Full wwPDB X-ray Structure Validation Report (i)

Mar 25, 2023 – 12:07 pm GMT

PDB ID	:	7ZXD
Title	:	Crystal structure of CYP125 from Mycobacterium tuberculosis in complex with an inhibitor
Authors	:	Snee, M.; Katariya, M.; Levy, C.; Leys, D.
Deposited on	:	2022-05-20
Resolution	:	2.09 Å(reported)

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

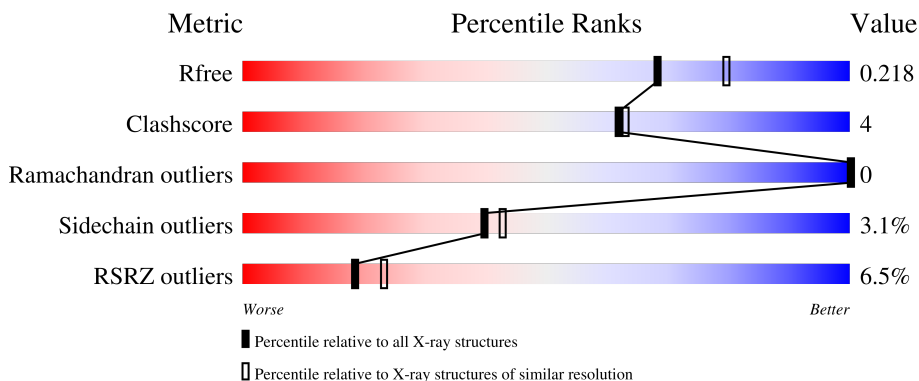|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.09 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		3.1%
RSRZ outliers		6.5%

Worse .... *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	418	% / 91% / 7% ··
1	B	418	9% / 87% / 10% ··
1	C	418	9% / 82% / 16% ·

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10380 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.
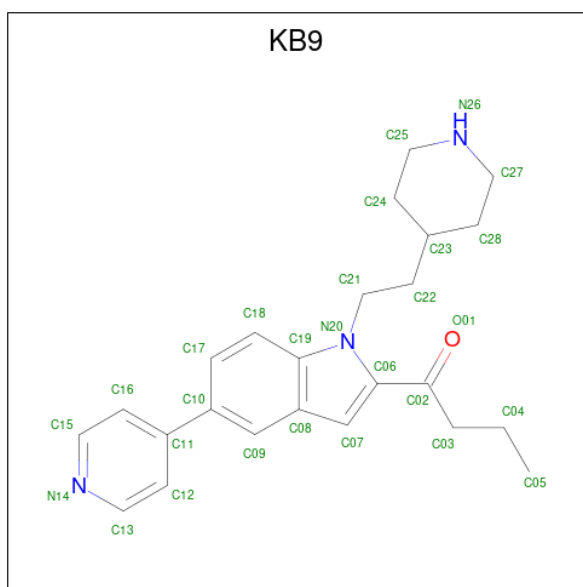
- Molecule 1 is a protein called Steroid C26-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	8	0
			3276	2077	578	607	14			
1	B	409	Total	C	N	O	S	0	4	0
			3242	2051	567	610	14			
1	C	409	Total	C	N	O	S	0	5	0
			3232	2046	563	609	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	-	expression tag	UNP P9WPP1
A	17	GLY	-	expression tag	UNP P9WPP1
B	16	ASN	-	expression tag	UNP P9WPP1
B	17	GLY	-	expression tag	UNP P9WPP1
C	16	ASN	-	expression tag	UNP P9WPP1
C	17	GLY	-	expression tag	UNP P9WPP1

- Molecule 2 is 1-[1-(2-piperidin-4-ylethyl)-5-pyridin-4-yl-indol-2-yl]butan-1-one (three-letter code: KB9) (formula: $C_{24}H_{29}N_3O$) (labeled as "Ligand of Interest" by depositor).

KB9

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	24	3	1		
2	A	1	Total	C	N	O	0	0
			28	24	3	1		
2	B	1	Total	C	N	O	0	0
			28	24	3	1		
2	C	1	Total	C	N	O	0	0
			28	24	3	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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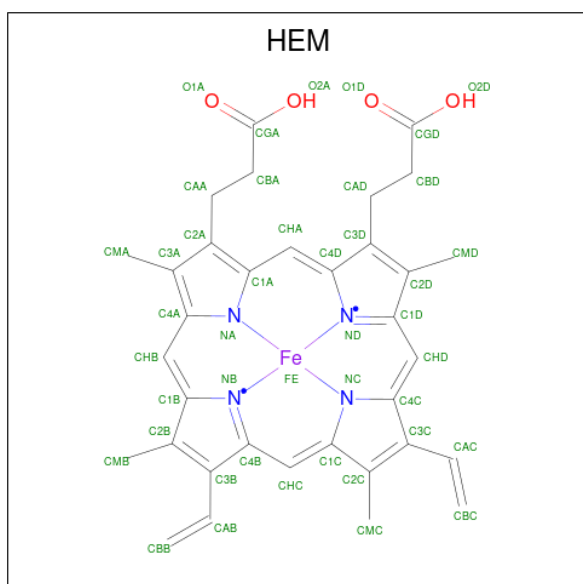
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	228	Total 228	O 228	0	0
6	B	85	Total 85	O 85	0	0
6	C	60	Total 60	O 60	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
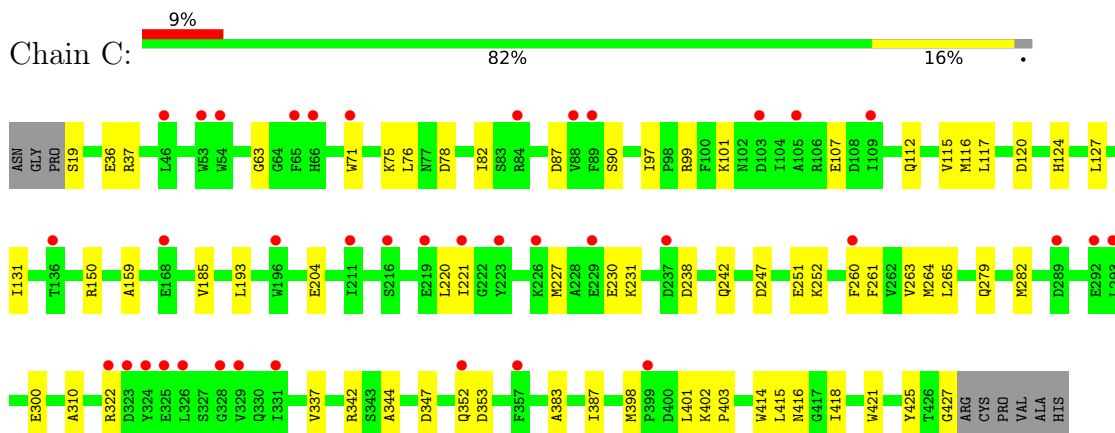
• Molecule 1: Steroid C26-monooxygenase
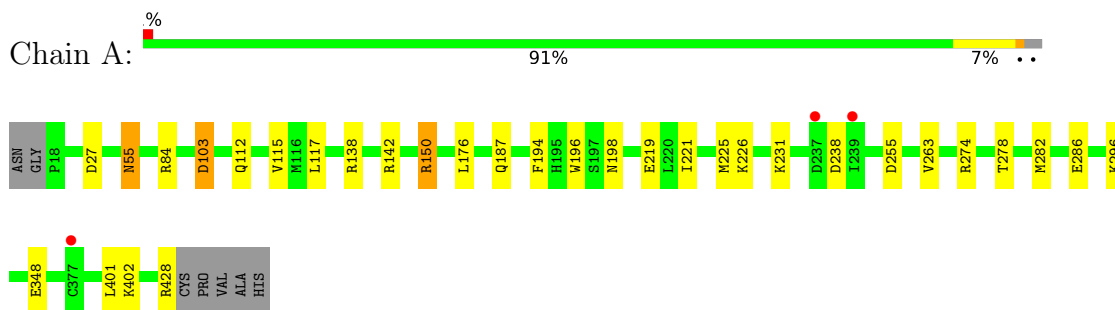
• Molecule 1: Steroid C26-monooxygenase
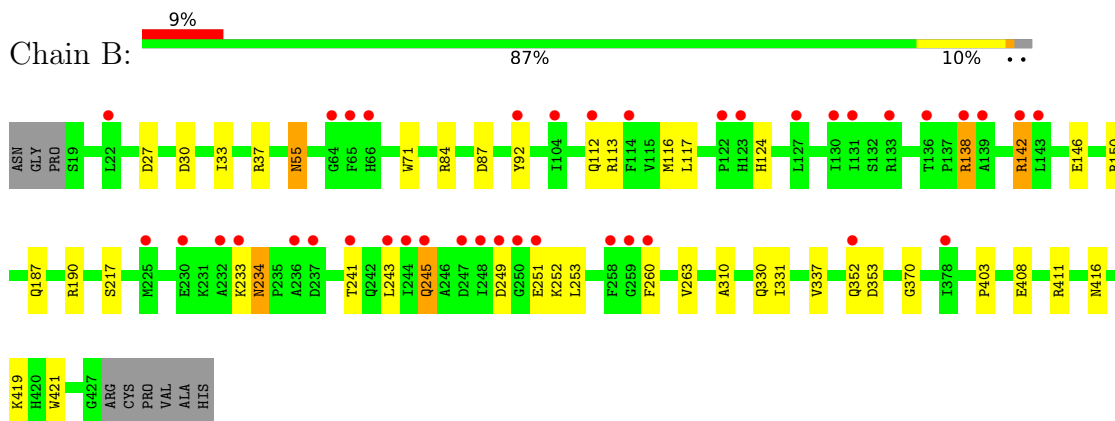
• Molecule 1: Steroid C26-monooxygenase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.24Å 69.22Å 144.14Å 90.00° 94.35° 90.00°	Depositor
Resolution (Å)	47.91 – 2.09 47.91 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.91-2.09) 96.9 (47.91-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.219 0.194 , 0.218	Depositor DCC
R_{free} test set	3938 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å²)	35.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 44.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10380	wwPDB-VP
Average B, all atoms (Å²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CL, SO4, HEM, KB9

