



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:08 AM UTC

PDB ID : 2BDM / pdb_00002bdm
Title : Structure of Cytochrome P450 2B4 with Bound Bifonazole
Authors : Zhao, Y.; White, M.A.; Muralidhara, B.K.; Sun, L.; Halpert, J.R.; Stout, C.D.
Deposited on : 2005-10-20
Resolution : 2.30 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

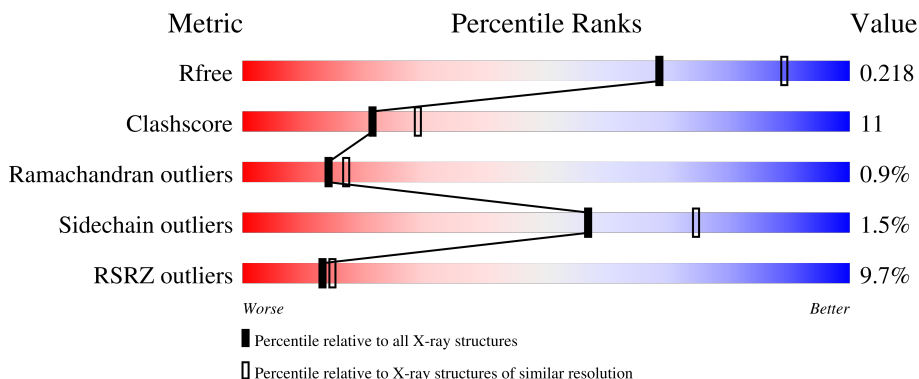
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	476	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TMI	A	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CM5	A	506	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4116 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.

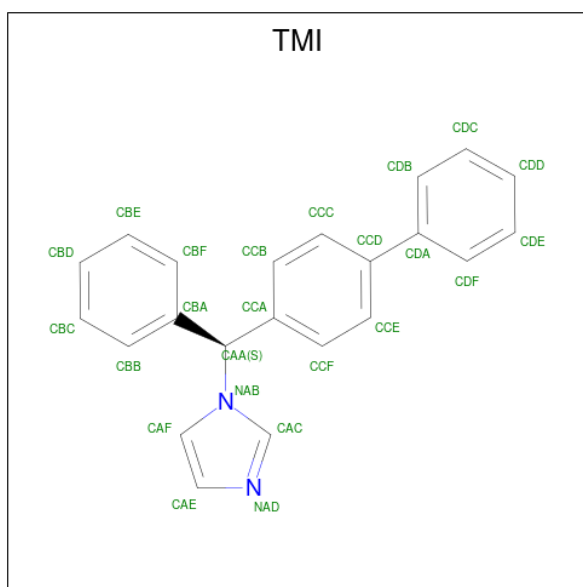
- Molecule 1 is a protein called Cytochrome P450 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3734	2405	649	669	11	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

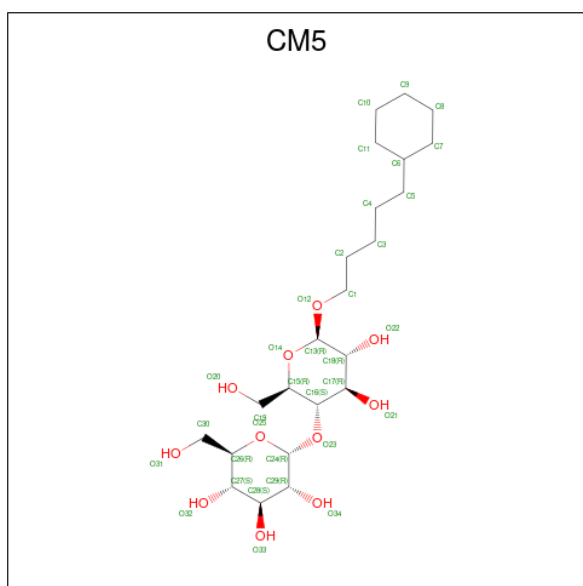
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C N	0	0
			24	22 2		
3	A	1	Total	C N	0	0
			24	22 2		
3	A	1	Total	C N	0	0
			24	22 2		

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (CCD ID: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	23	11		
4	A	1	Total	C	O	0	0
			34	23	11		
4	A	1	Total	C	O	0	0
			34	23	11		
4	A	1	Total	C	O	0	0
			34	23	11		

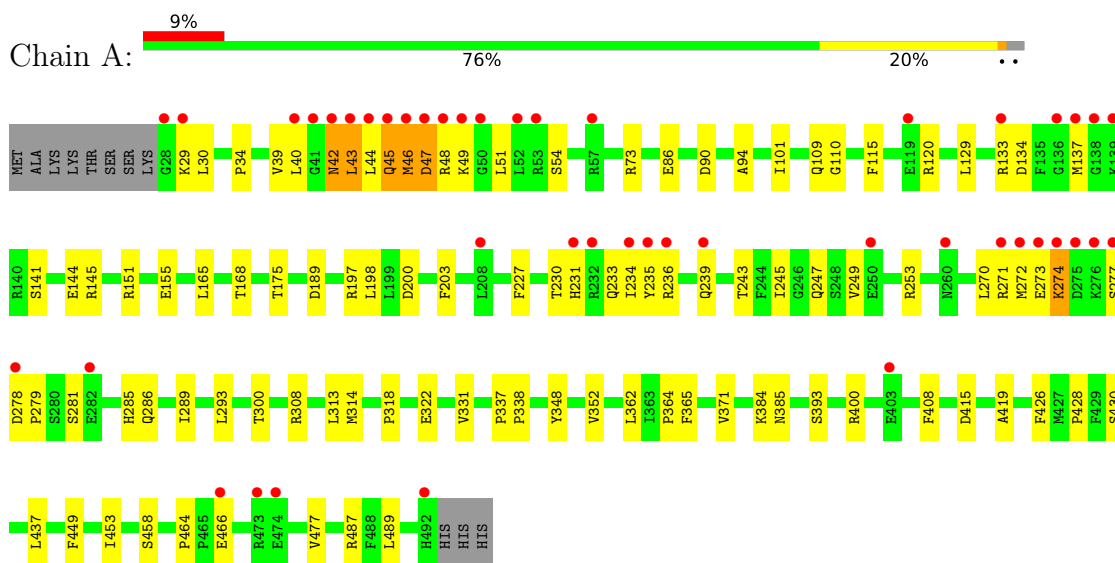
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		

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: Cytochrome P450 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.21Å 203.21Å 103.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 99.7 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.31Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.215 0.199 , 0.218	Depositor DCC
R_{free} test set	2750 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4116	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CM5, TMI, HEM

