48	0.48
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.96	0.48
1:A:145:ALA:HA	1:A:148:GLN:HB2	1.95	0.48
1:A:149:ARG:O	1:A:153:VAL:HG22	2.13	0.48
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.95	0.48
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.95	0.48
1:D:387:THR:HA	1:D:394:TRP:CD1	2.48	0.48
5:A:505:BTB:H51	5:A:505:BTB:H11	1.41	0.48
1:C:127:ALA:O	1:C:131:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:HIS:ND1	10:B:603:HOH:O	2.35	0.47
1:C:156:GLU:O	1:C:160:THR:HG22	2.14	0.47
1:A:167:GLU:HG2	6:A:507:GOL:H12	1.97	0.47
1:B:298:GLU:CD	5:B:505:BTB:H42	2.34	0.47
1:C:165:LEU:HG	1:C:346:LEU:HD12	1.95	0.47
1:C:296:PRO:O	1:C:298:GLU:HG2	2.14	0.47
1:A:125:SER:HA	1:A:128:ARG:NH1	2.30	0.47
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.50	0.47
1:D:290:PRO:HG2	1:D:302:LEU:HD11	1.97	0.46
1:A:359:SER:OG	1:A:419:ASP:HA	2.15	0.46
1:B:72:LYS:O	1:B:463:GLU:HG3	2.14	0.46
1:D:242:ARG:CZ	1:D:479:PRO:HG3	2.45	0.46
1:A:246:SER:OG	1:A:250:ARG:HD2	2.15	0.46
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.97	0.46
1:B:326:LEU:HD12	5:C:504:BTB:H72	1.97	0.46
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.97	0.46
1:D:359:SER:OG	1:D:419:ASP:HA	2.15	0.46
1:A:277:HIS:CD2	1:A:300:PRO:HG2	2.51	0.46
1:A:238:ARG:NH2	1:A:240:ASP:OD1	2.49	0.45
5:A:505:BTB:O3	5:A:505:BTB:O4	2.08	0.45
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.52	0.45
1:C:179:ARG:NH2	1:C:438:ARG:HG3	2.31	0.45
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.98	0.45
5:A:506:BTB:H11	5:A:506:BTB:H51	1.68	0.45
5:B:504:BTB:H82	5:B:504:BTB:O4	2.17	0.45
1:A:256:GLN:HB3	1:A:258:ASP:H	1.82	0.45
1:C:384:ASP:OD1	5:C:504:BTB:O3	2.34	0.45
1:A:387:THR:HA	1:A:394:TRP:CD1	2.52	0.45
5:D:505:BTB:O4	5:D:505:BTB:H51	2.16	0.45
1:A:238:ARG:HG2	1:A:239:GLY:N	2.32	0.44
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.98	0.44
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.58	0.44
1:A:231:PHE:HB2	1:A:350:ALA:O	2.18	0.44
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.52	0.44
5:A:504:BTB:H32	5:A:504:BTB:H51	1.36	0.44
1:C:244:TRP:CZ2	1:C:300:PRO:HG3	2.52	0.44
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.19	0.44
1:B:170:LEU:HD11	1:B:230:VAL:HG11	1.99	0.44
1:A:93:PRO:HB3	1:A:106:PRO:HB3	2.00	0.44
1:B:152:GLU:OE1	1:B:166:ARG:NH2	2.51	0.44
1:B:445:TRP:CE2	1:B:449:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:OE2	1:C:164:GLN:HG2	2.16	0.44
1:A:170:LEU:HD11	1:A:230:VAL:HG21	2.00	0.44
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.70	0.44
5:B:505:BTB:H42	5:B:505:BTB:H72	1.50	0.44
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.00	0.44
1:A:267:ASN:O	1:A:270:ILE:N	2.51	0.44
1:C:275:ILE:HA	1:C:279:TRP:O	2.18	0.44
1:C:367:LEU:HB3	1:C:375:ILE:HD13	1.99	0.44
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.00	0.43
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.53	0.43
1:A:322:TRP:CD1	5:A:504:BTB:H61	2.53	0.43
1:B:429:LYS:NZ	10:B:610:HOH:O	2.48	0.43
1:B:445:TRP:CZ2	1:B:449:VAL:HG21	2.53	0.43
1:C:247:GLN:HE21	4:C:503:K7U:C14	2.31	0.43
1:D:138:ILE:HD12	1:D:140:ARG:HE	1.83	0.43
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.99	0.43
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.53	0.43
5:C:506:BTB:H42	5:C:506:BTB:H51	1.68	0.43
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.53	0.43
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.34	0.43
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.43
5:C:505:BTB:H42	5:C:505:BTB:H51	1.62	0.43
1:A:239:GLY:N	1:A:297:ASP:OD2	2.49	0.43
1:A:250:ARG:HD3	1:A:267:ASN:OD1	2.19	0.43
1:D:455:SER:HA	1:D:460:PHE:CB	2.49	0.43
1:B:144:GLN:HB2	10:B:633:HOH:O	2.19	0.43
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.54	0.43
1:B:175:LYS:HE2	1:B:191:GLY:O	2.19	0.43
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	2.00	0.43
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.54	0.43
5:D:504:BTB:H12	5:D:504:BTB:H72	1.74	0.43
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.42
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.42
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.52	0.42
1:A:255:ARG:HG2	1:A:259:GLY:O	2.19	0.42
1:B:248:LEU:HB2	1:B:335:ALA:HB3	2.00	0.42
1:B:455:SER:HA	1:B:460:PHE:CB	2.49	0.42
1:D:290:PRO:HB3	1:D:304:LEU:HD23	2.00	0.42
1:D:428:MET:HG3	1:D:458:PRO:HB2	2.01	0.42
1:A:144:GLN:HG3	1:A:145:ALA:N	2.35	0.42
1:B:70:ARG:HD2	1:B:79:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:O	1:C:140:ARG:HG2	2.18	0.42
1:C:207:MET:HE3	1:C:293:LEU:HB3	2.01	0.42
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.55	0.42
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.00	0.42
1:C:306:PRO:O	1:C:309:LEU:HB2	2.20	0.42
1:A:224:LEU:HB2	1:A:416:THR:HB	2.02	0.41
1:A:279:TRP:HB2	1:A:302:LEU:HD13	2.02	0.41
1:A:125:SER:HA	1:A:128:ARG:HH12	1.84	0.41
5:B:505:BTB:H12	5:B:505:BTB:H51	1.57	0.41
5:C:505:BTB:H52	5:C:505:BTB:H81	1.59	0.41
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.56	0.41
1:C:181:ALA:HA	1:C:182:PRO:HD3	1.93	0.41
1:D:367:LEU:HA	1:D:373:TYR:HB2	2.03	0.41
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.02	0.41
1:B:342:GLU:HG3	1:B:474:ARG:HH12	1.85	0.41
1:D:247:GLN:HA	1:D:335:ALA:O	2.19	0.41
1:B:122:GLN:CD	1:B:122:GLN:H	2.22	0.41
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.03	0.41
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.56	0.41
1:B:298:GLU:HG2	10:B:694:HOH:O	2.19	0.41
1:B:364:THR:O	1:B:368:CYS:HB2	2.20	0.41
1:B:75:GLU:HG2	1:B:76:VAL:HG23	2.03	0.41
5:C:506:BTB:HO1	5:C:506:BTB:HO4	1.64	0.41
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.28	0.41
1:B:286:PHE:HZ	1:B:328:LEU:HD23	1.85	0.41
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.56	0.41
1:C:306:PRO:HA	1:C:307:PRO:HD3	1.96	0.41
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.56	0.41
1:C:188:ILE:HD12	1:C:188:ILE:HA	1.94	0.41
1:C:238:ARG:HH12	1:C:296:PRO:HG2	1.86	0.41
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.92	0.40
1:B:202:ARG:HE	1:B:202:ARG:HB2	1.72	0.40
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.57	0.40
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.53	0.40
1:C:71:VAL:HG21	1:C:465:VAL:HG23	2.03	0.40
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.96	0.40
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.57	0.40
1:B:214:HIS:CD2	1:B:214:HIS:C	2.95	0.40
1:B:301:GLU:HB3	1:B:303:PHE:HE1	1.85	0.40
1:B:447:TRP:HA	3:B:502:H4B:N1	2.36	0.40
1:C:367:LEU:HA	1:C:373:TYR:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:THR:HA	1:C:394:TRP:CD1	2.57	0.40
5:D:504:BTB:H51	5:D:504:BTB:H32	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	398/440 (90%)	371 (93%)	23 (6%)	4 (1%)	15 10
1	B	400/440 (91%)	387 (97%)	12 (3%)	1 (0%)	41 39
1	C	399/440 (91%)	384 (96%)	13 (3%)	2 (0%)	29 25
1	D	398/440 (90%)	389 (98%)	9 (2%)	0	100 100
All	All	1595/1760 (91%)	1531 (96%)	57 (4%)	7 (0%)	34 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	A	88	ALA
1	A	203	SER
1	A	239	GLY
1	C	89	GLN
1	C	277	HIS
1	B	89	GLN

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%)	323 (94%)	19 (6%)	21	18
1	B	343/373 (92%)	328 (96%)	15 (4%)	28	27
1	C	342/373 (92%)	327 (96%)	15 (4%)	28	27
1	D	341/373 (91%)	333 (98%)	8 (2%)	50	53
All	All	1368/1492 (92%)	1311 (96%)	57 (4%)	30	29

All (57) 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	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	202	ARG
1	A	205	GLN
1	A	209	THR
1	A	216	LYS
1	A	238	ARG
1	A	240	ASP
1	A	245	ASN
1	A	256	GLN
1	A	285	ARG
1	A	291	LEU
1	A	321	GLU
1	A	470	SER
1	B	90	GLN
1	B	97	ARG
1	B	106	PRO
1	B	122	GLN
1	B	128	ARG
1	B	136	SER
1	B	139	LYS
1	B	147	GLU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	255	ARG