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	0.25	0/3385	0.48	1/4588 (0.0%)
1	B	0.25	0/3329	0.48	0/4520
1	C	0.25	0/3330	0.47	0/4523
All	All	0.25	0/10044	0.48	1/13631 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	LEU	CA-CB-CG	5.40	127.73	115.30

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	3276	0	3178	20	0
1	B	3242	0	3097	23	0
1	C	3232	0	3094	39	0
2	A	56	0	0	1	0
2	B	28	0	0	1	0
2	C	28	0	0	2	0
3	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	4	0
3	C	43	0	30	2	0
4	A	15	0	0	1	0
5	A	1	0	0	0	0
6	A	228	0	0	2	0
6	B	85	0	0	1	0
6	C	60	0	0	2	0
All	All	10380	0	9459	85	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 4.

All (85) 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:37:ARG:HD2	1:C:37:ARG:HD2	1.52	0.90
3:C:502:HEM:HBC2	3:C:502:HEM:HHD	1.69	0.75
1:C:279:GLN:HG2	1:C:282:MET:HE3	1.70	0.74
1:A:150[B]:ARG:HH11	1:A:150[B]:ARG:HB2	1.56	0.71
1:A:84:ARG:NH2	4:A:505:SO4:O4	2.26	0.68
1:C:63:GLY:HA3	1:C:99:ARG:HD2	1.75	0.68
1:A:112[B]:GLN:OE1	6:A:601:HOH:O	2.15	0.65
1:A:103:ASP:OD1	6:A:602:HOH:O	2.15	0.63
1:C:99:ARG:NH1	6:C:602:HOH:O	2.32	0.63
1:C:159:ALA:HB2	1:C:398:MET:HG2	1.83	0.61
1:C:115:VAL:HB	1:C:264:MET:HG3	1.87	0.56
1:C:36:GLU:OE1	6:C:601:HOH:O	2.18	0.56
1:C:107:GLU:N	1:C:107:GLU:OE1	2.39	0.56
1:C:402:LYS:HD2	1:C:427:GLY:HA2	1.90	0.54
1:C:220:LEU:HB2	1:C:263:VAL:HG12	1.91	0.53
1:A:27:ASP:HA	1:A:55:ASN:HD21	1.74	0.52
1:A:221:ILE:O	1:A:225:MET:HG3	2.10	0.52
1:A:117:LEU:HD22	2:A:502:KB9:C16	2.41	0.51
1:C:117:LEU:HD22	2:C:501:KB9:C16	2.41	0.51
3:C:502:HEM:HMB2	3:C:502:HEM:HBB2	1.93	0.50
3:B:502:HEM:HMC1	3:B:502:HEM:HBC2	1.92	0.50
1:B:233:LYS:C	1:B:234:ASN:HD22	2.14	0.50
1:B:27:ASP:HA	1:B:55:ASN:HD21	1.75	0.49
1:C:185:VAL:HG21	1:C:193:LEU:HD22	1.94	0.48
1:A:150[A]:ARG:HH21	1:A:187:GLN:HE22	1.61	0.48
1:B:71:TRP:CD1	1:B:331:ILE:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:MET:HG2	1:B:124:HIS:CD2	2.49	0.48
1:C:238:ASP:O	1:C:242:GLN:HG2	2.13	0.48
1:C:247:ASP:OD1	1:C:251:GLU:N	2.44	0.48
1:C:101:LYS:HG2	1:C:204:GLU:HG2	1.95	0.48
1:C:279:GLN:HE22	1:C:416:ASN:ND2	2.12	0.47
1:B:146:GLU:O	1:B:150:ARG:HG3	2.14	0.47
3:B:502:HEM:HMB2	3:B:502:HEM:HBB2	1.96	0.47
1:B:92:TYR:CZ	1:B:113:ARG:HD3	2.50	0.47
1:B:30:ASP:HB3	1:B:33:ILE:HD12	1.97	0.46
1:B:403:PRO:HB3	1:B:421:TRP:CZ2	2.50	0.46
1:C:116:MET:H	1:C:264:MET:HE2	1.81	0.46
1:A:226[B]:LYS:HB2	1:A:226[B]:LYS:HE2	1.57	0.46
1:B:243:LEU:HB3	1:B:253:LEU:HD12	1.96	0.46
1:B:408:GLU:HG2	1:B:419:LYS:HE3	1.97	0.46
1:C:97[A]:ILE:HD11	2:C:501:KB9:C18	2.45	0.46
1:A:196:TRP:NE1	1:A:219[A]:GLU:OE1	2.49	0.46
1:C:353:ASP:N	1:C:353:ASP:OD1	2.49	0.46
1:B:117:LEU:HD22	2:B:501:KB9:C12	2.46	0.46
1:C:310:ALA:O	1:C:342:ARG:NH2	2.50	0.45
1:A:198:ASN:ND2	1:A:274:ARG:HH22	2.15	0.45
1:C:265:LEU:HD23	1:C:265:LEU:HA	1.78	0.45
1:C:260:PHE:HA	1:C:263:VAL:HG22	1.97	0.45
1:A:226[B]:LYS:NZ	1:B:353[B]:ASP:OD2	2.50	0.44
1:B:353[B]:ASP:N	1:B:353[B]:ASP:OD1	2.48	0.44
1:C:87:ASP:N	1:C:87:ASP:OD1	2.50	0.44
1:C:131:ILE:HD12	1:C:261:PHE:CD1	2.52	0.44
1:B:138:ARG:O	1:B:142:ARG:HB2	2.17	0.44
1:B:241:THR:O	1:B:245:GLN:HG3	2.18	0.44
1:A:150[B]:ARG:HH11	1:A:150[B]:ARG:CB	2.27	0.43
1:B:71:TRP:HB2	1:B:337:VAL:HG12	2.01	0.43
1:B:260:PHE:HA	1:B:263:VAL:HG12	2.00	0.43
1:C:78:ASP:O	1:C:82:ILE:HG13	2.18	0.43
1:C:403:PRO:HB3	1:C:421:TRP:CZ2	2.54	0.43
1:C:71:TRP:HB2	1:C:337:VAL:HG12	2.00	0.43
1:B:92:TYR:CE2	1:B:113:ARG:HD3	2.54	0.42
1:C:116:MET:HG2	1:C:124:HIS:CD2	2.54	0.42
1:A:176:LEU:HB3	1:A:194:PHE:CE1	2.54	0.42
3:B:502:HEM:O2A	6:B:601:HOH:O	2.21	0.42
1:A:238:ASP:OD1	1:A:238:ASP:N	2.52	0.42
1:A:278:THR:O	1:A:282:MET:HG3	2.19	0.42
1:C:414:TRP:CZ3	1:C:415:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:SER:OG	1:C:120:ASP:OD2	2.28	0.42
1:C:127:LEU:O	1:C:131:ILE:HG12	2.20	0.42
1:B:310:ALA:O	1:B:416:ASN:ND2	2.52	0.42
1:C:221:ILE:HG13	1:C:263:VAL:HG11	2.02	0.42
1:C:76:LEU:HD12	1:C:344:ALA:O	2.20	0.41
1:B:370:GLY:HA3	3:B:502:HEM:HBA1	2.02	0.41
1:A:348:GLU:H	1:A:348:GLU:CD	2.23	0.41
1:C:401:LEU:HD12	1:C:425:TYR:HD1	1.85	0.41
1:C:282:MET:CE	1:C:418:ILE:HG13	2.50	0.41
1:C:383:ALA:O	1:C:387:ILE:HG13	2.20	0.41
1:B:87:ASP:OD1	1:B:87:ASP:N	2.52	0.41
1:A:221:ILE:HG13	1:A:263:VAL:HG21	2.02	0.41
1:C:75:LYS:NZ	1:C:347:ASP:OD1	2.53	0.41
1:C:112:GLN:O	1:C:115:VAL:HG22	2.20	0.41
1:B:187:GLN:HA	1:B:190:ARG:HG3	2.03	0.41
1:C:227:MET:O	1:C:231:LYS:HG2	2.21	0.40
1:A:225:MET:HE3	1:A:255:ASP:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/418 (100%)	407 (98%)	10 (2%)	0	100	100
1	B	411/418 (98%)	401 (98%)	10 (2%)	0	100	100
1	C	412/418 (99%)	404 (98%)	8 (2%)	0	100	100
All	All	1240/1254 (99%)	1212 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/341 (100%)	330 (97%)	11 (3%)	39	41
1	B	335/341 (98%)	320 (96%)	15 (4%)	27	27
1	C	335/341 (98%)	327 (98%)	8 (2%)	49	53
All	All	1011/1023 (99%)	977 (97%)	34 (3%)	40	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	103	ASP
1	A	138	ARG
1	A	142	ARG
1	A	150[A]	ARG
1	A	150[B]	ARG
1	A	231	LYS
1	A	286	GLU
1	A	296	LYS
1	A	402	LYS
1	A	428	ARG
1	B	55	ASN
1	B	84	ARG
1	B	112	GLN
1	B	138	ARG
1	B	142	ARG
1	B	217	SER
1	B	234	ASN
1	B	245	GLN
1	B	249	ASP
1	B	251	GLU
1	B	252	LYS
1	B	330	GLN
1	B	352[A]	GLN
1	B	352[B]	GLN
1	B	411	ARG