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	0.40	0/3828	0.88	8/5181 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	SER	N-CA-C	-7.28	98.35	109.85
1	A	362	LEU	N-CA-C	6.70	118.58	111.28
1	A	234	ILE	N-CA-C	6.64	118.62	111.58
1	A	331	VAL	N-CA-C	6.23	117.24	111.45
1	A	189	ASP	N-CA-C	-6.22	101.27	110.48
1	A	227	PHE	CA-C-N	6.13	126.04	119.85
1	A	227	PHE	C-N-CA	6.13	126.04	119.85
1	A	203	PHE	N-CA-C	6.08	121.62	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3734	0	3744	78	0
2	A	43	0	30	2	0
3	A	72	0	54	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	136	0	168	23	0
5	A	131	0	0	1	0
All	All	4116	0	3996	87	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 11.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	3:A:502:TMI:HDB	1.61	0.83
1:A:29:LYS:HD3	1:A:30:LEU:N	1.94	0.81
1:A:29:LYS:HD3	1:A:30:LEU:H	1.48	0.77
4:A:507:CM5:H31A	4:A:507:CM5:H72	1.69	0.73
1:A:253:ARG:HH22	4:A:506:CM5:H18	1.55	0.72
1:A:141:SER:OG	1:A:144:GLU:HG3	1.91	0.70
1:A:249:VAL:HG11	4:A:506:CM5:H12	1.73	0.70
1:A:101:ILE:HD12	4:A:505:CM5:C3	2.27	0.64
1:A:273:GLU:O	1:A:274:LYS:HB2	1.98	0.63
1:A:43:LEU:HD12	1:A:43:LEU:H	1.64	0.63
1:A:45:GLN:HE21	1:A:45:GLN:H	1.44	0.62
1:A:134:ASP:HA	1:A:137:MET:HE2	1.81	0.62
1:A:129:LEU:HB2	4:A:504:CM5:H192	1.82	0.62
1:A:51:LEU:HD22	1:A:365:PHE:CZ	2.36	0.59
1:A:198:LEU:HD21	3:A:502:TMI:HDC	1.85	0.59
1:A:46:MET:HE1	5:A:729:HOH:O	2.01	0.59
1:A:51:LEU:HD23	1:A:51:LEU:O	2.03	0.59
1:A:51:LEU:HD21	4:A:507:CM5:H41	1.84	0.58
4:A:507:CM5:H31A	4:A:507:CM5:C7	2.32	0.58
3:A:501:TMI:HDB	4:A:504:CM5:H32A	1.85	0.58
4:A:505:CM5:H192	4:A:505:CM5:O25	2.03	0.58
1:A:39:VAL:HG13	1:A:40:LEU:HD22	1.86	0.57
1:A:235:TYR:HE1	1:A:239:GLN:NE2	2.02	0.57
4:A:506:CM5:H12	4:A:506:CM5:O22	2.03	0.57
1:A:46:MET:O	1:A:47:ASP:HB2	2.03	0.57
1:A:43:LEU:HD12	1:A:43:LEU:N	2.18	0.57
1:A:54:SER:OG	4:A:507:CM5:H13	2.05	0.57
1:A:314:MET:HA	1:A:314:MET:HE2	1.88	0.55
1:A:101:ILE:HD12	4:A:505:CM5:H31A	1.89	0.55
4:A:506:CM5:H192	4:A:506:CM5:O25	2.07	0.53
1:A:165:LEU:C	1:A:165:LEU:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:145:ARG:HG3	2.10	0.52
1:A:285:HIS:O	1:A:289:ILE:HG13	2.10	0.52
1:A:39:VAL:CG1	1:A:40:LEU:HD22	2.40	0.51
1:A:129:LEU:HG	1:A:133:ARG:NH2	2.25	0.51
1:A:293:LEU:HD13	3:A:502:TMI:HDE	1.93	0.51
1:A:45:GLN:H	1:A:45:GLN:NE2	2.08	0.50
1:A:277:SER:OG	1:A:281:SER:HB3	2.12	0.50
1:A:47:ASP:O	1:A:51:LEU:HB2	2.11	0.49
1:A:48:ARG:HG3	3:A:503:TMI:HBC	1.95	0.49
1:A:364:PRO:HA	1:A:393:SER:HB2	1.93	0.49
1:A:39:VAL:O	1:A:43:LEU:HD11	2.13	0.49
1:A:231:HIS:O	1:A:235:TYR:HB2	2.12	0.49
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.77	0.48
1:A:477:VAL:HG22	3:A:503:TMI:CBE	2.43	0.48
1:A:253:ARG:HH22	4:A:506:CM5:C18	2.25	0.48
1:A:230:THR:OG1	1:A:233:GLN:HG3	2.15	0.47
1:A:464:PRO:HB2	1:A:466:GLU:OE1	2.14	0.47
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.79	0.47
1:A:73:ARG:NH1	1:A:110:GLY:O	2.48	0.47
1:A:151:ARG:NH1	1:A:155:GLU:OE2	2.48	0.47
1:A:270:LEU:C	1:A:272:MET:H	2.23	0.46
1:A:101:ILE:HD12	4:A:505:CM5:H32A	1.96	0.46
1:A:415:ASP:OD2	1:A:419:ALA:HB3	2.16	0.46
1:A:384:LYS:O	1:A:385:ASN:HB2	2.16	0.45
1:A:34:PRO:HG3	4:A:507:CM5:H192	2.00	0.44
1:A:94:ALA:O	1:A:371:VAL:HA	2.18	0.44
1:A:430:SER:CB	2:A:500:HEM:HBA1	2.47	0.44
1:A:286:GLN:HG2	4:A:506:CM5:H32A	1.99	0.44
1:A:46:MET:HE3	3:A:503:TMI:CAF	2.47	0.44
1:A:47:ASP:OD1	1:A:49:LYS:N	2.51	0.44
1:A:243:THR:O	1:A:247:GLN:HG2	2.18	0.43
1:A:278:ASP:HB2	1:A:279:PRO:HD2	2.00	0.43
3:A:503:TMI:CDF	4:A:507:CM5:H81	2.48	0.43
1:A:46:MET:O	1:A:47:ASP:CB	2.67	0.43
4:A:507:CM5:H26	4:A:507:CM5:H191	2.01	0.43
1:A:271:ARG:HH21	1:A:271:ARG:HG3	1.84	0.43
1:A:175:THR:HB	1:A:300:THR:HB	2.01	0.42
1:A:313:LEU:HD21	1:A:408:PHE:CD1	2.54	0.42
1:A:449:PHE:O	1:A:453:ILE:HG13	2.19	0.42
1:A:348:TYR:O	1:A:352:VAL:HG23	2.19	0.42
4:A:506:CM5:H13	4:A:506:CM5:H22A	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:O	1:A:249:VAL:HG23	2.19	0.42
1:A:273:GLU:O	1:A:274:LYS:CB	2.66	0.41
1:A:115:PHE:CE1	4:A:505:CM5:H22A	2.56	0.41
1:A:29:LYS:CD	1:A:30:LEU:H	2.26	0.41
1:A:43:LEU:HD23	1:A:109:GLN:OE1	2.20	0.41
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.96	0.41
1:A:86:GLU:O	1:A:90:ASP:HB2	2.21	0.41
1:A:487:ARG:HD2	1:A:489:LEU:HD21	2.02	0.41
1:A:120:ARG:HA	1:A:120:ARG:HD3	1.77	0.41
1:A:318:PRO:O	1:A:322:GLU:HG3	2.21	0.41
1:A:51:LEU:CD2	4:A:507:CM5:H41	2.50	0.41
1:A:430:SER:HB3	2:A:500:HEM:HBA1	2.03	0.41
1:A:168:THR:HA	1:A:308:ARG:HD3	2.02	0.40
1:A:426:PHE:CZ	1:A:428:PRO:HG3	2.56	0.40
1:A:437:LEU:HD11	4:A:504:CM5:H17	2.04	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	463/476 (97%)	440 (95%)	19 (4%)	4 (1%)	14 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	47	ASP
1	A	236	ARG
1	A	274	LYS