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Mol	Chain	Res	Type
1	B	257	GLN
1	B	326	LEU
1	B	378	ASP
1	B	396	ASP
1	C	67	LYS
1	C	70	ARG
1	C	89	GLN
1	C	97	ARG
1	C	98	ARG
1	C	125	SER
1	C	131	ILE
1	C	140	ARG
1	C	202	ARG
1	C	233	GLN
1	C	234	ARG
1	C	238	ARG
1	C	255	ARG
1	C	308	GLU
1	C	354	SER
1	D	98	ARG
1	D	107	ARG
1	D	124	LEU
1	D	167	GLU
1	D	192	LYS
1	D	200	ASP
1	D	326	LEU
1	D	396	ASP

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

Mol	Chain	Res	Type
1	C	87	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	K7U	D	503	-	16,18,18	2.81	6 (37%)	17,26,26	1.77	5 (29%)
6	GOL	A	507	-	5,5,5	0.32	0	5,5,5	0.22	0
6	GOL	D	506	-	5,5,5	0.25	0	5,5,5	0.53	0
2	HEM	B	501	1	41,50,50	1.51	5 (12%)	45,82,82	1.64	8 (17%)
6	GOL	C	510	-	5,5,5	0.39	0	5,5,5	0.12	0
3	H4B	C	502	-	16,18,18	0.97	0	11,26,26	2.78	6 (54%)
2	HEM	A	501	1	41,50,50	1.55	5 (12%)	45,82,82	1.64	8 (17%)
5	BTB	D	504	8	13,13,13	0.40	0	7,16,16	0.66	0
6	GOL	C	508	-	5,5,5	0.79	0	5,5,5	1.77	1 (20%)
6	GOL	A	508	-	5,5,5	0.45	0	5,5,5	0.79	0
6	GOL	C	507	-	5,5,5	0.36	0	5,5,5	0.18	0
5	BTB	C	506	-	13,13,13	0.47	0	7,16,16	0.39	0
5	BTB	C	505	-	13,13,13	0.42	0	7,16,16	0.82	0
5	BTB	A	506	-	13,13,13	0.36	0	7,16,16	0.63	0
5	BTB	A	505	-	13,13,13	0.49	0	7,16,16	0.73	0
4	K7U	B	503	-	16,18,18	2.46	4 (25%)	17,26,26	2.05	4 (23%)
6	GOL	B	506	-	5,5,5	0.33	0	5,5,5	0.51	0
4	K7U	A	503	-	16,18,18	2.70	5 (31%)	17,26,26	1.69	4 (23%)
3	H4B	B	502	-	16,18,18	0.92	0	11,26,26	2.56	6 (54%)
2	HEM	C	501	1	41,50,50	1.48	6 (14%)	45,82,82	1.78	9 (20%)
4	K7U	C	503	-	16,18,18	2.83	6 (37%)	17,26,26	2.09	7 (41%)
5	BTB	B	505	-	13,13,13	0.55	0	7,16,16	0.87	0
5	BTB	B	504	8	13,13,13	0.45	0	7,16,16	1.01	1 (14%)
5	BTB	A	504	8	13,13,13	0.69	0	7,16,16	1.19	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BTB	C	504	8	13,13,13	0.35	0	7,16,16	1.00	0
2	HEM	D	501	1	41,50,50	1.43	5 (12%)	45,82,82	1.77	10 (22%)
3	H4B	D	502	-	16,18,18	0.92	1 (6%)	11,26,26	2.54	5 (45%)
6	GOL	C	509	-	5,5,5	0.33	0	5,5,5	0.29	0
3	H4B	A	502	-	16,18,18	0.90	0	11,26,26	2.60	5 (45%)
5	BTB	D	505	-	13,13,13	0.49	0	7,16,16	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	K7U	D	503	-	-	0/3/16/16	0/2/2/2
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	D	506	-	-	0/4/4/4	-
2	HEM	B	501	1	-	1/12/54/54	-
6	GOL	C	510	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
2	HEM	A	501	1	-	2/12/54/54	-
5	BTB	D	504	8	-	2/21/21/21	-
6	GOL	C	508	-	-	4/4/4/4	-
6	GOL	A	508	-	-	3/4/4/4	-
6	GOL	C	507	-	-	4/4/4/4	-
5	BTB	C	506	-	-	7/21/21/21	-
5	BTB	C	505	-	-	14/21/21/21	-
5	BTB	A	506	-	-	3/21/21/21	-
5	BTB	A	505	-	-	10/21/21/21	-
4	K7U	B	503	-	-	0/3/16/16	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
4	K7U	A	503	-	-	1/3/16/16	0/2/2/2
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	1/12/54/54	-
4	K7U	C	503	-	-	0/3/16/16	0/2/2/2
5	BTB	B	505	-	-	11/21/21/21	-
5	BTB	B	504	8	-	8/21/21/21	-
5	BTB	A	504	8	-	9/21/21/21	-
5	BTB	C	504	8	-	6/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	1	-	1/12/54/54	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
6	GOL	C	509	-	-	2/4/4/4	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
5	BTB	D	505	-	-	7/21/21/21	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	K7U	C06-C08	-9.39	1.28	1.44
4	A	503	K7U	C06-C08	-9.24	1.29	1.44
4	C	503	K7U	C06-C08	-9.16	1.29	1.44
4	B	503	K7U	C06-C08	-8.41	1.30	1.44
2	B	501	HEM	C3C-CAC	4.15	1.56	1.47
2	A	501	HEM	C3C-CAC	3.89	1.55	1.47
2	C	501	HEM	C3C-CAC	3.75	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.53	1.35	1.40
2	D	501	HEM	FE-NB	3.50	2.14	1.96
4	C	503	K7U	F16-C13	-3.28	1.32	1.38
4	A	503	K7U	F15-C13	-3.27	1.32	1.38
2	B	501	HEM	CAB-C3B	3.23	1.56	1.47
4	C	503	K7U	F15-C13	-3.21	1.32	1.38
2	D	501	HEM	C3C-CAC	3.21	1.54	1.47
2	C	501	HEM	CAB-C3B	3.20	1.56	1.47
2	D	501	HEM	CAB-C3B	3.09	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.08	1.36	1.40
2	A	501	HEM	CAB-C3B	3.07	1.55	1.47
4	B	503	K7U	F15-C13	-3.00	1.33	1.38
2	A	501	HEM	FE-NB	2.91	2.11	1.96
4	D	503	K7U	C14-C13	-2.86	1.51	1.54
2	B	501	HEM	C3C-C2C	-2.85	1.36	1.40
4	D	503	K7U	C10-N11	-2.82	1.43	1.46
4	D	503	K7U	F16-C13	-2.77	1.33	1.38
4	A	503	K7U	F16-C13	-2.76	1.33	1.38
4	C	503	K7U	C10-N11	2.73	1.49	1.46
4	C	503	K7U	C14-C13	-2.72	1.51	1.54
4	D	503	K7U	F15-C13	-2.58	1.33	1.38
2	A	501	HEM	FE-ND	2.58	2.09	1.96
2	C	501	HEM	FE-ND	2.49	2.09	1.96
4	D	503	K7U	C12-C13	-2.47	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	K7U	F16-C13	-2.44	1.33	1.38
2	B	501	HEM	FE-ND	2.44	2.08	1.96
4	B	503	K7U	C12-C13	-2.30	1.52	1.54
4	A	503	K7U	C12-C13	-2.29	1.52	1.54
4	A	503	K7U	C14-C13	-2.25	1.52	1.54
4	C	503	K7U	C12-C13	-2.24	1.52	1.54
2	C	501	HEM	FE-NB	2.22	2.07	1.96
2	B	501	HEM	FE-NB	2.20	2.07	1.96
3	D	502	H4B	C4A-C4	-2.15	1.38	1.41
2	D	501	HEM	CMD-C2D	2.11	1.55	1.50
2	C	501	HEM	CMB-C2B	2.02	1.55	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	H4B	C8A-C4A-C4	6.04	119.93	114.57
3	D	502	H4B	C8A-C4A-C4	5.58	119.52	114.57
3	A	502	H4B	C8A-C4A-C4	5.31	119.29	114.57
2	C	501	HEM	CBA-CAA-C2A	-5.27	103.63	112.62
4	B	503	K7U	C05-C06-N01	-5.13	118.35	123.61
3	B	502	H4B	C8A-C4A-C4	4.64	118.69	114.57
4	D	503	K7U	F16-C13-F15	4.51	116.75	107.49
2	C	501	HEM	C4B-CHC-C1C	4.47	128.46	122.56
2	A	501	HEM	C4B-CHC-C1C	4.37	128.32	122.56
2	D	501	HEM	CBA-CAA-C2A	-4.14	105.56	112.62
4	A	503	K7U	C05-C06-N01	-3.94	119.58	123.61
4	C	503	K7U	C05-C06-N01	-3.86	119.66	123.61
4	C	503	K7U	C08-C06-N01	3.83	122.75	116.55
2	C	501	HEM	C1B-NB-C4B	3.81	109.01	105.07
2	B	501	HEM	CBA-CAA-C2A	-3.76	106.21	112.62
2	A	501	HEM	C1B-NB-C4B	3.63	108.82	105.07
2	D	501	HEM	CBD-CAD-C3D	-3.62	102.56	112.63
2	D	501	HEM	C4B-CHC-C1C	3.60	127.31	122.56
4	B	503	K7U	C06-N01-C02	3.56	122.70	116.90
3	B	502	H4B	N1-C2-N3	-3.55	119.86	125.42
2	B	501	HEM	C3B-C2B-C1B	3.49	109.08	106.49
2	B	501	HEM	CBD-CAD-C3D	-3.47	102.99	112.63
3	C	502	H4B	N1-C2-N3	-3.39	120.10	125.42
2	B	501	HEM	C1B-NB-C4B	3.37	108.55	105.07
4	B	503	K7U	C08-C06-N01	3.36	121.98	116.55
2	B	501	HEM	C4B-CHC-C1C	3.35	126.98	122.56
2	D	501	HEM	CMC-C2C-C3C	3.33	130.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	H4B	N1-C2-N3	-3.27	120.29	125.42
6	C	508	GOL	O1-C1-C2	-3.24	94.69	110.20
2	D	501	HEM	C4C-CHD-C1D	3.21	126.80	122.56
3	C	502	H4B	C2-N3-C4	3.16	120.94	115.93
3	B	502	H4B	C2-N1-C8A	3.14	121.58	114.54
3	B	502	H4B	C4-C4A-N5	3.12	121.74	119.12
3	A	502	H4B	C2-N3-C4	3.10	120.86	115.93
2	D	501	HEM	C3B-C2B-C1B	3.07	108.76	106.49
2	D	501	HEM	C1B-NB-C4B	3.02	108.20	105.07
2	C	501	HEM	CBD-CAD-C3D	-3.00	104.29	112.63
2	D	501	HEM	C4D-ND-C1D	2.99	108.16	105.07
3	D	502	H4B	N1-C2-N3	-2.98	120.74	125.42
3	D	502	H4B	C2-N3-C4	2.98	120.67	115.93
2	A	501	HEM	C3B-C2B-C1B	2.96	108.68	106.49
3	B	502	H4B	C2-N3-C4	2.85	120.46	115.93
3	C	502	H4B	C2-N1-C8A	2.84	120.90	114.54
4	C	503	K7U	F16-C13-F15	2.81	113.27	107.49
4	A	503	K7U	C06-N01-C02	2.80	121.46	116.90
3	A	502	H4B	C4-C4A-N5	2.80	121.47	119.12
2	C	501	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	C	501	HEM	C3B-C2B-C1B	2.77	108.54	106.49
2	A	501	HEM	C4D-ND-C1D	2.77	107.94	105.07
4	A	503	K7U	F16-C13-F15	2.76	113.15	107.49
2	A	501	HEM	CBA-CAA-C2A	-2.75	107.93	112.62
3	A	502	H4B	C2-N1-C8A	2.75	120.70	114.54
2	B	501	HEM	CMC-C2C-C3C	2.67	129.68	124.68
3	D	502	H4B	C2-N1-C8A	2.64	120.46	114.54
4	C	503	K7U	C06-N01-C02	2.62	121.16	116.90
4	C	503	K7U	N02-C02-N01	2.62	120.62	116.49
4	B	503	K7U	F16-C13-F15	2.58	112.79	107.49
2	C	501	HEM	CHC-C4B-C3B	2.51	128.41	124.57
2	B	501	HEM	CHC-C4B-C3B	2.49	128.38	124.57
4	A	503	K7U	C08-C06-N01	2.48	120.56	116.55
4	D	503	K7U	C06-N01-C02	2.43	120.86	116.90
3	C	502	H4B	C4-C4A-N5	2.43	121.16	119.12
2	C	501	HEM	C3D-C4D-ND	-2.39	107.50	110.17
2	C	501	HEM	CMC-C2C-C3C	2.37	129.12	124.68
2	A	501	HEM	CBD-CAD-C3D	-2.35	106.11	112.63
2	A	501	HEM	CHC-C4B-C3B	2.33	128.13	124.57
3	C	502	H4B	N2-C2-N3	2.32	120.86	117.25
4	D	503	K7U	C05-C06-N01	-2.31	121.25	123.61
2	B	501	HEM	C4D-ND-C1D	2.31	107.45	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504	BTB	O4-C4-C2	2.30	117.73	111.44
4	C	503	K7U	C05-C06-C08	-2.26	117.40	119.83
4	D	503	K7U	C14-N11-C12	2.23	92.82	89.83
4	C	503	K7U	C14-N11-C12	2.23	92.81	89.83
3	B	502	H4B	N2-C2-N1	2.21	120.69	117.25
4	D	503	K7U	C08-C06-N01	2.19	120.09	116.55
3	D	502	H4B	C4A-N5-C6	-2.14	115.33	121.16
2	A	501	HEM	CHD-C1D-C2D	2.08	128.23	124.98
2	D	501	HEM	C2B-C1B-NB	-2.08	107.38	109.84
2	D	501	HEM	C3D-C4D-ND	-2.04	107.90	110.17
5	B	504	BTB	C6-C5-N	2.01	119.45	111.59