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Mol	Chain	Res	Type
1	C	19	SER
1	C	150	ARG
1	C	230	GLU
1	C	252	LYS
1	C	300	GLU
1	C	322	ARG
1	C	352[A]	GLN
1	C	352[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	330	GLN
1	B	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	KB9	A	502	-	27,31,31	0.87	1 (3%)	34,42,42	1.08	2 (5%)
3	HEM	A	503	6,1	41,50,50	1.44	3 (7%)	45,82,82	1.44	6 (13%)
4	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	506	-	4,4,4	0.15	0	6,6,6	0.04	0
2	KB9	A	501	-	27,31,31	0.86	1 (3%)	34,42,42	1.04	0
4	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.05	0
2	KB9	B	501	-	27,31,31	0.85	1 (3%)	34,42,42	1.49	5 (14%)
3	HEM	C	502	6,1	41,50,50	1.52	4 (9%)	45,82,82	1.49	11 (24%)
2	KB9	C	501	-	27,31,31	0.89	1 (3%)	34,42,42	1.12	2 (5%)
3	HEM	B	502	6,1	41,50,50	1.44	4 (9%)	45,82,82	1.47	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KB9	A	502	-	-	2/12/24/24	0/4/4/4
3	HEM	A	503	6,1	-	0/12/54/54	-
2	KB9	A	501	-	-	2/12/24/24	0/4/4/4
2	KB9	B	501	-	-	4/12/24/24	0/4/4/4
3	HEM	C	502	6,1	-	0/12/54/54	-
2	KB9	C	501	-	-	5/12/24/24	0/4/4/4
3	HEM	B	502	6,1	-	1/12/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	HEM	C3C-C2C	-5.07	1.33	1.40
3	B	502	HEM	C3C-CAC	3.81	1.55	1.47
3	A	503	HEM	C3C-C2C	-3.80	1.35	1.40
3	A	503	HEM	C3C-CAC	3.79	1.55	1.47
3	B	502	HEM	C3C-C2C	-3.65	1.35	1.40
3	C	502	HEM	C3C-CAC	3.18	1.54	1.47
3	C	502	HEM	CAB-C3B	3.02	1.55	1.47
3	B	502	HEM	CAB-C3B	3.02	1.55	1.47
3	A	503	HEM	CAB-C3B	2.90	1.55	1.47
2	A	502	KB9	O01-C02	-2.27	1.18	1.22
2	A	501	KB9	O01-C02	-2.15	1.18	1.22
2	B	501	KB9	O01-C02	-2.14	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KB9	O01-C02	-2.13	1.18	1.22
3	B	502	HEM	CAA-C2A	2.12	1.55	1.52
3	C	502	HEM	FE-NB	2.00	2.06	1.96

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	KB9	C27-C28-C23	4.33	118.84	112.14
3	C	502	HEM	C4C-CHD-C1D	3.53	127.22	122.56
2	B	501	KB9	C28-C23-C24	3.40	117.64	109.33
3	C	502	HEM	C4D-ND-C1D	3.24	108.42	105.07
3	A	503	HEM	C4C-CHD-C1D	3.04	126.56	122.56
3	B	502	HEM	C4D-ND-C1D	2.99	108.17	105.07
3	A	503	HEM	C4D-ND-C1D	2.95	108.12	105.07
3	B	502	HEM	C1B-NB-C4B	2.93	108.10	105.07
3	B	502	HEM	C4C-CHD-C1D	2.88	126.36	122.56
3	A	503	HEM	CBA-CAA-C2A	-2.72	107.97	112.62
2	B	501	KB9	C21-C22-C23	-2.65	109.02	115.07
3	C	502	HEM	C2C-C3C-C4C	2.63	108.73	106.90
2	C	501	KB9	C21-C22-C23	-2.50	109.37	115.07
3	A	503	HEM	C1B-NB-C4B	2.49	107.65	105.07
3	A	503	HEM	CMC-C2C-C3C	2.38	129.12	124.68
3	B	502	HEM	C4B-CHC-C1C	2.37	125.68	122.56
3	B	502	HEM	C3B-C2B-C1B	2.33	108.22	106.49
3	C	502	HEM	C1B-NB-C4B	2.32	107.47	105.07
3	B	502	HEM	CMC-C2C-C3C	2.25	128.89	124.68
3	C	502	HEM	C4B-CHC-C1C	2.22	125.49	122.56
2	A	502	KB9	C17-C10-C11	-2.21	117.53	121.36
3	C	502	HEM	C3C-C4C-NC	-2.20	106.80	110.94
3	C	502	HEM	C3B-C2B-C1B	2.19	108.11	106.49
2	C	501	KB9	C03-C02-C06	2.19	120.26	118.03
3	C	502	HEM	CBA-CAA-C2A	-2.19	108.88	112.62
3	C	502	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
3	C	502	HEM	C3D-C4D-ND	-2.15	107.77	110.17
2	B	501	KB9	C28-C27-N26	2.14	114.97	110.64
3	B	502	HEM	C3D-C4D-ND	-2.14	107.79	110.17
3	A	503	HEM	C3D-C4D-ND	-2.12	107.81	110.17
2	A	502	KB9	C15-N14-C13	2.12	121.83	116.85
3	C	502	HEM	C2D-C1D-ND	-2.02	107.47	109.88
2	B	501	KB9	C03-C02-C06	2.01	120.08	118.03