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	411/421 (98%)	405 (98%)	6 (2%)	57 75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	43	LEU
1	A	44	LEU
1	A	45	GLN
1	A	46	MET
1	A	200	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	239	GLN
1	A	284	HIS
1	A	286	GLN
1	A	376	GLN
1	A	492	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	CM5	A	504	-	36,36,36	0.56	1 (2%)	49,49,49	0.77	1 (2%)
4	CM5	A	506	-	36,36,36	0.57	1 (2%)	49,49,49	1.08	4 (8%)
3	TMI	A	503	-	27,27,27	0.98	1 (3%)	35,36,36	1.24	2 (5%)
3	TMI	A	501	2	27,27,27	0.98	1 (3%)	35,36,36	1.15	2 (5%)
4	CM5	A	507	-	36,36,36	0.57	1 (2%)	49,49,49	0.81	2 (4%)
4	CM5	A	505	-	36,36,36	0.56	1 (2%)	49,49,49	0.71	1 (2%)
3	TMI	A	502	-	27,27,27	0.98	1 (3%)	35,36,36	1.25	2 (5%)
2	HEM	A	500	1,3	50,50,50	2.42	25 (50%)	67,82,82	1.36	11 (16%)

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	CM5	A	504	-	-	2/17/65/65	0/3/3/3
4	CM5	A	506	-	1/1/11/11	7/17/65/65	0/3/3/3
3	TMI	A	503	-	1/1/1/1	0/16/16/16	0/4/4/4
3	TMI	A	501	2	-	1/16/16/16	0/4/4/4
4	CM5	A	507	-	-	0/17/65/65	0/3/3/3
4	CM5	A	505	-	-	2/17/65/65	0/3/3/3
3	TMI	A	502	-	-	0/16/16/16	0/4/4/4
2	HEM	A	500	1,3	-	4/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C4A-NA	-4.41	1.31	1.39
2	A	500	HEM	C4D-ND	-4.40	1.32	1.40
2	A	500	HEM	C1D-ND	-4.19	1.30	1.38
2	A	500	HEM	FE-NB	4.03	2.07	1.94
3	A	503	TMI	CDA-CCD	-3.93	1.39	1.49
3	A	501	TMI	CDA-CCD	-3.92	1.39	1.49
2	A	500	HEM	C1B-NB	-3.91	1.33	1.40
3	A	502	TMI	CDA-CCD	-3.90	1.39	1.49
2	A	500	HEM	CBB-CAB	3.89	1.49	1.30
2	A	500	HEM	C1C-NC	-3.77	1.32	1.39
2	A	500	HEM	FE-ND	3.69	2.06	1.94
2	A	500	HEM	C1C-C2C	-3.66	1.38	1.45
2	A	500	HEM	CMA-C3A	3.53	1.58	1.50
2	A	500	HEM	CAC-C3C	-3.50	1.38	1.47
2	A	500	HEM	C4B-NB	-3.34	1.32	1.38
2	A	500	HEM	FE-NA	3.08	2.05	1.95
2	A	500	HEM	FE-NC	3.01	2.05	1.95
2	A	500	HEM	CMC-C2C	2.86	1.56	1.50
2	A	500	HEM	CBD-CGD	2.78	1.57	1.50
2	A	500	HEM	C4D-C3D	-2.74	1.40	1.45
2	A	500	HEM	C3B-C2B	2.68	1.42	1.37
2	A	500	HEM	C4C-NC	-2.57	1.34	1.39
2	A	500	HEM	C1A-C2A	-2.43	1.39	1.44
4	A	506	CM5	O12-C13	2.38	1.44	1.40
2	A	500	HEM	CBC-CAC	2.37	1.41	1.30
4	A	507	CM5	O12-C13	2.33	1.44	1.40
2	A	500	HEM	O2A-CGA	-2.33	1.23	1.30
4	A	505	CM5	O12-C13	2.26	1.44	1.40
2	A	500	HEM	CAD-C3D	2.26	1.57	1.51
4	A	504	CM5	O12-C13	2.25	1.43	1.40
2	A	500	HEM	CMD-C2D	2.14	1.55	1.50
2	A	500	HEM	C3C-C2C	2.06	1.41	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	TMI	CAF-NAB-CAC	5.30	109.54	106.32
3	A	503	TMI	CAF-NAB-CAC	5.28	109.53	106.32
3	A	501	TMI	CAF-NAB-CAC	4.91	109.31	106.32
4	A	506	CM5	O12-C13-C18	3.88	114.17	108.27
3	A	502	TMI	NAB-CAC-NAD	-3.67	106.76	112.21
3	A	503	TMI	NAB-CAC-NAD	-3.61	106.86	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	TMI	NAB-CAC-NAD	-3.32	107.29	112.21
2	A	500	HEM	CHD-C4C-NC	-3.11	121.07	124.45
4	A	504	CM5	C24-O23-C16	-3.06	110.72	117.98
4	A	507	CM5	C24-O23-C16	-2.91	111.08	117.98
2	A	500	HEM	C3B-C4B-NB	2.84	111.51	109.47
2	A	500	HEM	C1C-CHC-C4B	2.83	132.04	126.02
2	A	500	HEM	C4B-C3B-C2B	-2.76	104.74	107.28
2	A	500	HEM	C3B-C2B-C1B	-2.69	104.39	106.41
4	A	505	CM5	C24-O23-C16	-2.57	111.88	117.98
2	A	500	HEM	C4C-C3C-C2C	-2.55	104.61	106.81
4	A	506	CM5	O14-C13-C18	-2.42	105.39	110.37
2	A	500	HEM	CHB-C1B-NB	-2.32	121.50	124.37
4	A	506	CM5	C19-C15-C16	-2.30	106.92	113.38
2	A	500	HEM	C4D-ND-C1D	2.23	107.84	105.21
4	A	507	CM5	C1-O12-C13	-2.20	109.92	113.68
2	A	500	HEM	C1B-NB-C4B	2.20	107.81	105.21
4	A	506	CM5	C1-O12-C13	-2.10	110.10	113.68
2	A	500	HEM	C4A-CHB-C1B	2.09	131.17	126.25
2	A	500	HEM	CAD-CBD-CGD	2.03	119.04	113.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	503	TMI	CAA
4	A	506	CM5	C24