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
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	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	C1-C2-C4-O4
5	A	506	BTB	C3-C2-C4-O4
5	A	506	BTB	N-C2-C4-O4
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	504	BTB	C1-C2-C3-O3
5	B	504	BTB	C1-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	B	504	BTB	C3-C2-C4-O4
5	B	504	BTB	N-C2-C4-O4
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-C5
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C8-C7-N-C5
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	C	506	BTB	C4-C2-N-C7
5	D	504	BTB	C3-C2-C4-O4
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	A	508	GOL	C1-C2-C3-O3
6	C	507	GOL	O1-C1-C2-C3
6	C	507	GOL	C1-C2-C3-O3
6	C	508	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	508	GOL	C1-C2-C3-O3
6	C	509	GOL	O1-C1-C2-O2
6	C	509	GOL	O1-C1-C2-C3
5	C	506	BTB	N-C5-C6-O6
6	C	507	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
5	D	505	BTB	N-C7-C8-O8
5	B	505	BTB	N-C5-C6-O6
5	C	505	BTB	N-C5-C6-O6
6	A	508	GOL	O1-C1-C2-C3
6	B	506	GOL	C1-C2-C3-O3
6	C	510	GOL	O1-C1-C2-C3
6	C	510	GOL	C1-C2-C3-O3
5	B	505	BTB	N-C7-C8-O8
6	A	508	GOL	O2-C2-C3-O3
6	B	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O2-C2-C3-O3
6	C	508	GOL	O1-C1-C2-O2
6	C	508	GOL	O2-C2-C3-O3
2	A	501	HEM	C2A-CAA-CBA-CGA
6	C	510	GOL	O2-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
3	A	502	H4B	C7-C6-C9-O9
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
5	A	505	BTB	C1-C2-C4-O4
5	C	504	BTB	C1-C2-C3-O3
5	A	504	BTB	O1-C1-C2-N
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
2	D	501	HEM	C3D-CAD-CBD-CGD
3	A	502	H4B	C7-C6-C9-C10
6	C	510	GOL	O1-C1-C2-O2
4	A	503	K7U	C08-C09-C10-N11
5	A	505	BTB	N-C5-C6-O6
5	C	504	BTB	N-C7-C8-O8
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
5	A	505	BTB	C3-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	B	504	BTB	C4-C2-C3-O3
5	C	504	BTB	C4-C2-C3-O3
5	D	504	BTB	C1-C2-C4-O4

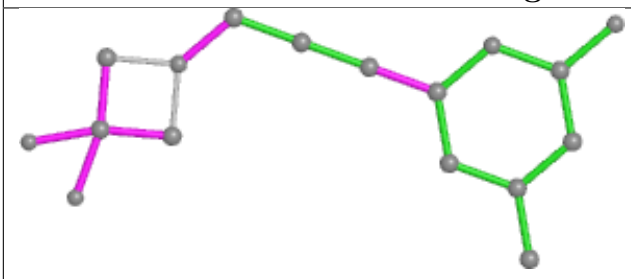
There are no ring outliers.

18 monomers are involved in 37 short contacts:

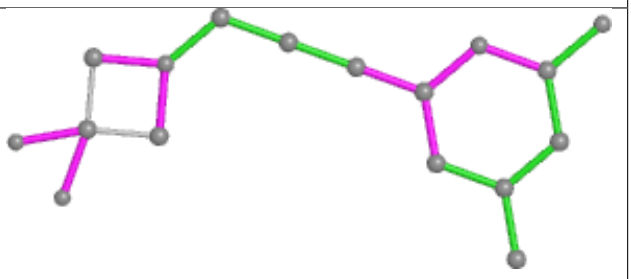
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	GOL	1	0
2	B	501	HEM	2	0
2	A	501	HEM	3	0
5	D	504	BTB	2	0
5	C	506	BTB	2	0
5	C	505	BTB	3	0
5	A	506	BTB	1	0
5	A	505	BTB	2	0
3	B	502	H4B	1	0
2	C	501	HEM	3	0
4	C	503	K7U	2	0
5	B	505	BTB	5	0
5	B	504	BTB	1	0
5	A	504	BTB	2	0
5	C	504	BTB	3	0
2	D	501	HEM	2	0
3	A	502	H4B	1	0
5	D	505	BTB	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.