There are no chirality outliers.
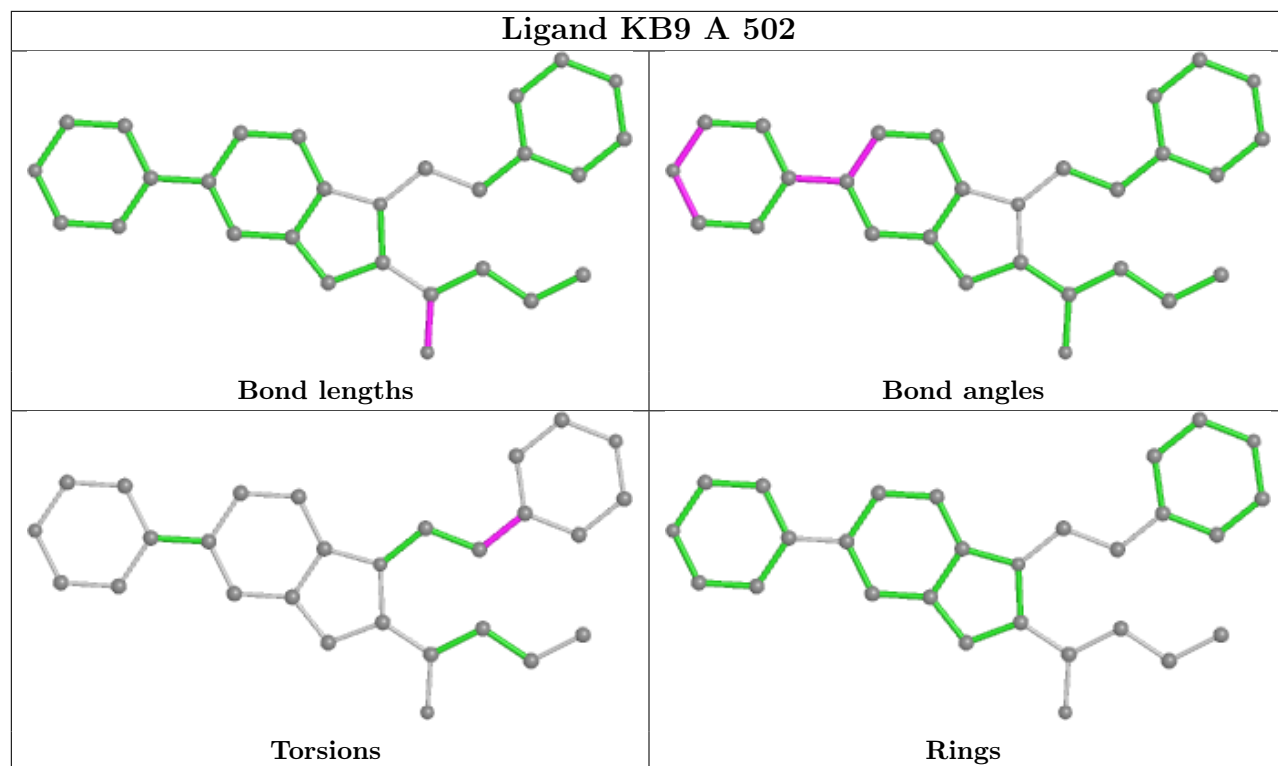
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	KB9	C02-C03-C04-C05
2	C	501	KB9	C02-C03-C04-C05
2	C	501	KB9	C06-C02-C03-C04
2	B	501	KB9	O01-C02-C03-C04
2	C	501	KB9	O01-C02-C03-C04
2	B	501	KB9	C06-C02-C03-C04
2	A	501	KB9	C06-C02-C03-C04
2	A	502	KB9	C21-C22-C23-C28
2	C	501	KB9	C21-C22-C23-C28
2	A	501	KB9	O01-C02-C03-C04
2	A	502	KB9	C21-C22-C23-C24
2	B	501	KB9	C21-C22-C23-C28
2	C	501	KB9	C21-C22-C23-C24
3	B	502	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	KB9	1	0
4	A	505	SO4	1	0
2	B	501	KB9	1	0
3	C	502	HEM	2	0
2	C	501	KB9	2	0
3	B	502	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.
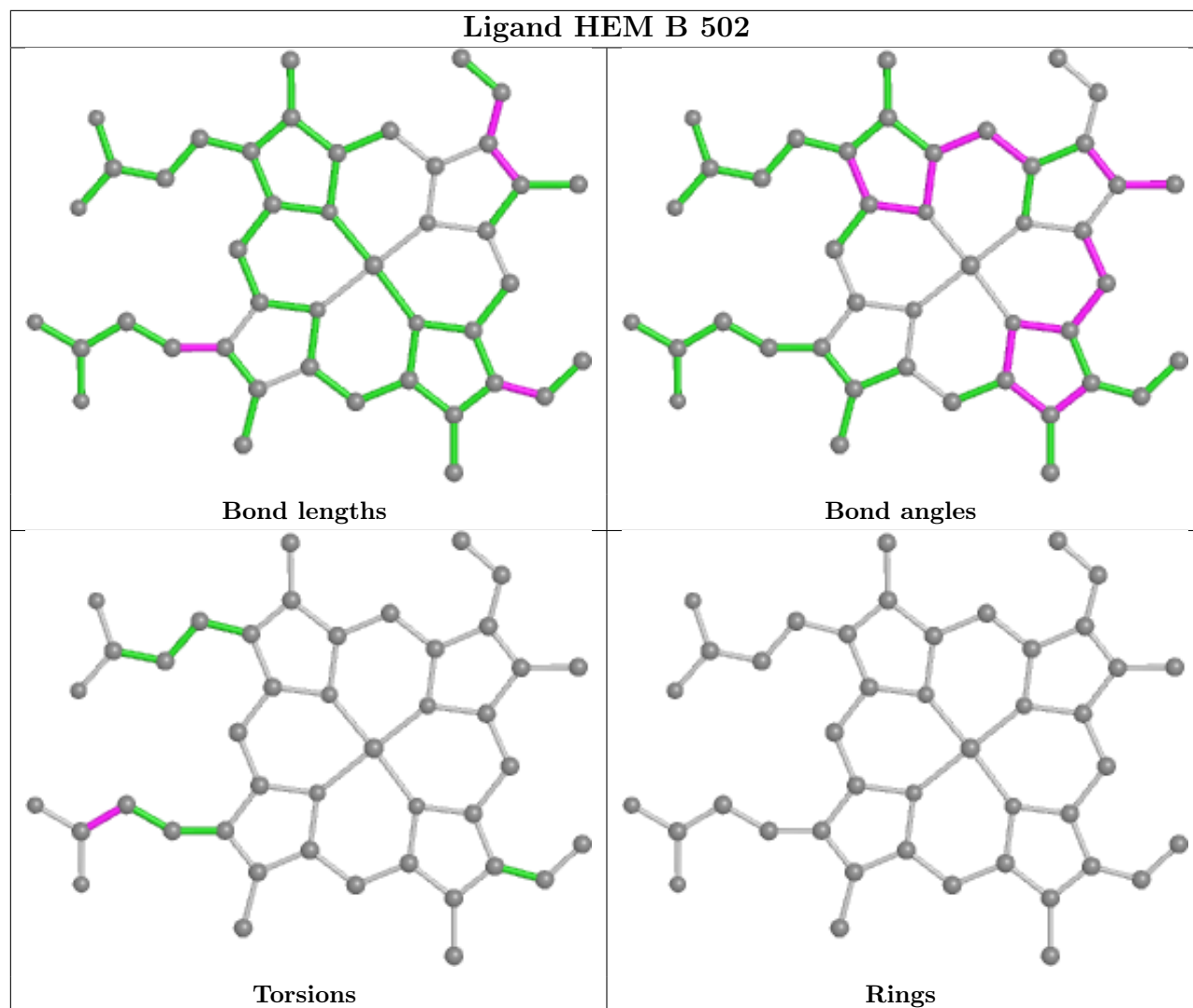
Ligand KB9 A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand KB9 A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand KB9 B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand KB9 C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 502