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	CM5	C2-C1-O12-C13
4	A	506	CM5	C2-C1-O12-C13
4	A	506	CM5	O14-C13-O12-C1
4	A	506	CM5	C29-C24-O23-C16
4	A	506	CM5	C18-C13-O12-C1
4	A	506	CM5	C1-C2-C3-C4
4	A	504	CM5	O25-C26-C30-O31
4	A	505	CM5	O25-C26-C30-O31
4	A	506	CM5	O25-C26-C30-O31
4	A	506	CM5	O25-C24-O23-C16
3	A	501	TMI	CCA-CAA-NAB-CAC
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A

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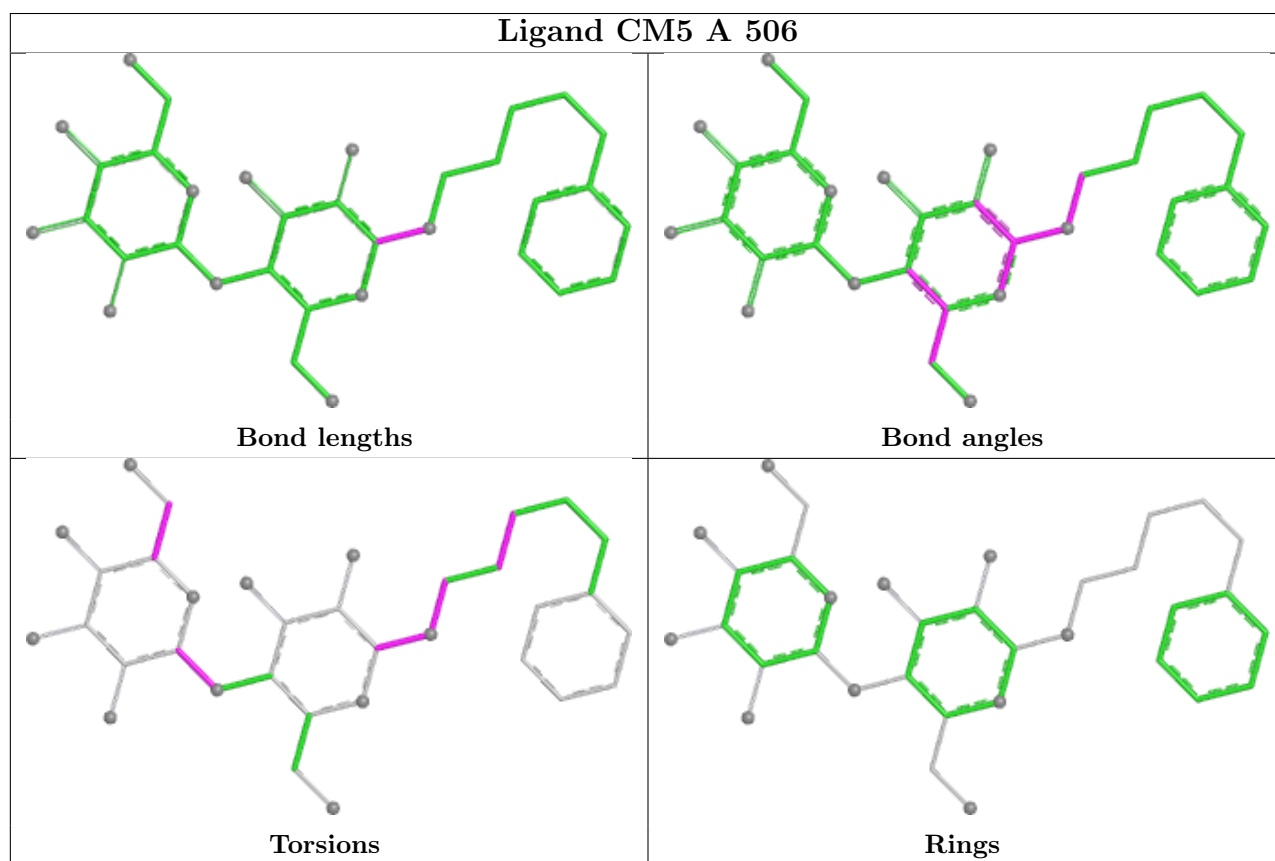
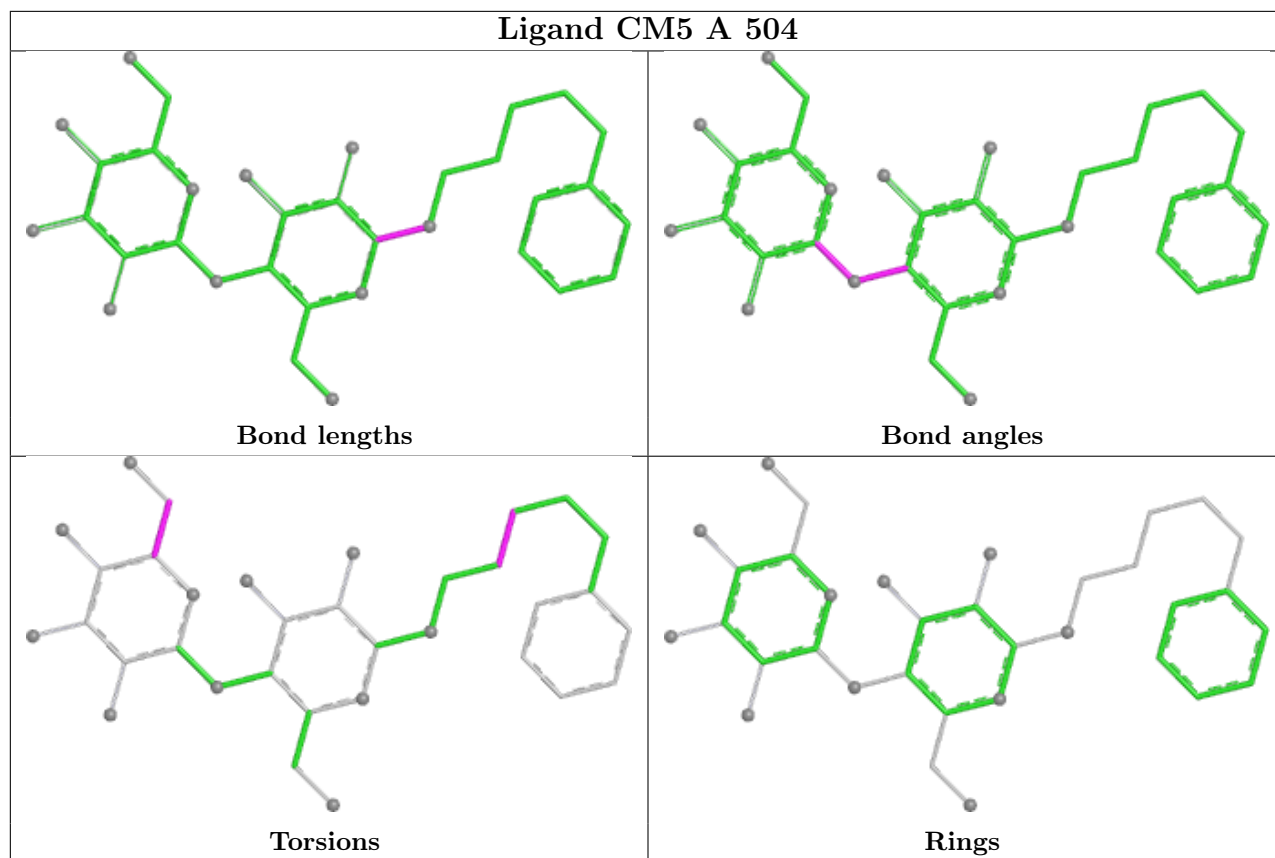
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C4C-C3C-CAC-CBC
4	A	504	CM5	C1-C2-C3-C4
2	A	500	HEM	C2C-C3C-CAC-CBC