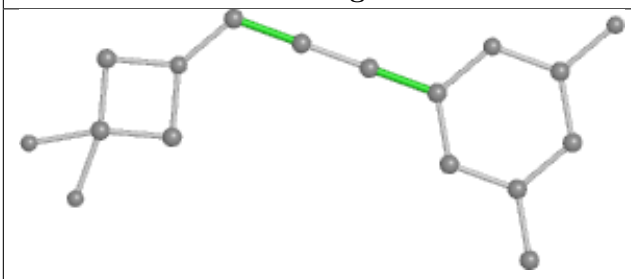
Ligand K7U D 503



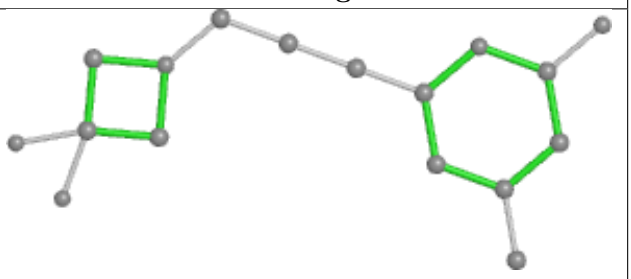
Bond lengths



Bond angles

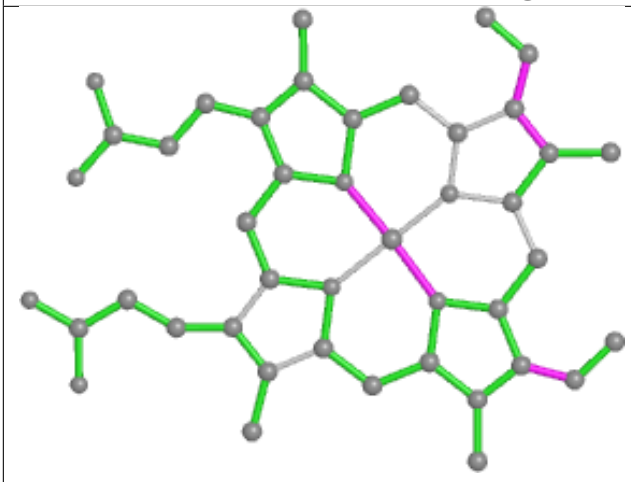


Torsions

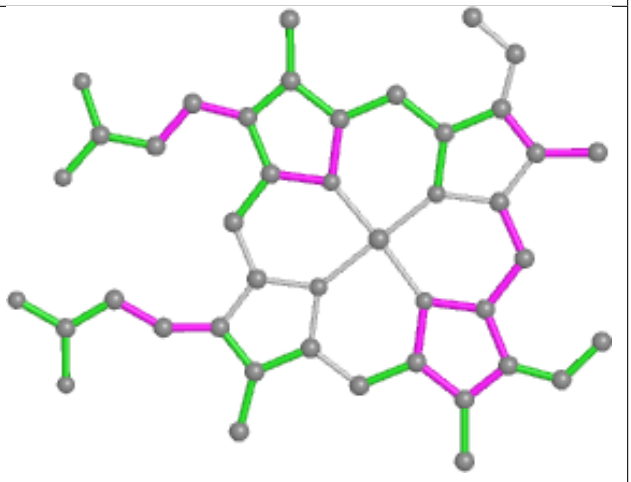


Rings

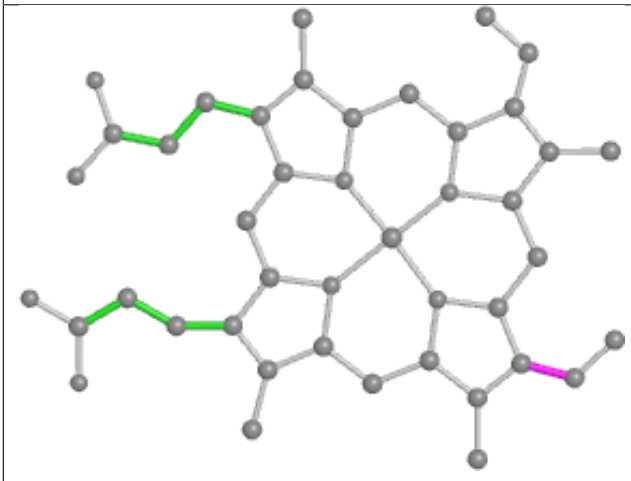
Ligand HEM B 501



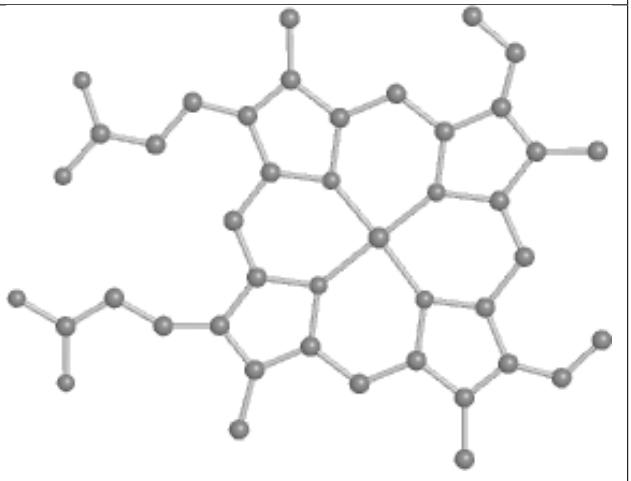
Bond lengths



Bond angles

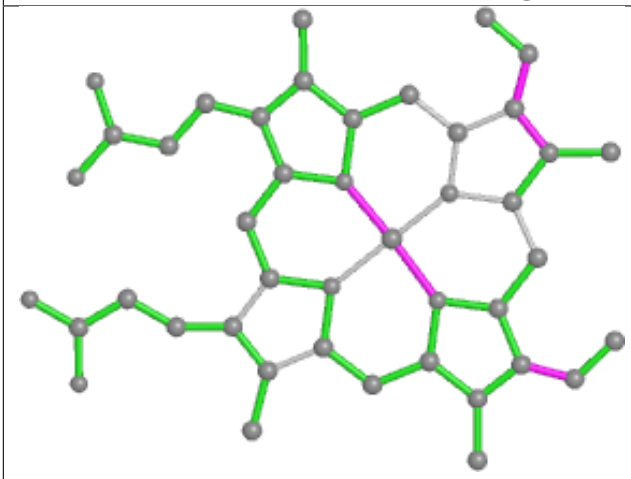


Torsions

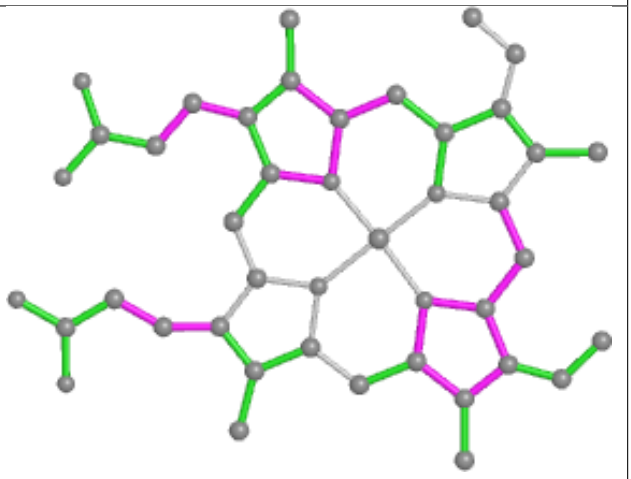


Rings

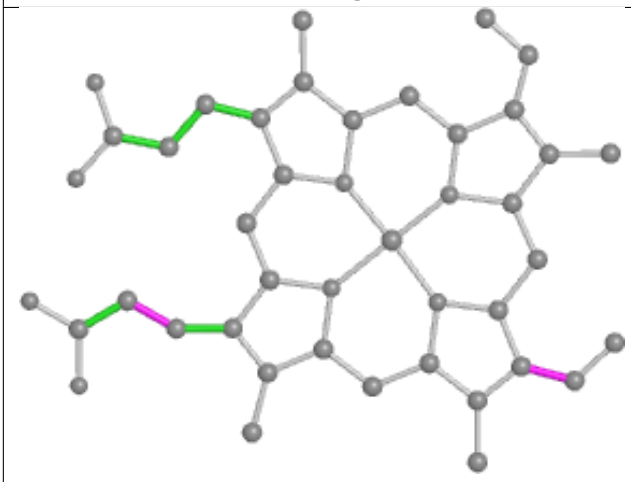
Ligand HEM A 501



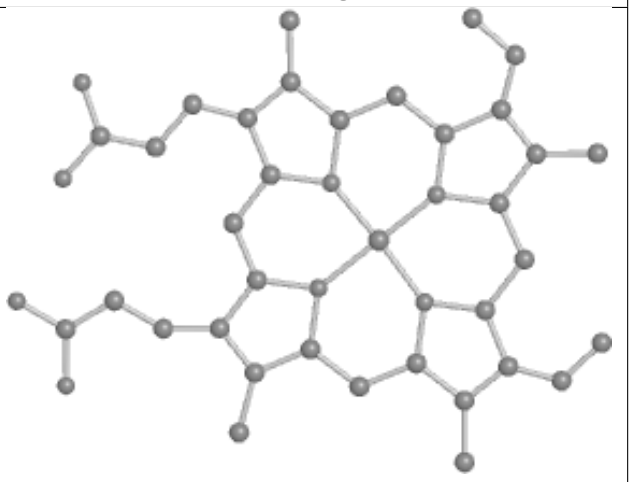
Bond lengths



Bond angles

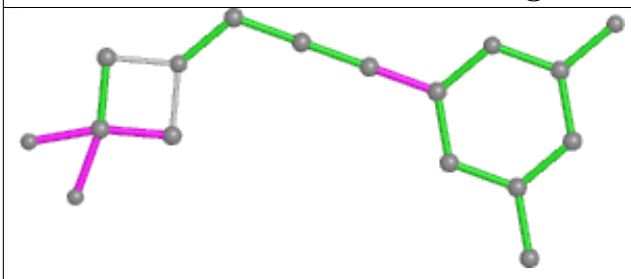


Torsions

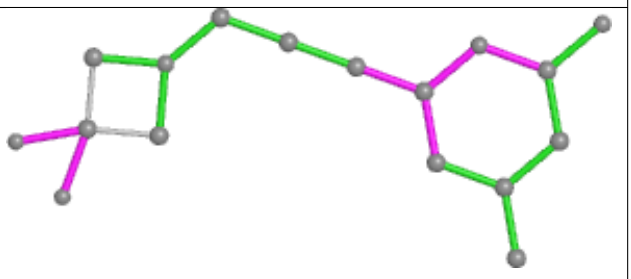


Rings

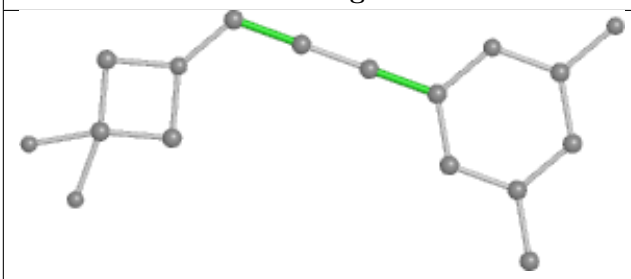
Ligand K7U B 503



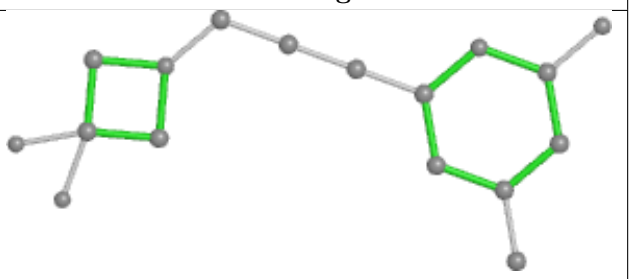
Bond lengths



Bond angles

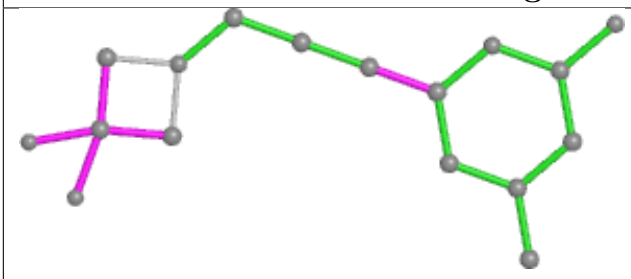


Torsions

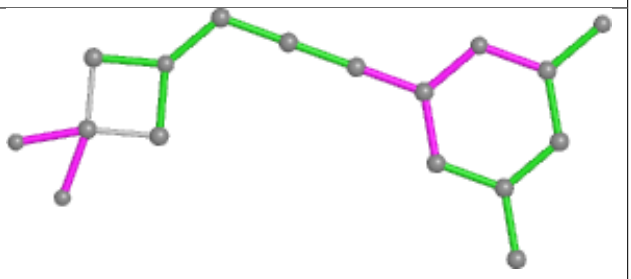


Rings

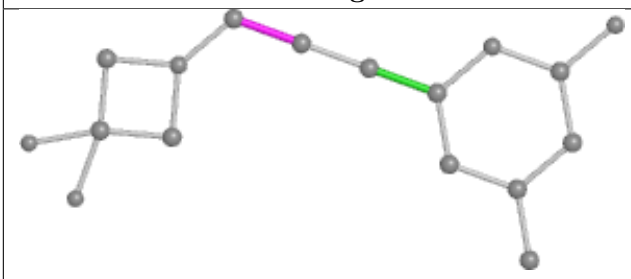
Ligand K7U A 503



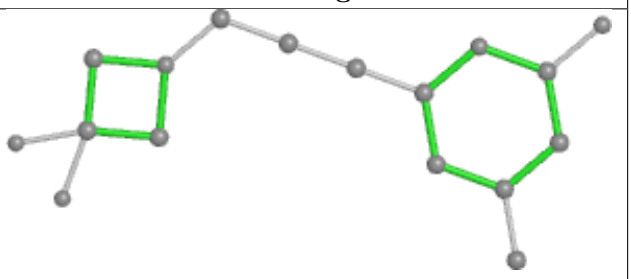
Bond lengths



Bond angles

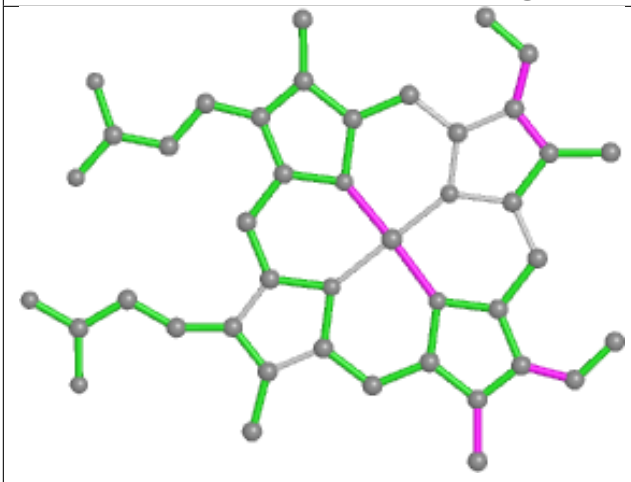


Torsions

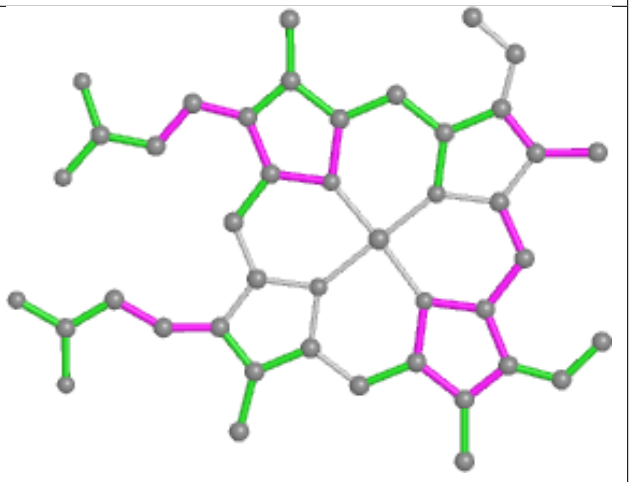


Rings

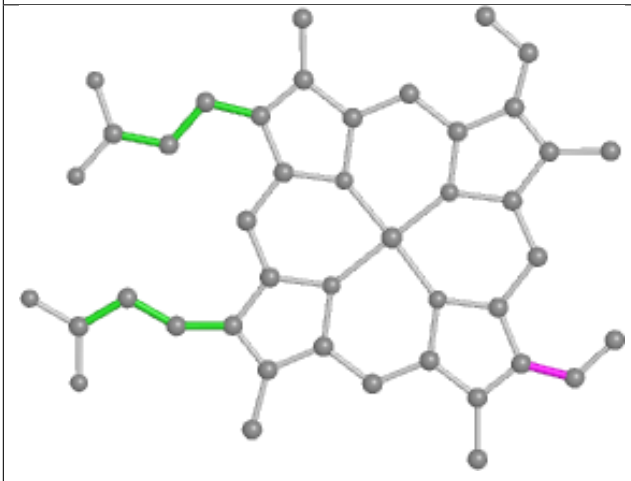
Ligand HEM C 501



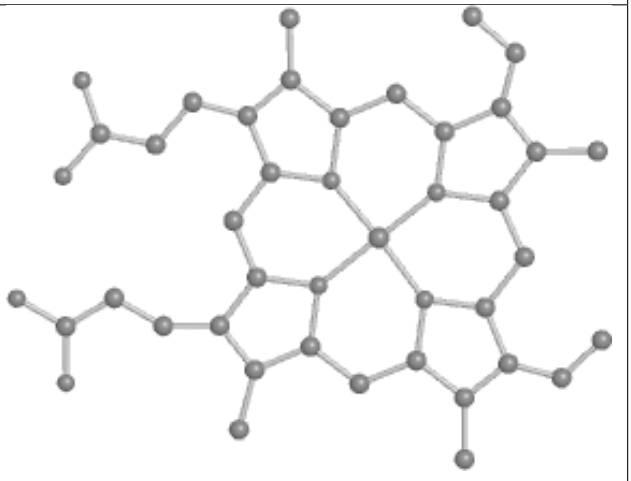
Bond lengths



Bond angles

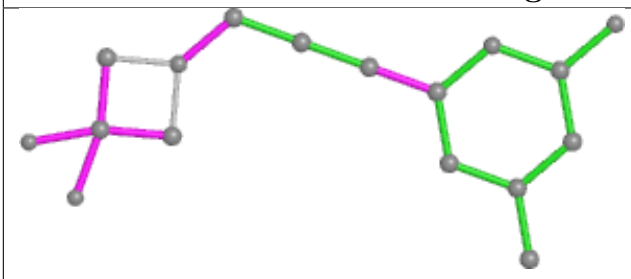


Torsions

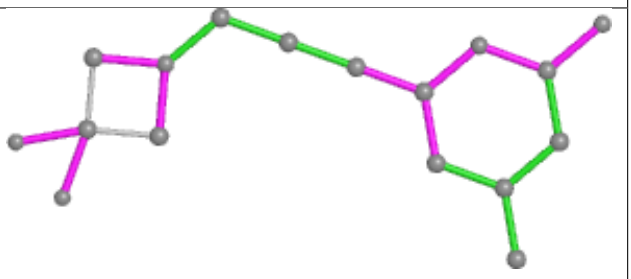


Rings

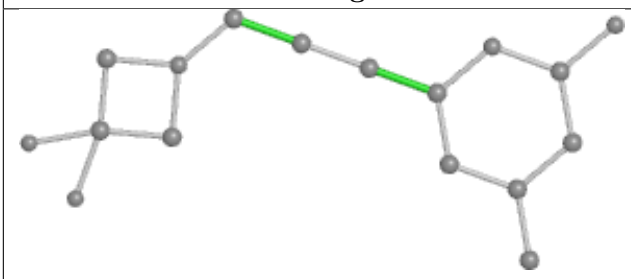
Ligand K7U C 503



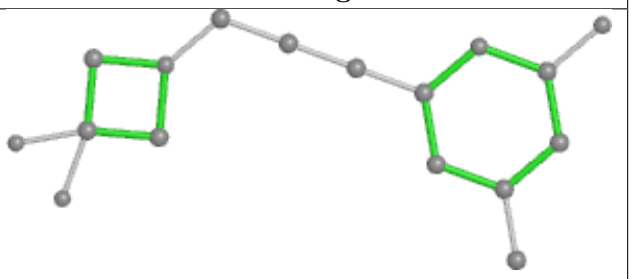
Bond lengths



Bond angles

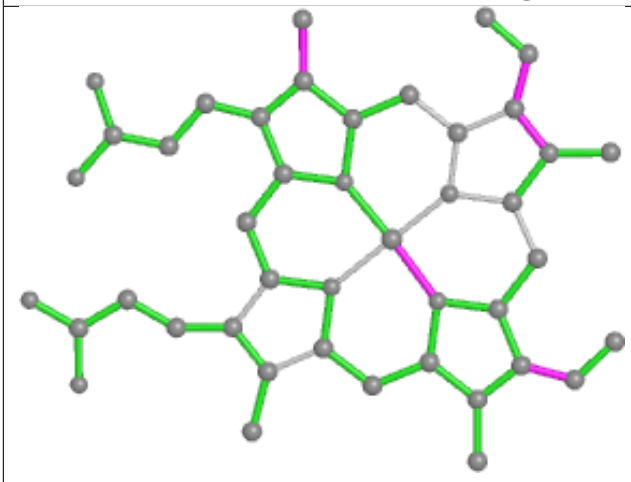


Torsions

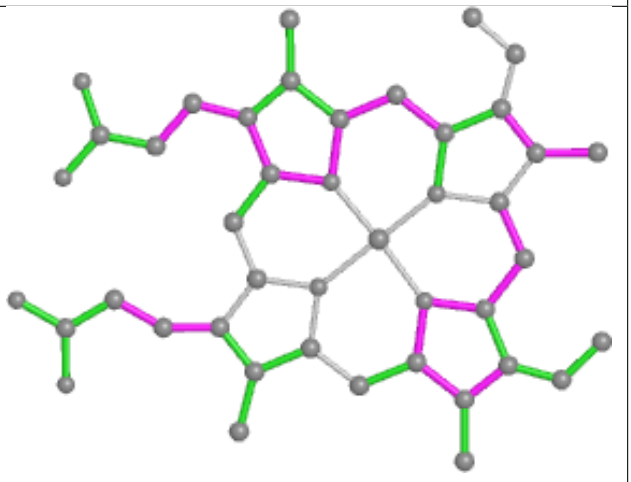


Rings

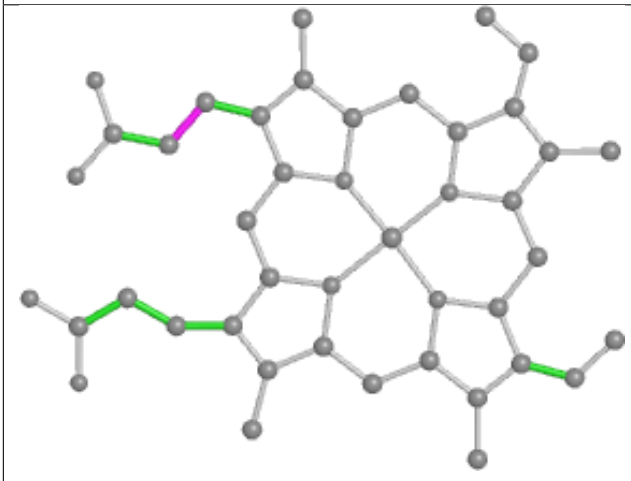
Ligand HEM D 501



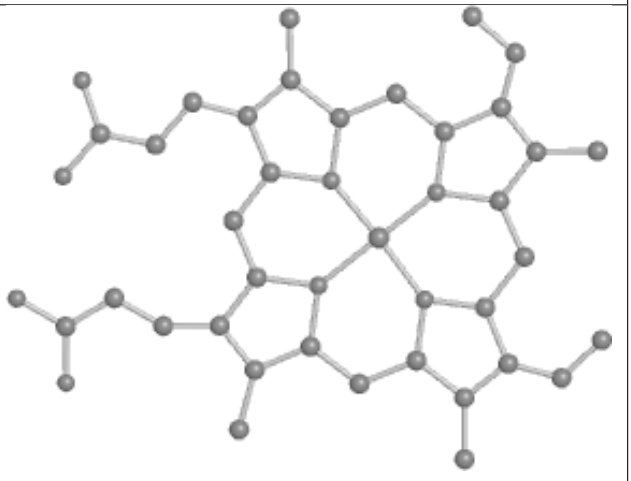
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	0.64	47 (11%) 4 5	30, 61, 111, 137	0