Bond lengths

Bond angles

Torsions

Rings
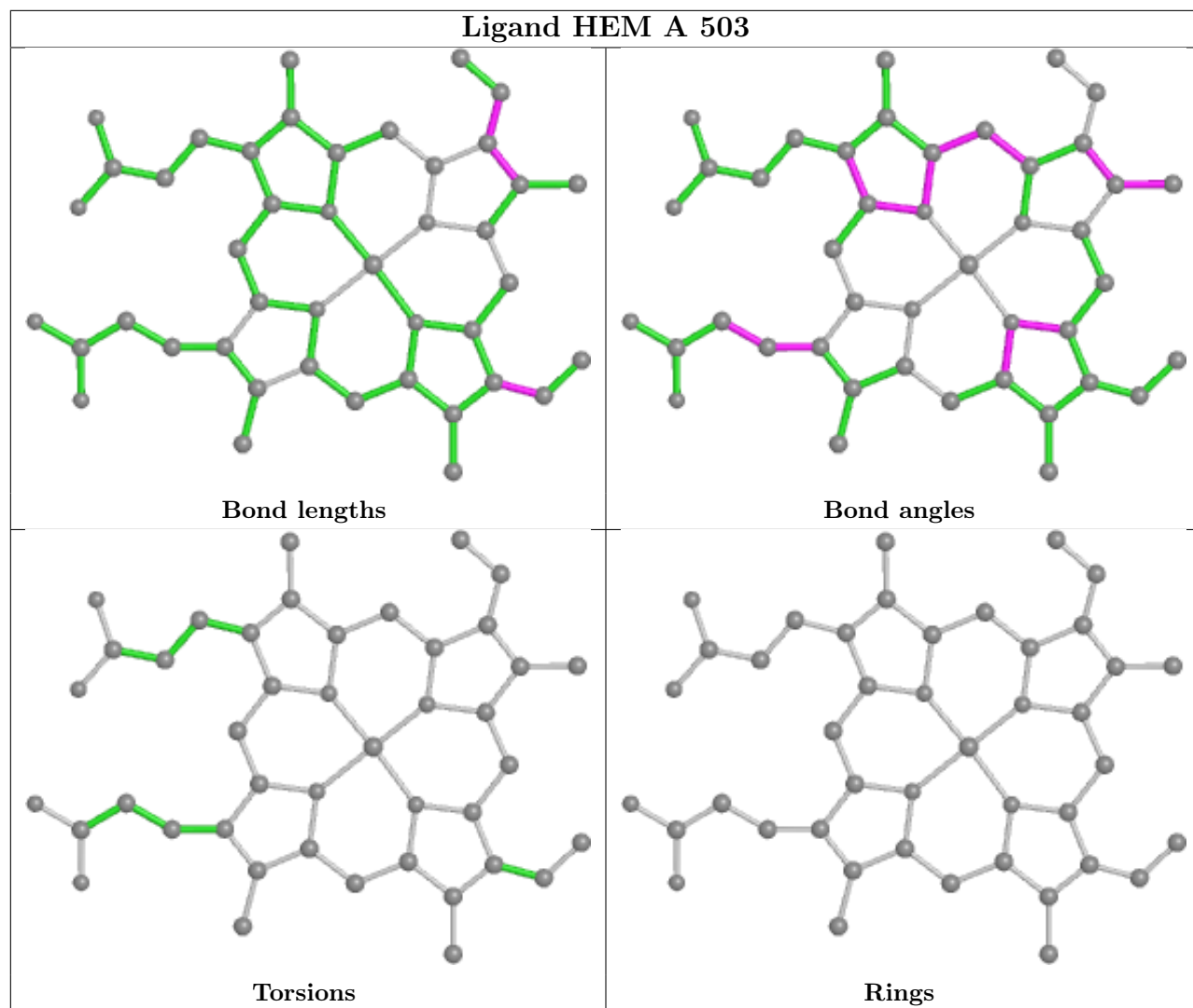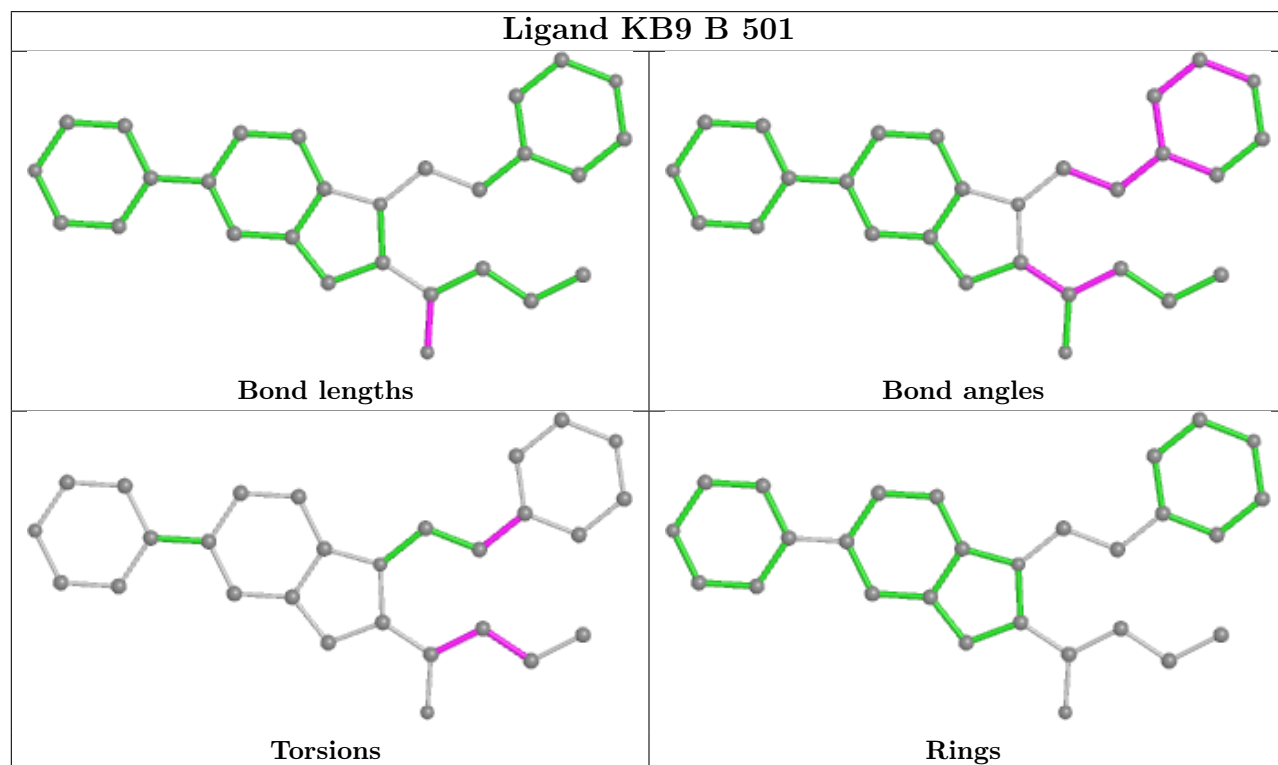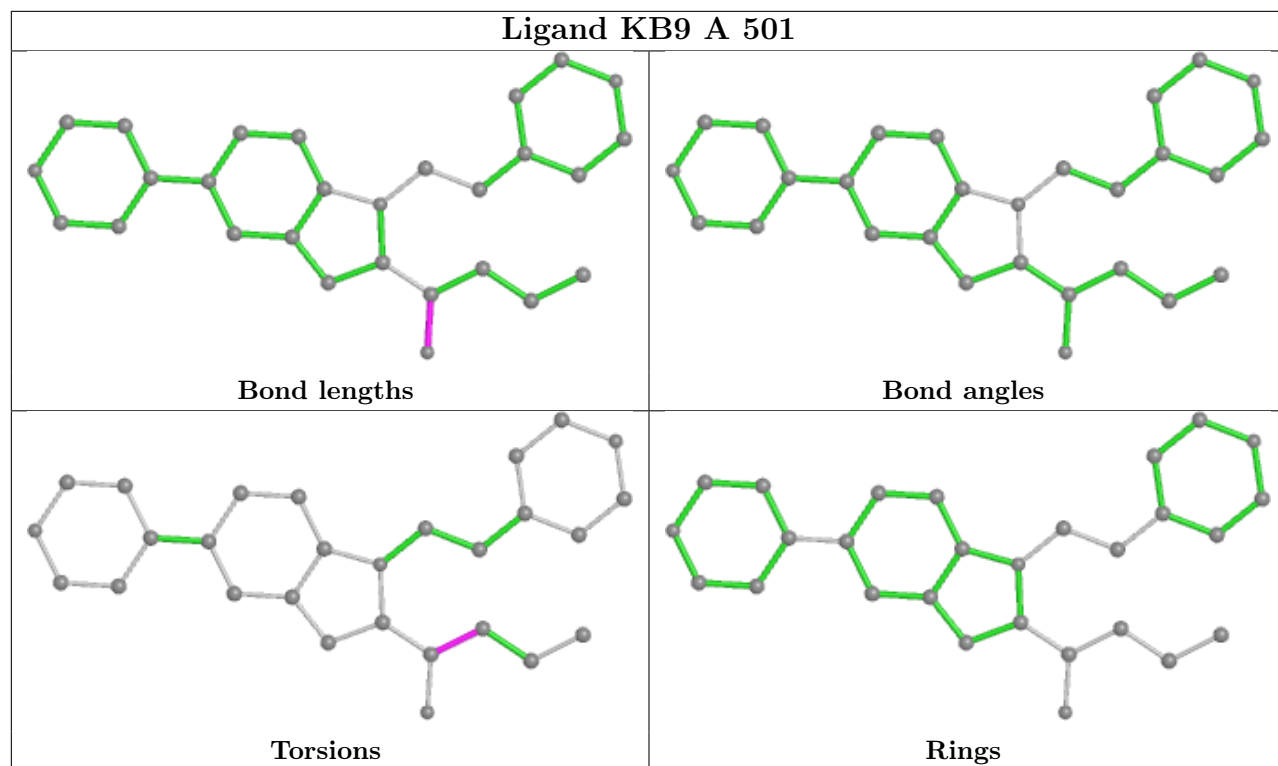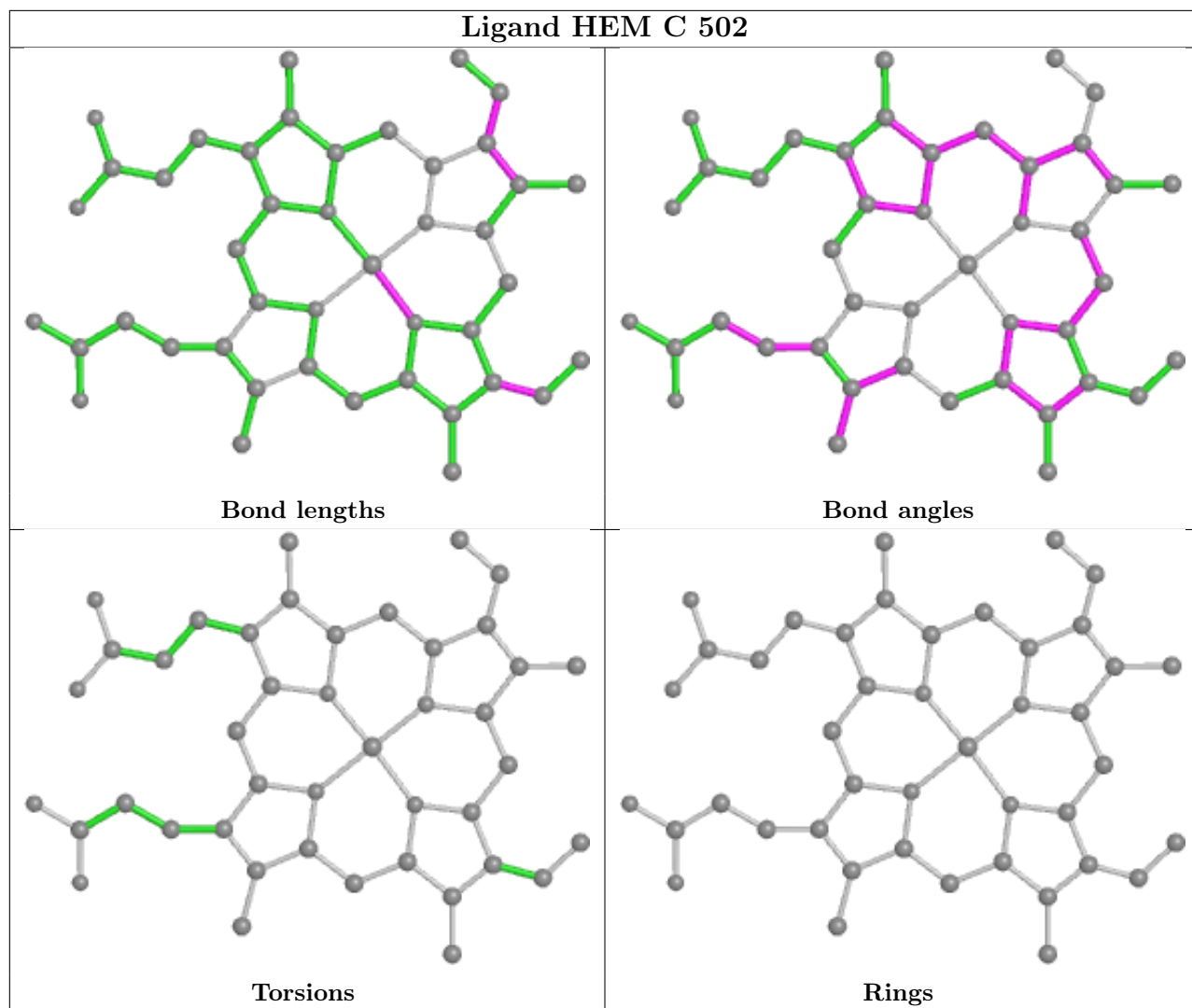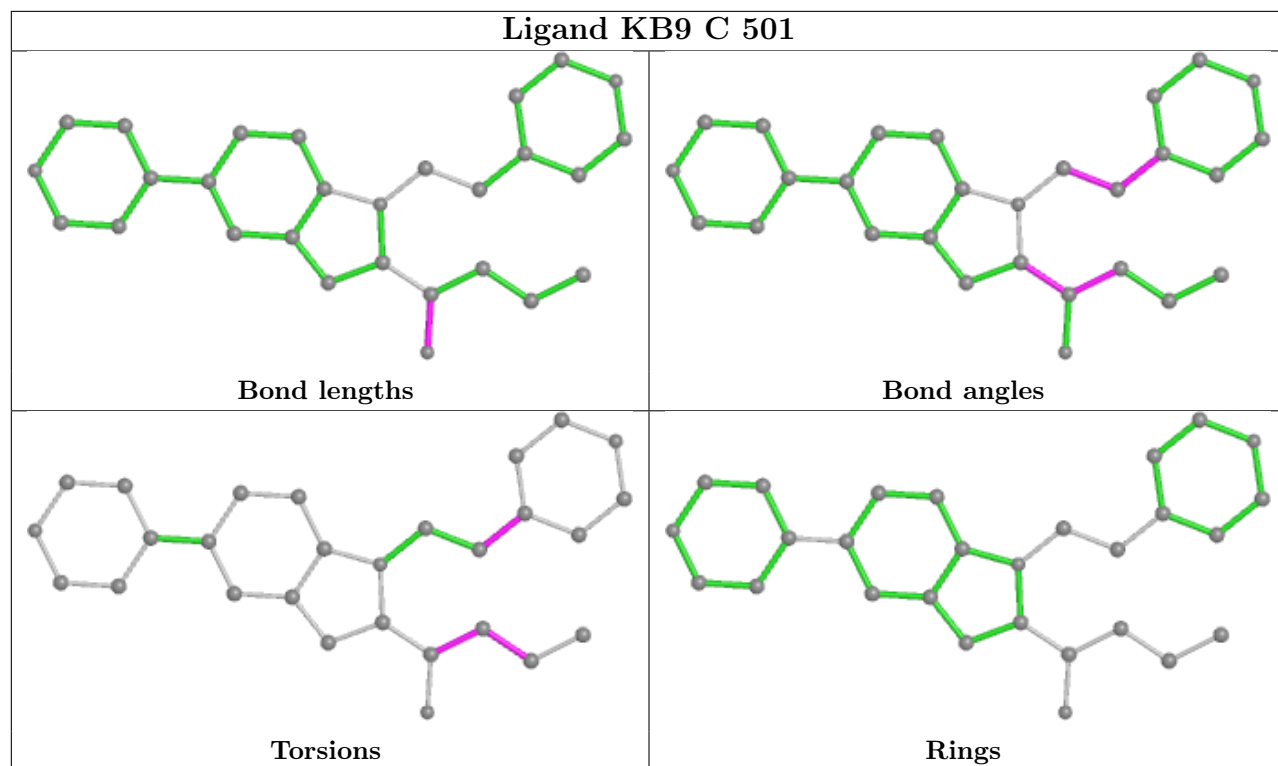
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/418 (98%)	0.20	3 (0%)	87	89	21, 33, 56, 101	0
1	B	409/418 (97%)	0.51	39 (9%)	8	10	34, 54, 90, 128	0
1	C	409/418 (97%)	0.63	38 (9%)	8	11	47, 61, 84, 103	1 (0%)
All	All	1229/1254 (98%)	0.45	80 (6%)	18	23	21, 52, 82, 128	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	PRO	4.9
1	B	248	ILE	4.8
1	C	237[A]	ASP	4.6
1	B	114	PHE	4.6
1	C	53	TRP	4.5
1	C	109	ILE	4.1
1	B	245	GLN	4.1
1	B	92	TYR	4.0
1	C	289	ASP	3.9
1	B	136	THR	3.7
1	B	138	ARG	3.7
1	C	326	LEU	3.6
1	C	71	TRP	3.6
1	B	112	GLN	3.6
1	C	89	PHE	3.4
1	B	130	ILE	3.3
1	B	131	ILE	3.3
1	B	250	GLY	3.3
1	C	196	TRP	3.2
1	C	331	ILE	3.1
1	B	123	HIS	3.1
1	C	216	SER	3.1
1	B	247	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	3.1