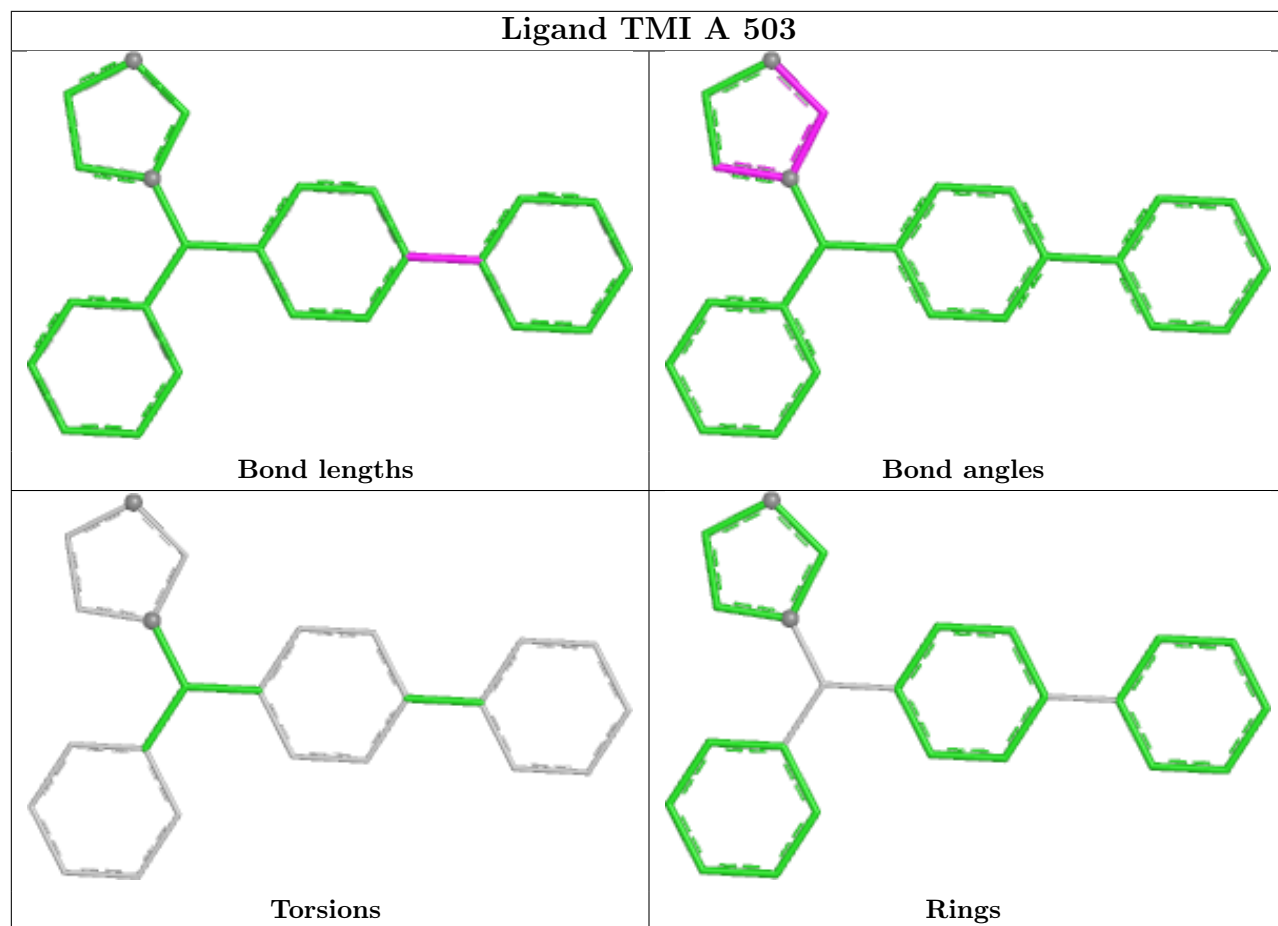
There are no ring outliers.