1	B	401/440 (91%)	-0.00	3 (0%) 87 89	24, 41, 73, 96	0
1	C	402/440 (91%)	0.39	34 (8%) 10 13	28, 53, 93, 115	0
1	D	402/440 (91%)	-0.08	1 (0%) 95 95	23, 39, 64, 98	0
All	All	1606/1760 (91%)	0.24	85 (5%) 26 31	23, 47, 96, 137	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	6.5
1	A	153	VAL	5.4
1	C	238	ARG	5.2
1	A	280	THR	5.0
1	A	480	TRP	4.9
1	A	305	LEU	4.9
1	A	254	TYR	4.9
1	B	89	GLN	4.6
1	A	120	PRO	4.5
1	C	236	PRO	4.3
1	A	89	GLN	4.3
1	A	244	TRP	4.2
1	C	204	ALA	4.1
1	A	304	LEU	4.0
1	A	300	PRO	4.0
1	A	279	TRP	4.0
1	C	480	TRP	3.9
1	C	89	GLN	3.9
1	C	292	LEU	3.8
1	A	122	GLN	3.7
1	A	275	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	304	LEU	3.6
1	A	346	LEU	3.5
1	A	284	GLY	3.5
1	A	303	PHE	3.5
1	A	479	PRO	3.5
1	A	302	LEU	3.5
1	C	305	LEU	3.5
1	C	307	PRO	3.4
1	D	89	GLN	3.4
1	C	120	PRO	3.4
1	A	142	GLY	3.3
1	A	238	ARG	3.3
1	C	308	GLU	3.1
1	C	90	GLN	3.1
1	C	293	LEU	3.0
1	C	303	PHE	3.0
1	A	291	LEU	3.0
1	A	308	GLU	2.9
1	A	163	TYR	2.9
1	C	302	LEU	2.9
1	C	121	GLU	2.9
1	A	289	LEU	2.8
1	A	293	LEU	2.8
1	A	283	ASN	2.7
1	B	106	PRO	2.7
1	C	208	PHE	2.7
1	A	121	GLU	2.6
1	C	68	PHE	2.6
1	C	122	GLN	2.6
1	A	237	GLY	2.6
1	A	145	ALA	2.6
1	A	256	GLN	2.6
1	A	306	PRO	2.6
1	A	301	GLU	2.5
1	C	252	ALA	2.5
1	A	207	MET	2.5
1	A	281	PRO	2.5
1	C	275	ILE	2.5
1	A	307	PRO	2.5
1	C	310	VAL	2.5
1	B	97	ARG	2.4
1	C	301	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	237	GLY	2.4
1	C	283	ASN	2.3
1	C	155	ALA	2.3
1	A	124	LEU	2.3
1	C	314	PRO	2.3
1	C	119	ALA	2.3
1	C	140	ARG	2.3
1	C	106	PRO	2.3
1	A	127	ALA	2.2
1	C	309	LEU	2.2
1	A	123	LEU	2.2
1	A	314	PRO	2.2
1	C	439	GLY	2.2
1	A	478	ASP	2.2
1	C	468	PHE	2.2
1	A	288	VAL	2.1
1	A	192	LYS	2.1
1	A	285	ARG	2.1
1	A	221	ARG	2.1
1	A	242	ARG	2.1
1	C	300	PRO	2.0
1	A	295	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, 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