1	B	233	LYS	3.0
1	C	46	LEU	3.0
1	C	325	GLU	2.9
1	C	223	TYR	2.9
1	B	237	ASP	2.8
1	B	225	MET	2.8
1	C	88	VAL	2.8
1	C	105	ALA	2.7
1	A	377	CYS	2.7
1	B	232	ALA	2.7
1	C	357	PHE	2.6
1	A	237	ASP	2.5
1	C	322	ARG	2.5
1	C	293	LEU	2.5
1	B	236	ALA	2.5
1	C	54	TRP	2.5
1	C	260	PHE	2.5
1	B	127	LEU	2.5
1	B	142	ARG	2.5
1	C	324	TYR	2.5
1	C	211	ILE	2.5
1	B	241	THR	2.4
1	C	226	LYS	2.4
1	C	328	GLY	2.4
1	B	65	PHE	2.4
1	B	251	GLU	2.4
1	B	249	ASP	2.4
1	B	104	ILE	2.3
1	B	230	GLU	2.3
1	C	399	PRO	2.3
1	C	65	PHE	2.3
1	C	136	THR	2.3
1	C	352[A]	GLN	2.3
1	B	258	PHE	2.3
1	B	260	PHE	2.3
1	C	229	GLU	2.3
1	B	378	ILE	2.3
1	B	66	HIS	2.2
1	C	329	VAL	2.2
1	B	259	GLY	2.2
1	C	103	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	168[A]	GLU	2.2
1	C	323	ASP	2.1
1	B	244	ILE	2.1
1	C	219	GLU	2.1
1	B	139	ALA	2.1
1	C	66	HIS	2.1
1	C	292	GLU	2.1
1	C	221	ILE	2.1
1	B	143	LEU	2.1
1	B	352[A]	GLN	2.1
1	C	84	ARG	2.0
1	B	243	LEU	2.0
1	B	64	GLY	2.0
1	A	239	ILE	2.0