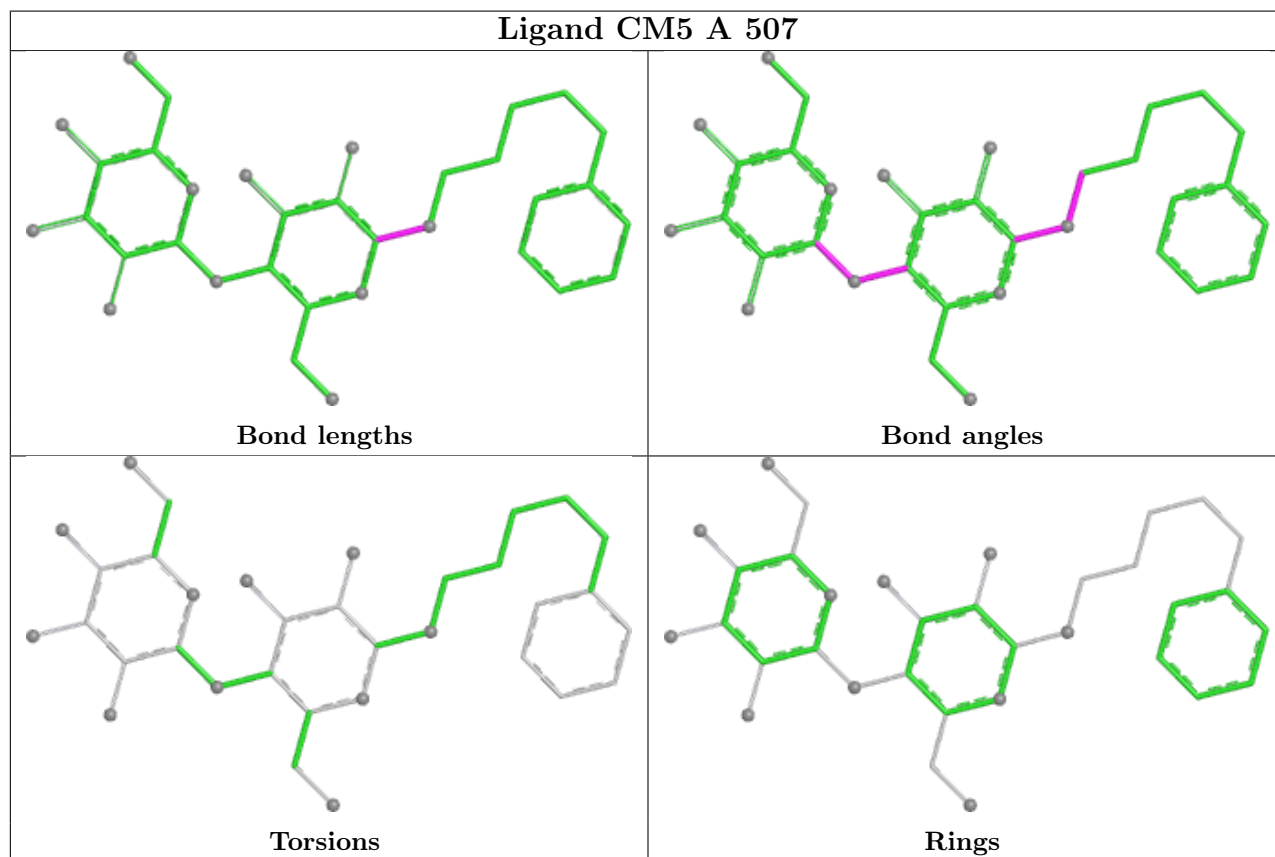
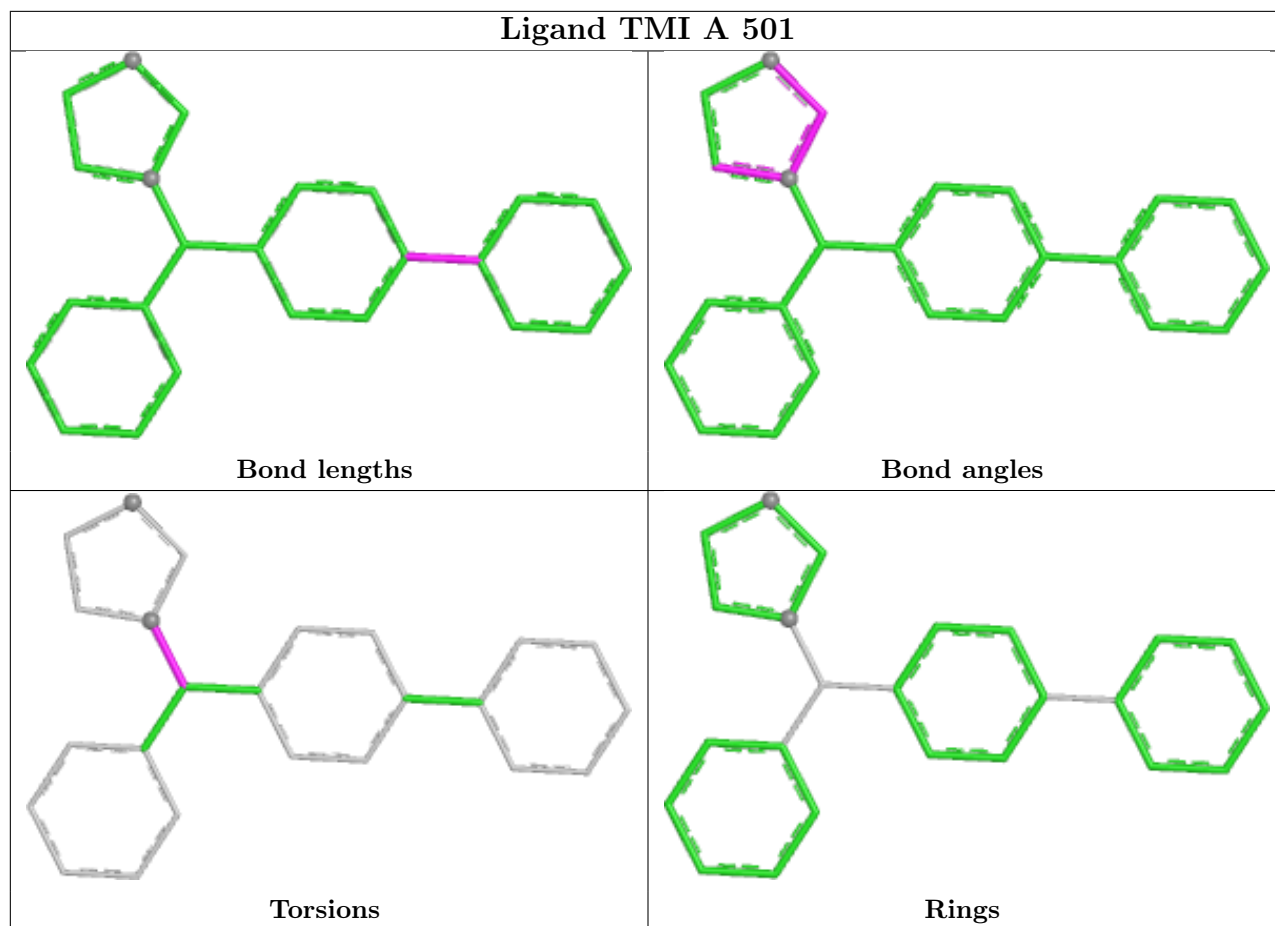
8 monomers are involved in 31 short contacts:

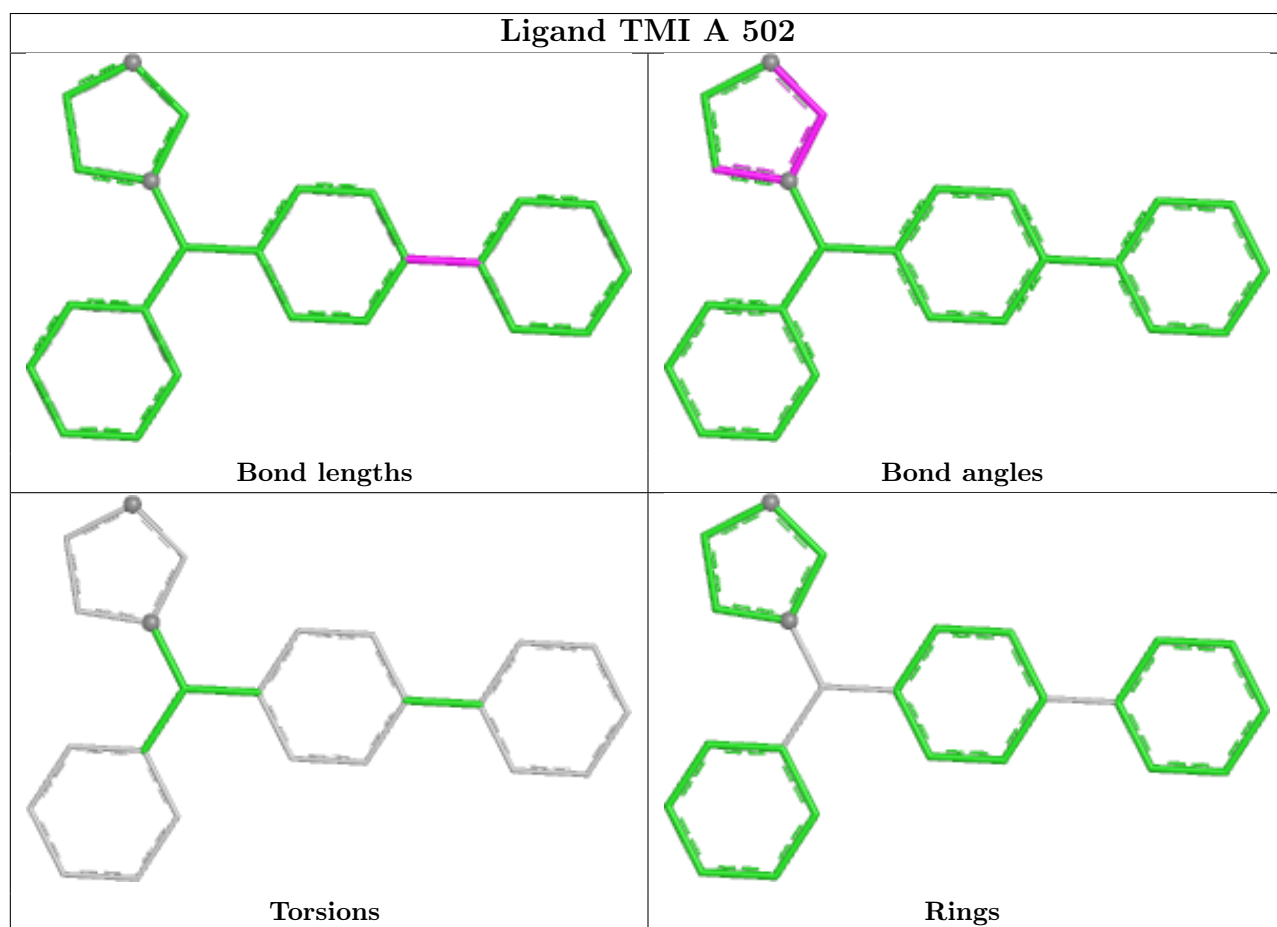
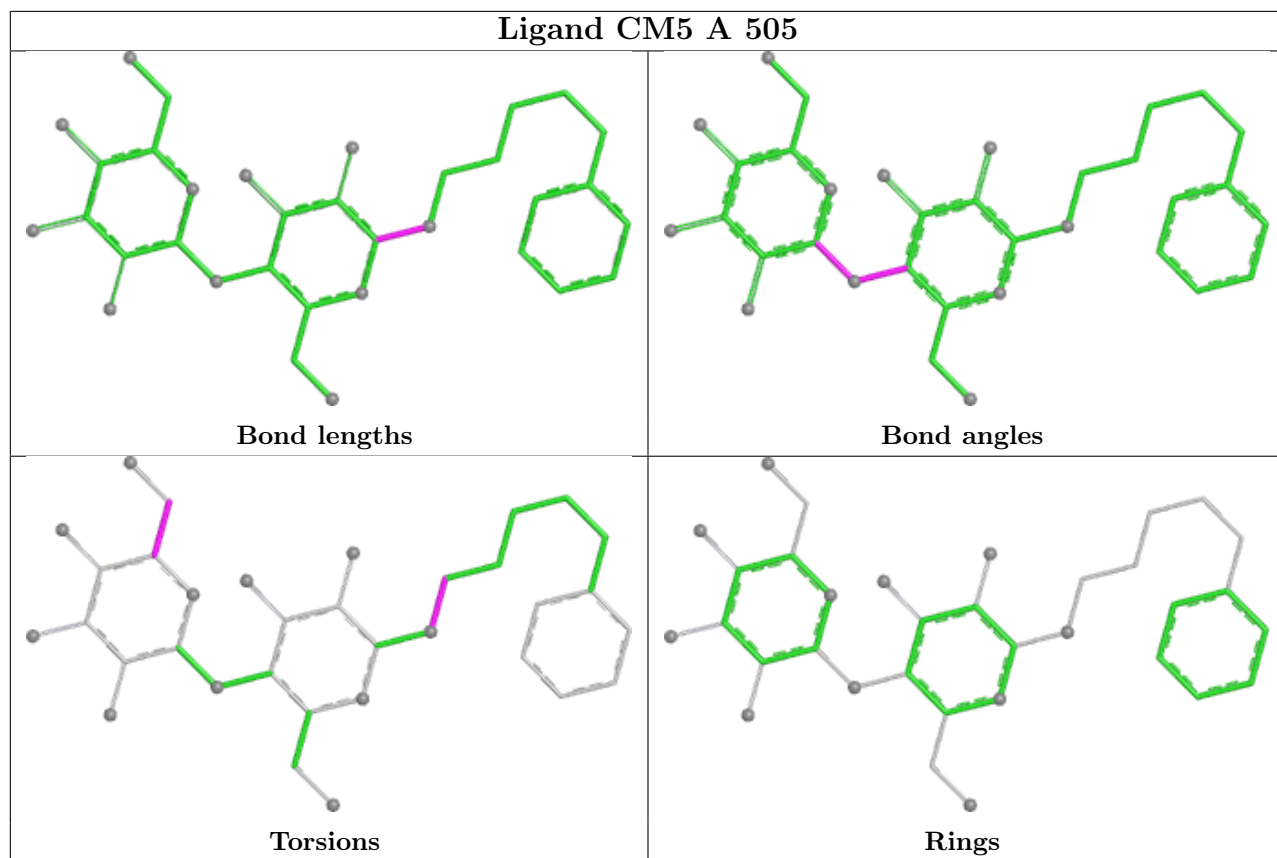
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	CM5	3	0
4	A	506	CM5	7	0
3	A	503	TMI	4	0
3	A	501	TMI	1	0
4	A	507	CM5	8	0
4	A	505	CM5	5	0
3	A	502	TMI	3	0
2	A	500	HEM	2	0