8	GD	A	510	1/1	0.55	0.13	92,92,92,92	1

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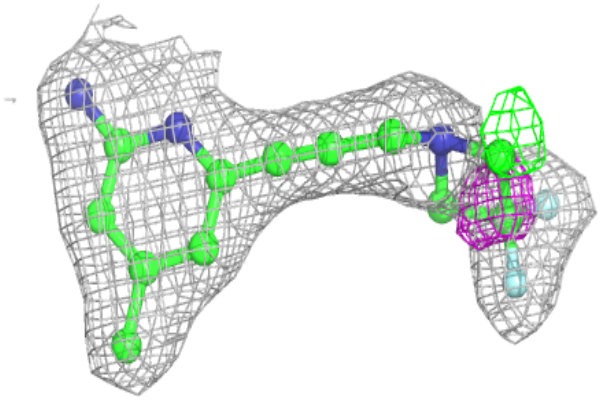
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	509	6/6	0.62	0.16	64,68,71,72	0
6	GOL	C	510	6/6	0.71	0.14	69,74,75,78	0
6	GOL	A	507	6/6	0.78	0.24	52,63,71,79	0
5	BTB	A	506	14/14	0.78	0.12	77,86,92,94	0
5	BTB	D	504	14/14	0.80	0.14	35,59,80,84	0
5	BTB	A	505	14/14	0.83	0.23	60,72,84,85	0
5	BTB	C	506	14/14	0.83	0.14	86,95,100,100	0
6	GOL	C	507	6/6	0.83	0.25	57,62,65,67	0
5	BTB	D	505	14/14	0.84	0.25	43,75,83,87	0
5	BTB	B	505	14/14	0.88	0.23	35,66,75,76	0
3	H4B	C	502	17/17	0.88	0.16	40,55,66,67	0
4	K7U	B	503	17/17	0.88	0.15	21,29,81,81	0
6	GOL	B	506	6/6	0.89	0.21	78,79,83,88	0
3	H4B	A	502	17/17	0.90	0.13	52,59,64,67	0
3	H4B	B	502	17/17	0.90	0.13	31,44,56,59	0
4	K7U	D	503	17/17	0.90	0.16	23,36,91,92	0
5	BTB	C	505	14/14	0.90	0.26	26,57,69,73	0
6	GOL	A	508	6/6	0.90	0.28	65,71,77,79	0
4	K7U	A	503	17/17	0.91	0.17	40,59,89,92	0
4	K7U	C	503	17/17	0.92	0.20	30,42,110,110	0
5	BTB	A	504	14/14	0.92	0.14	44,72,80,83	0
6	GOL	C	508	6/6	0.93	0.23	18,29,55,55	0
5	BTB	C	504	14/14	0.93	0.17	25,63,68,72	0
5	BTB	B	504	14/14	0.93	0.12	34,51,68,69	0
6	GOL	D	506	6/6	0.93	0.16	85,86,86,87	0
3	H4B	D	502	17/17	0.93	0.14	34,53,61,69	0
7	CL	A	509	1/1	0.95	0.08	66,66,66,66	0
2	HEM	A	501	43/43	0.95	0.14	35,55,68,70	0
7	CL	C	511	1/1	0.96	0.09	60,60,60,60	0
7	CL	D	507	1/1	0.96	0.05	44,44,44,44	0
7	CL	B	507	1/1	0.96	0.11	49,49,49,49	0
2	HEM	C	501	43/43	0.97	0.12	26,44,57,68	0
2	HEM	D	501	43/43	0.97	0.12	21,32,56,75	0
2	HEM	B	501	43/43	0.97	0.11	12,33,48,64	0
8	GD	D	508	1/1	0.98	0.18	49,49,49,49	0
8	GD	C	512	1/1	0.99	0.13	73,73,73,73	1
8	GD	B	508	1/1	0.99	0.18	45,45,45,45	0
9	ZN	A	511	1/1	0.99	0.13	48,48,48,48	0
9	ZN	C	513	1/1	1.00	0.12	38,38,38,38	0