1	B	22	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	SO4	A	505	5/5	0.70	0.24	72,97,114,138	0
4	SO4	A	504	5/5	0.74	0.19	69,74,102,126	0
2	KB9	B	501	28/28	0.84	0.28	58,76,91,93	0
4	SO4	A	506	5/5	0.84	0.24	44,60,83,86	0
2	KB9	C	501	28/28	0.88	0.29	56,67,73,75	0
2	KB9	A	502	28/28	0.89	0.15	26,36,39,41	0
2	KB9	A	501	28/28	0.91	0.14	36,39,46,48	0
3	HEM	C	502	43/43	0.94	0.15	49,54,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	B	502	43/43	0.96	0.13	40,47,57,60	0
5	CL	A	507	1/1	0.98	0.11	36,36,36,36	0
3	HEM	A	503	43/43	0.99	0.18	19,22,28,29	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 KB9 B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
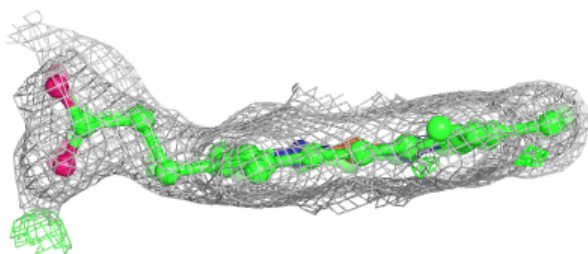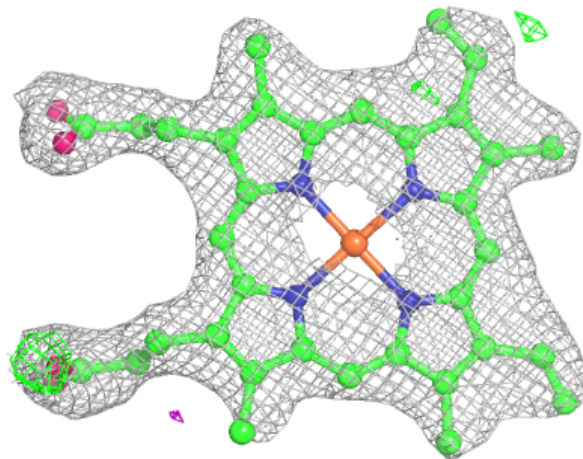and green (positive)
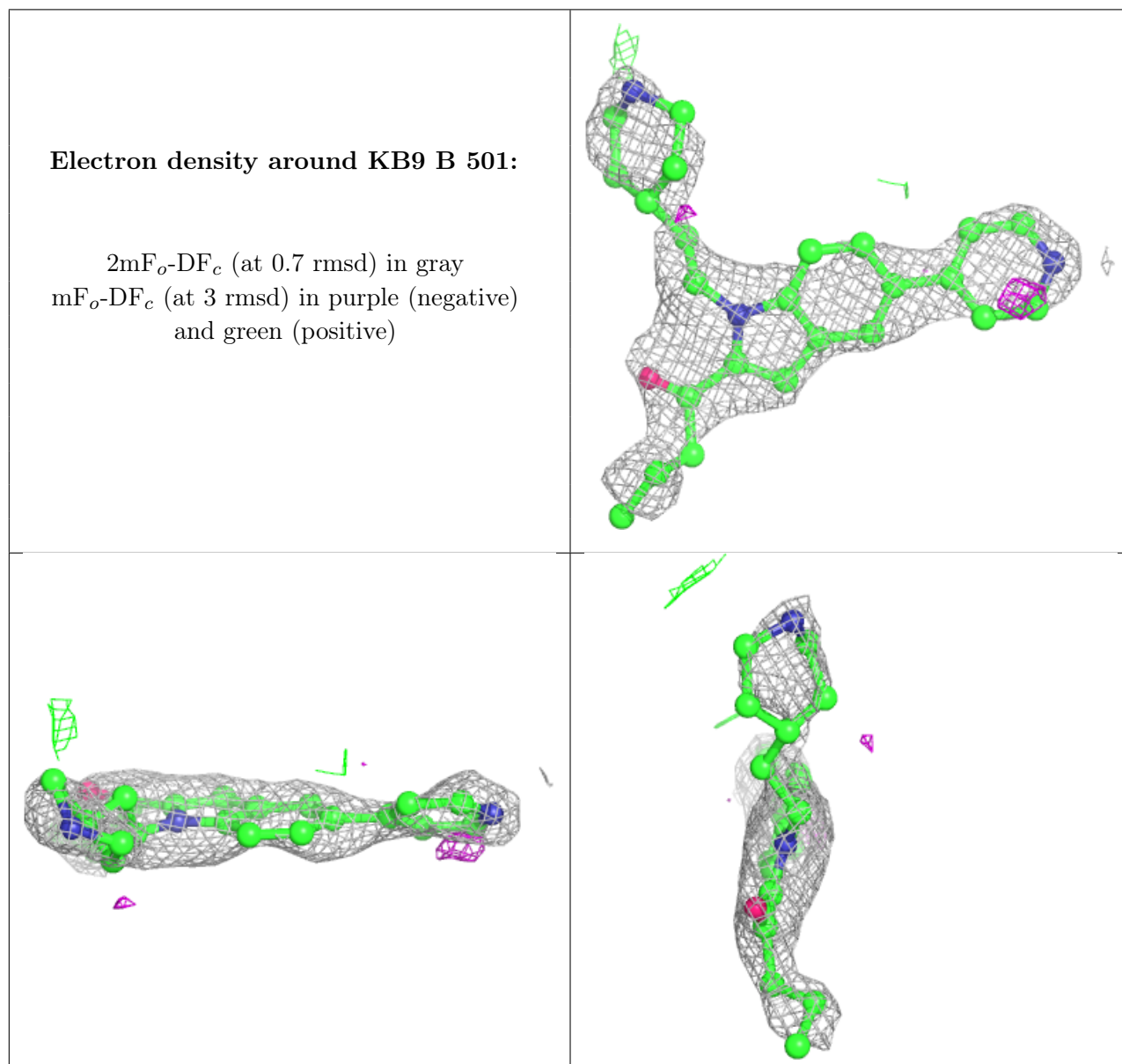
Electron density around KB9 C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
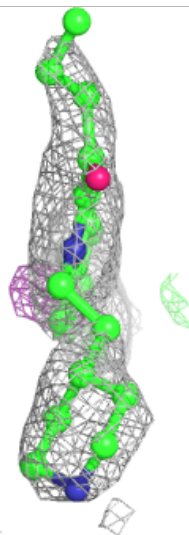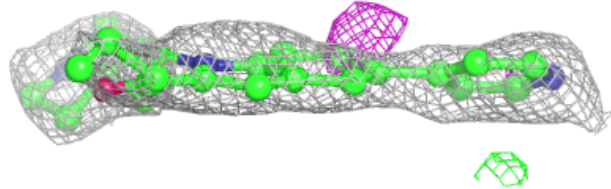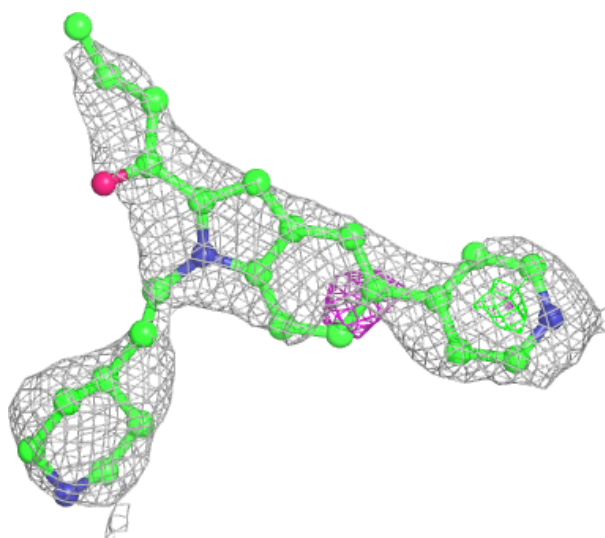