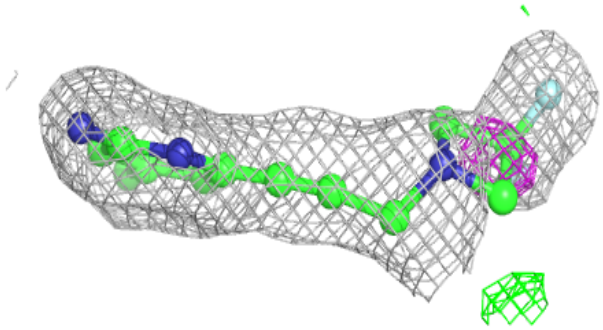
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

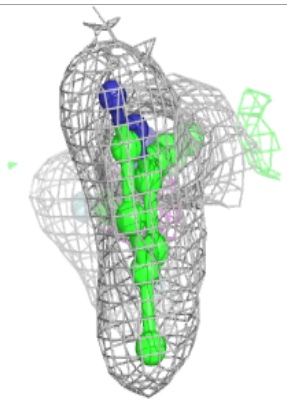
orientation to approximate a three-dimensional view.

Electron density around K7U 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)

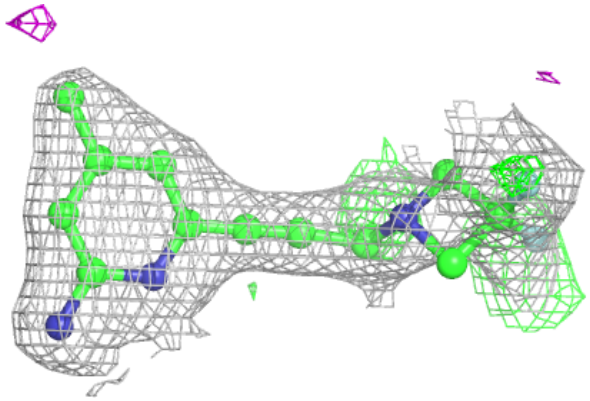


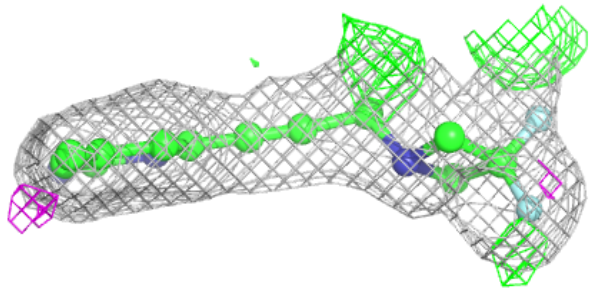


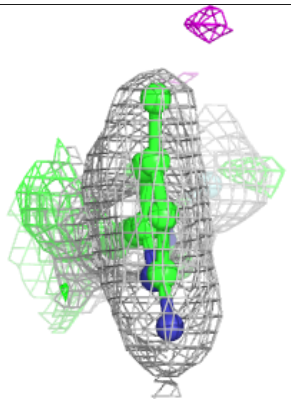


Electron density around K7U D 503:

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

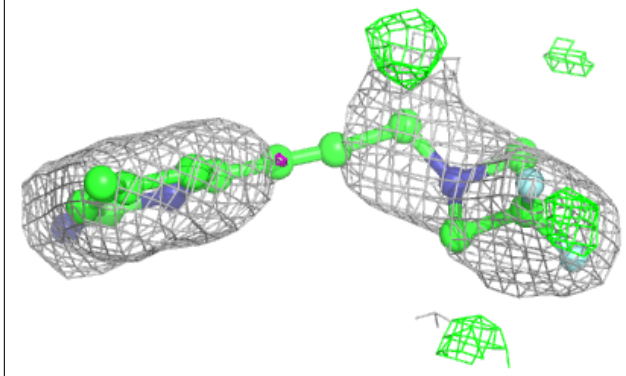


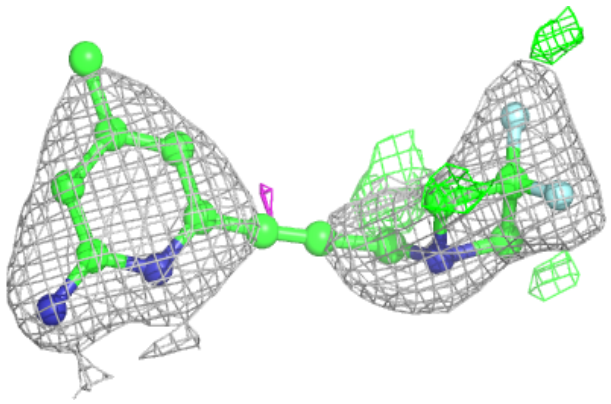


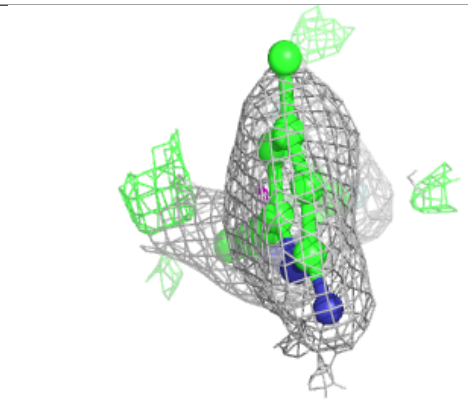


Electron density around K7U A 503:

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

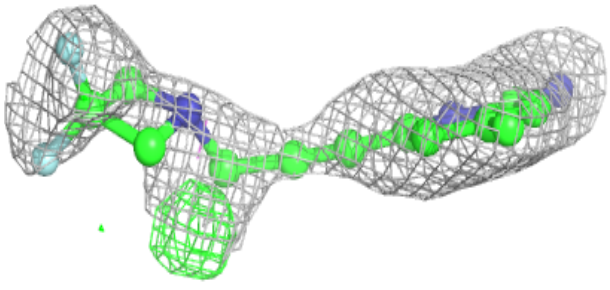


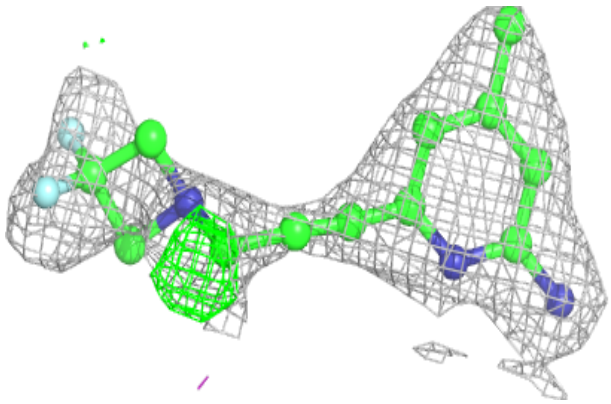


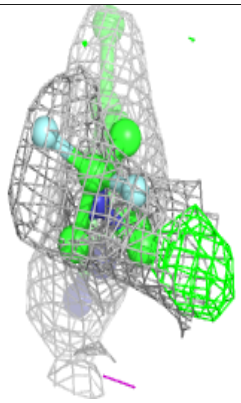


Electron density around K7U C 503:

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

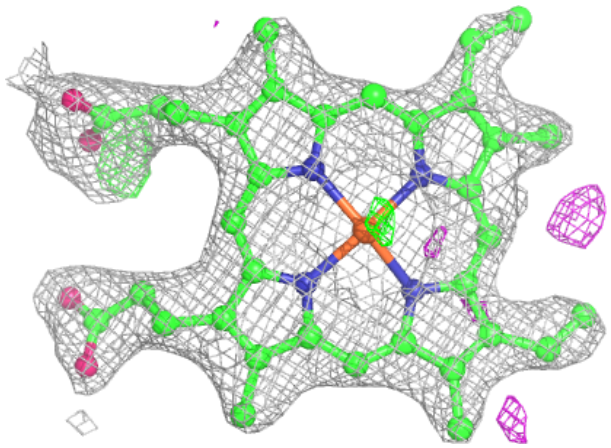


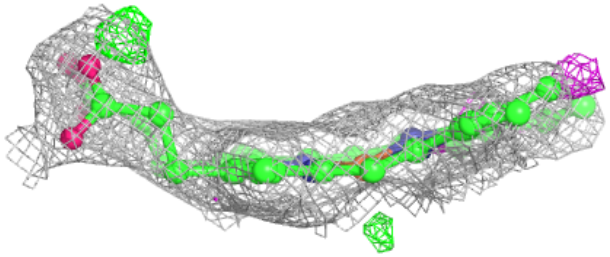


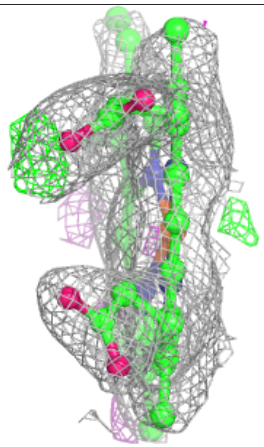


Electron density around HEM A 501:

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

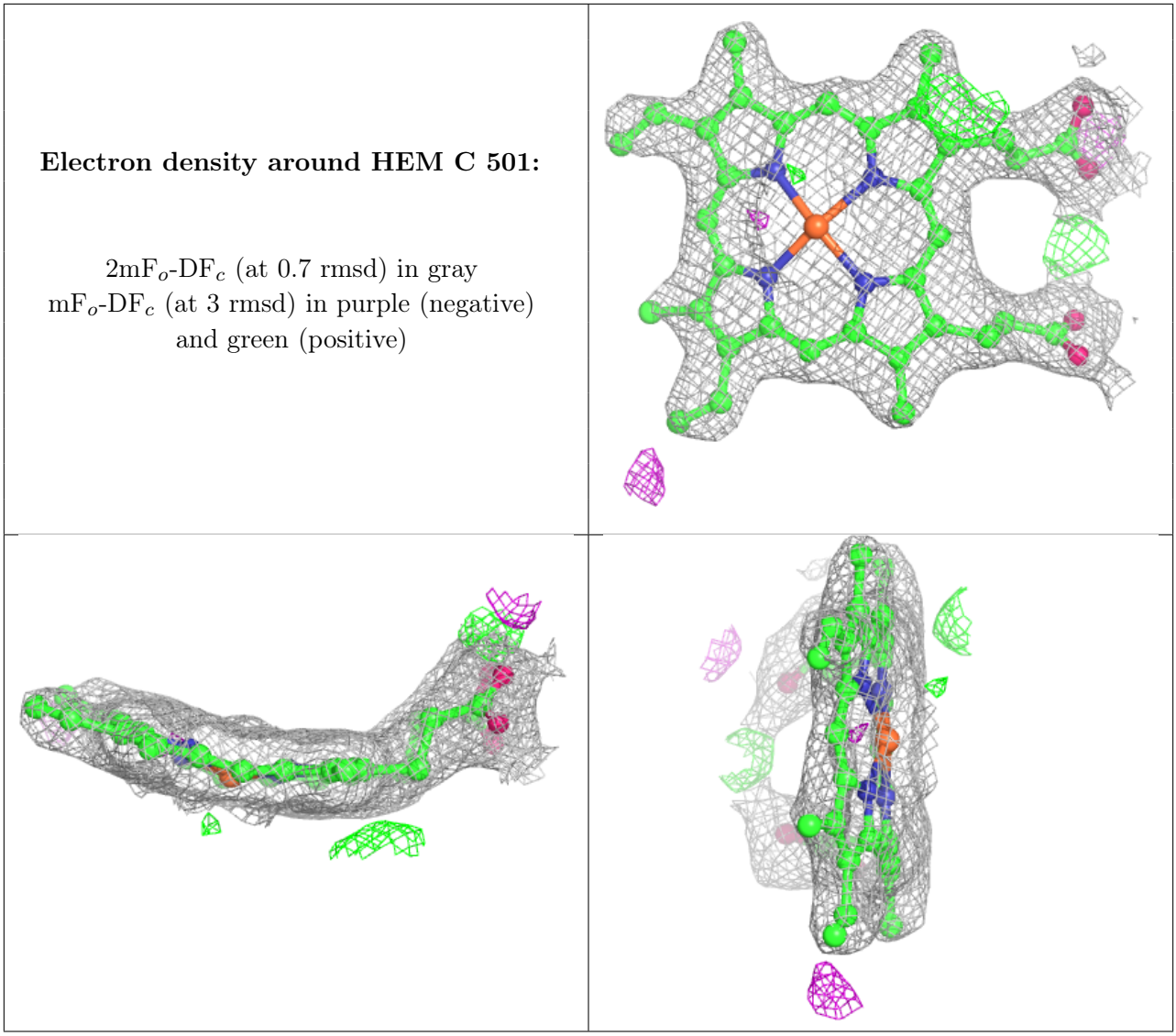






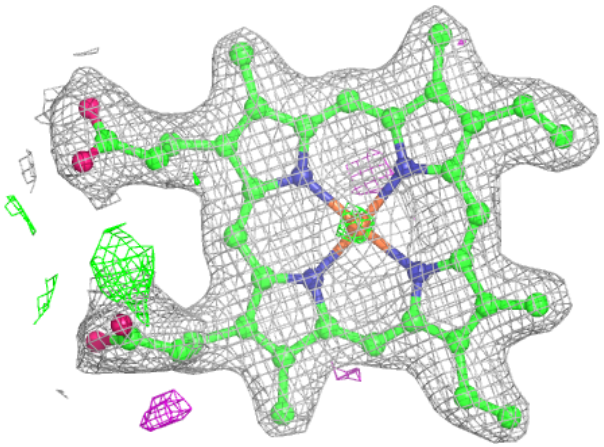
Electron density around HEM C 501:

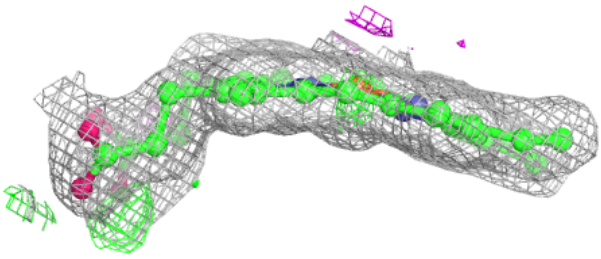
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

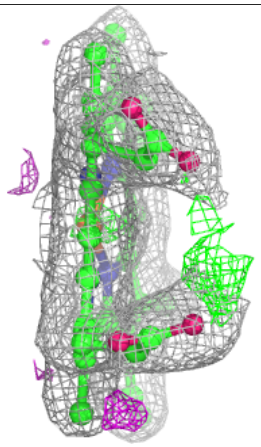


Electron density around HEM D 501:

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

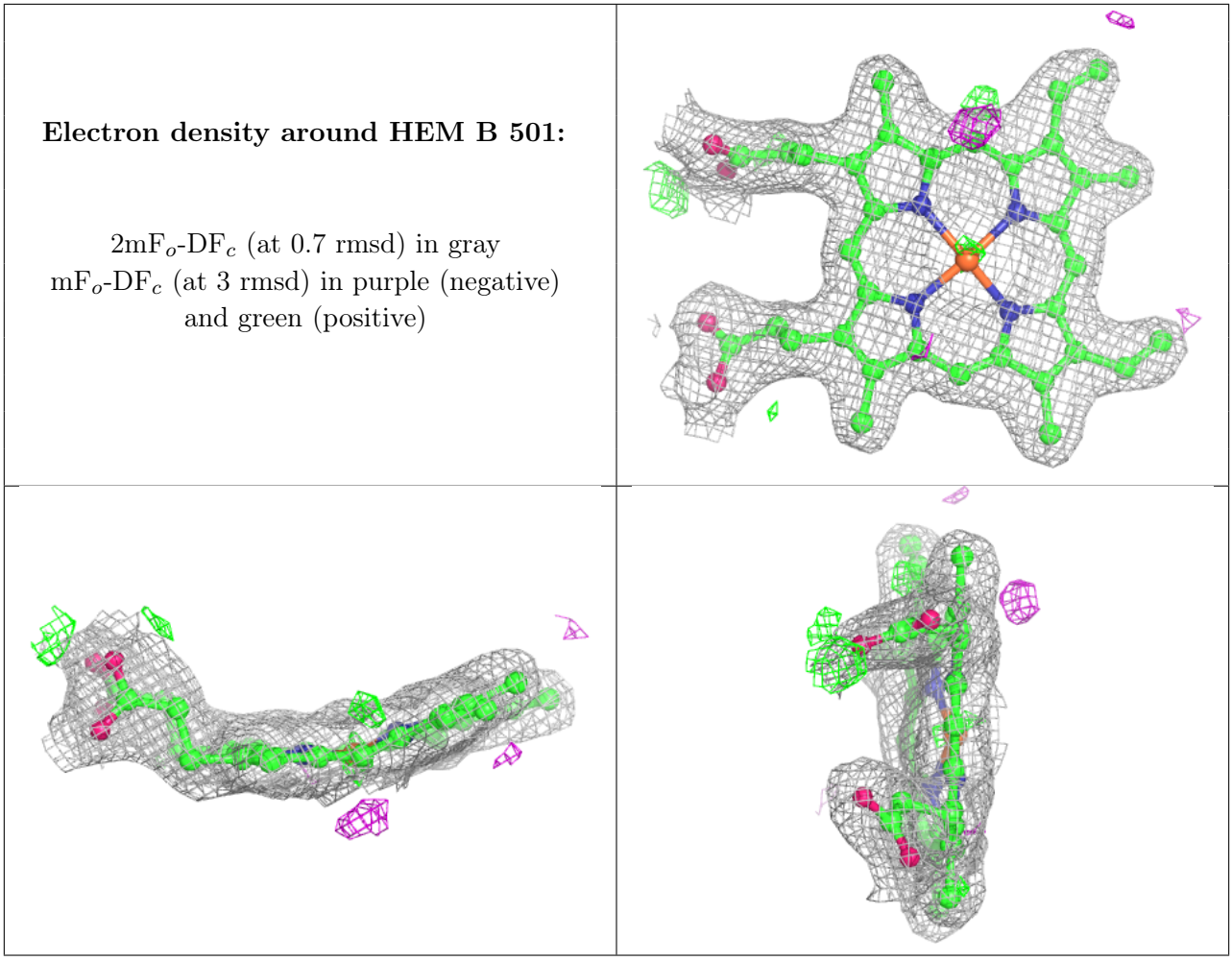






Electron density around HEM B 501:

$2mF_o$-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.