Electron density around KB9 A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
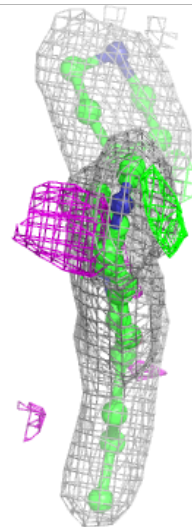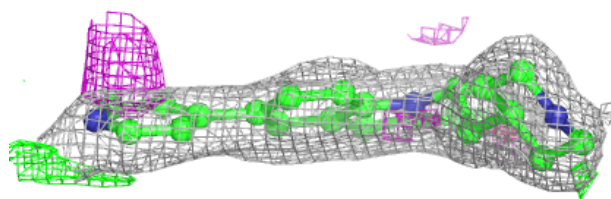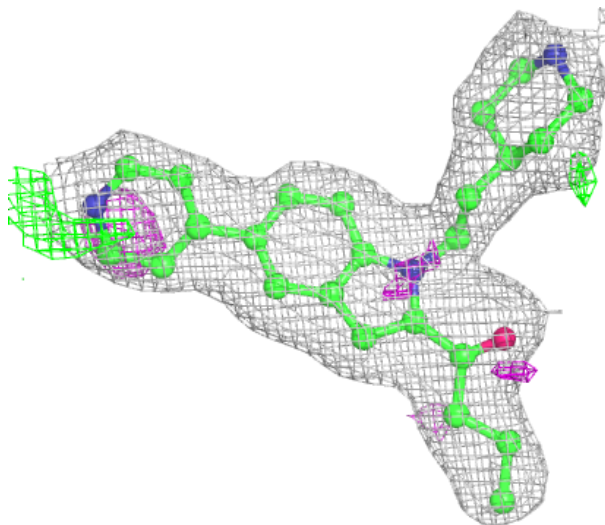
Electron density around KB9 A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
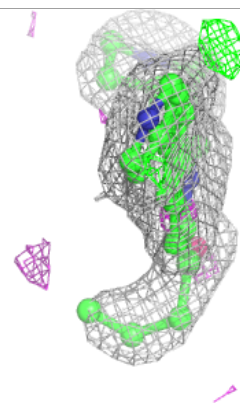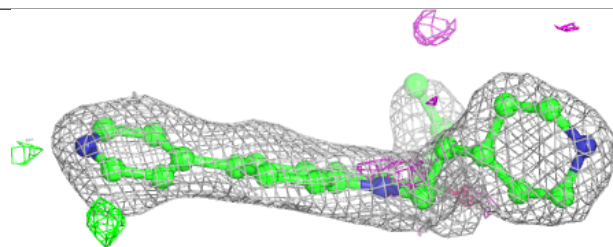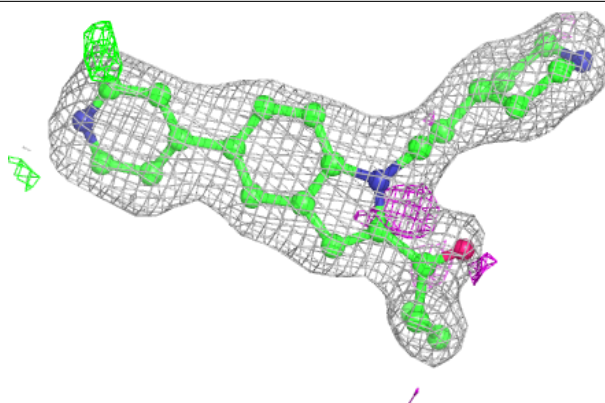
Electron density around HEM C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
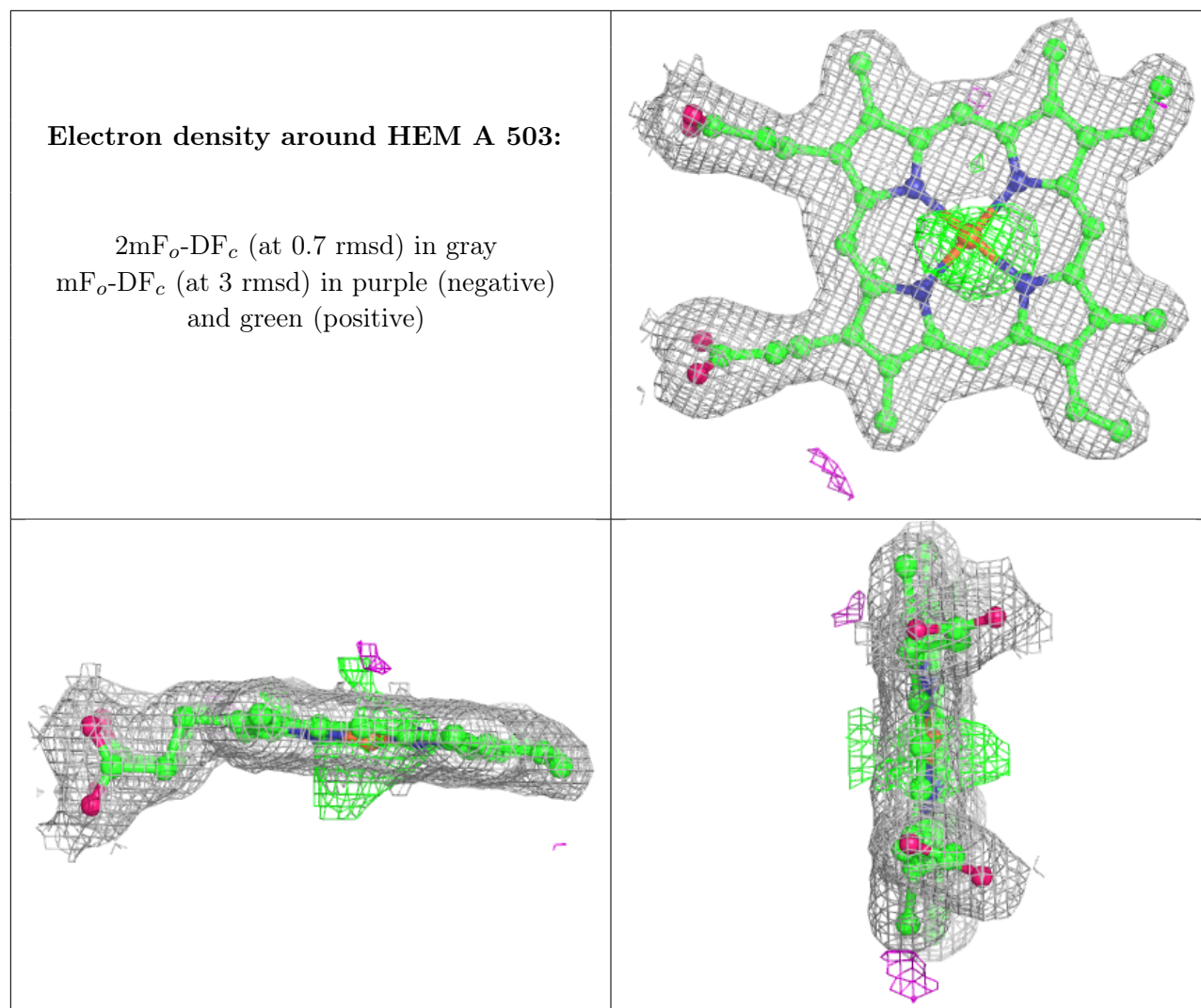mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
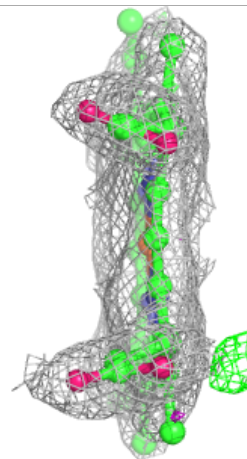
Electron density around HEM B 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
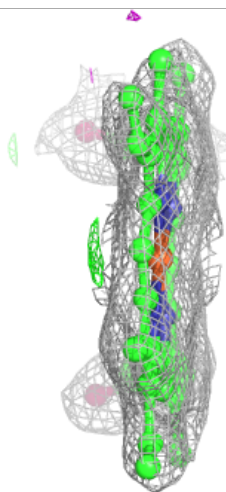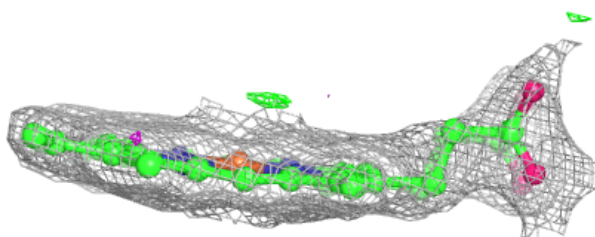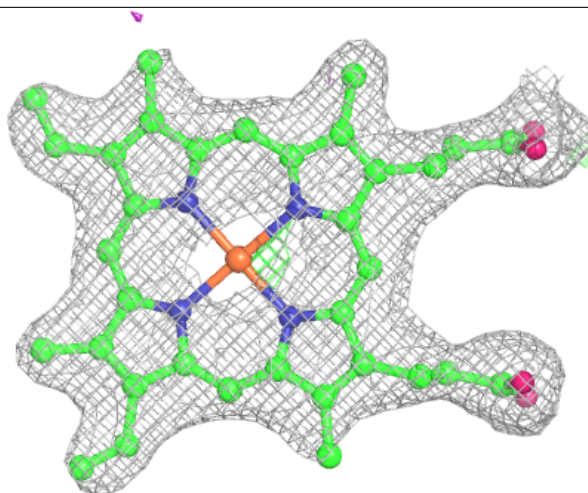
6.5 Other polymers (i)

There are no such residues in this entry.