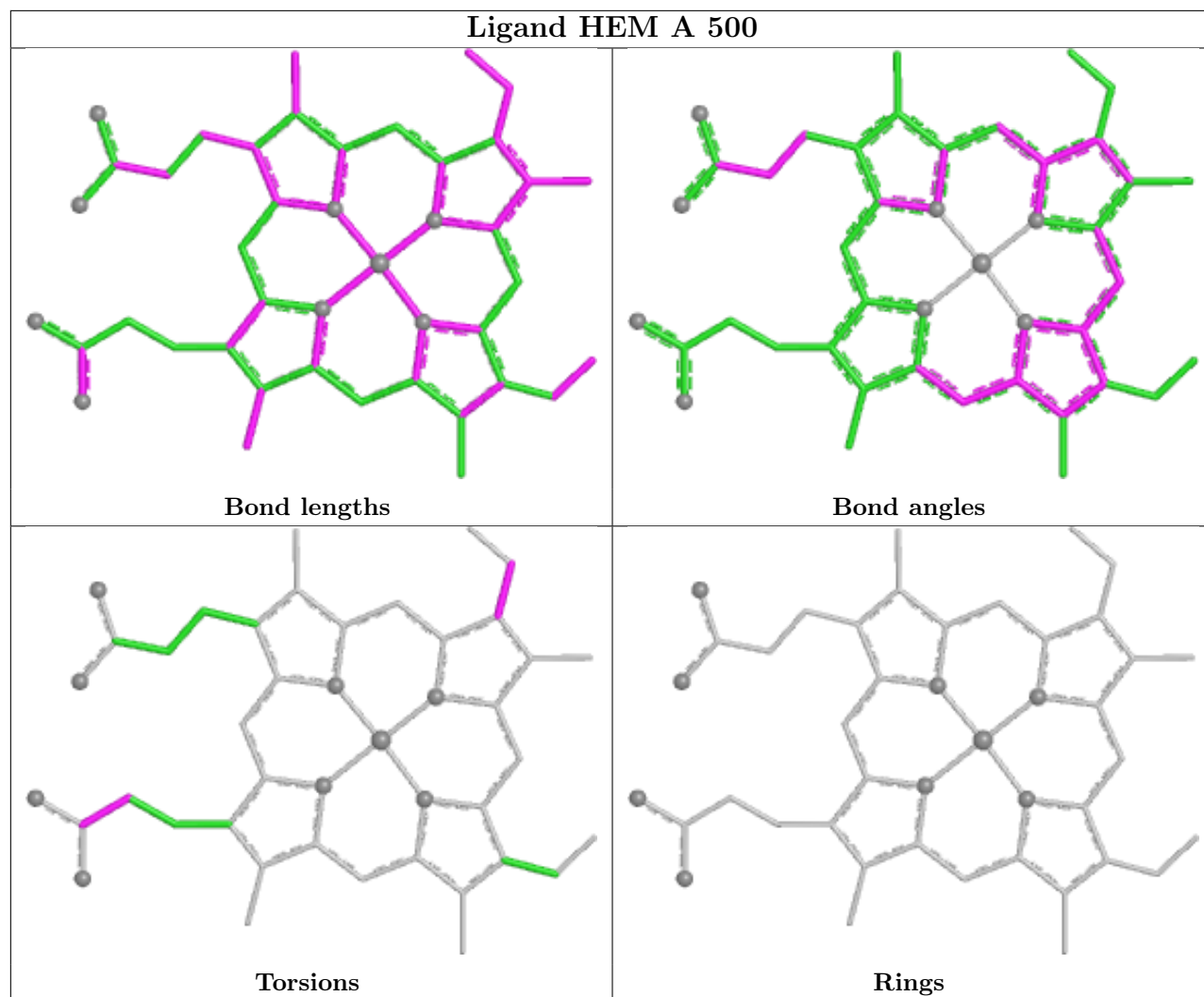
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	465/476 (97%)	0.34	45 (9%) 13 15	39, 53, 111, 184	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ASN	8.6
1	A	43	LEU	7.3
1	A	45	GLN	7.2
1	A	46	MET	6.6
1	A	492	HIS	5.5
1	A	274	LYS	5.5
1	A	44	LEU	5.1
1	A	272	MET	5.1
1	A	139	LYS	4.9
1	A	231	HIS	4.5
1	A	236	ARG	4.3
1	A	235	TYR	4.2
1	A	275	ASP	4.1
1	A	49	LYS	4.0
1	A	53	ARG	4.0
1	A	136	GLY	3.7
1	A	208	LEU	3.4
1	A	232	ARG	3.2
1	A	138	GLY	3.2
1	A	41	GLY	3.2
1	A	47	ASP	3.1
1	A	278	ASP	2.9
1	A	133	ARG	2.9
1	A	29	LYS	2.8
1	A	234	ILE	2.8
1	A	277	SER	2.7
1	A	276	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	466	GLU	2.7
1	A	473	ARG	2.5
1	A	48	ARG	2.5
1	A	403	GLU	2.5
1	A	271	ARG	2.5
1	A	260	ASN	2.3
1	A	273	GLU	2.3
1	A	28	GLY	2.3
1	A	137	MET	2.3
1	A	239	GLN	2.3
1	A	474	GLU	2.3
1	A	40	LEU	2.3
1	A	57	ARG	2.2
1	A	250	GLU	2.2
1	A	282	GLU	2.1
1	A	50	GLY	2.1
1	A	52	LEU	2.1
1	A	119	GLU	2.1

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 oligosaccharides 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.

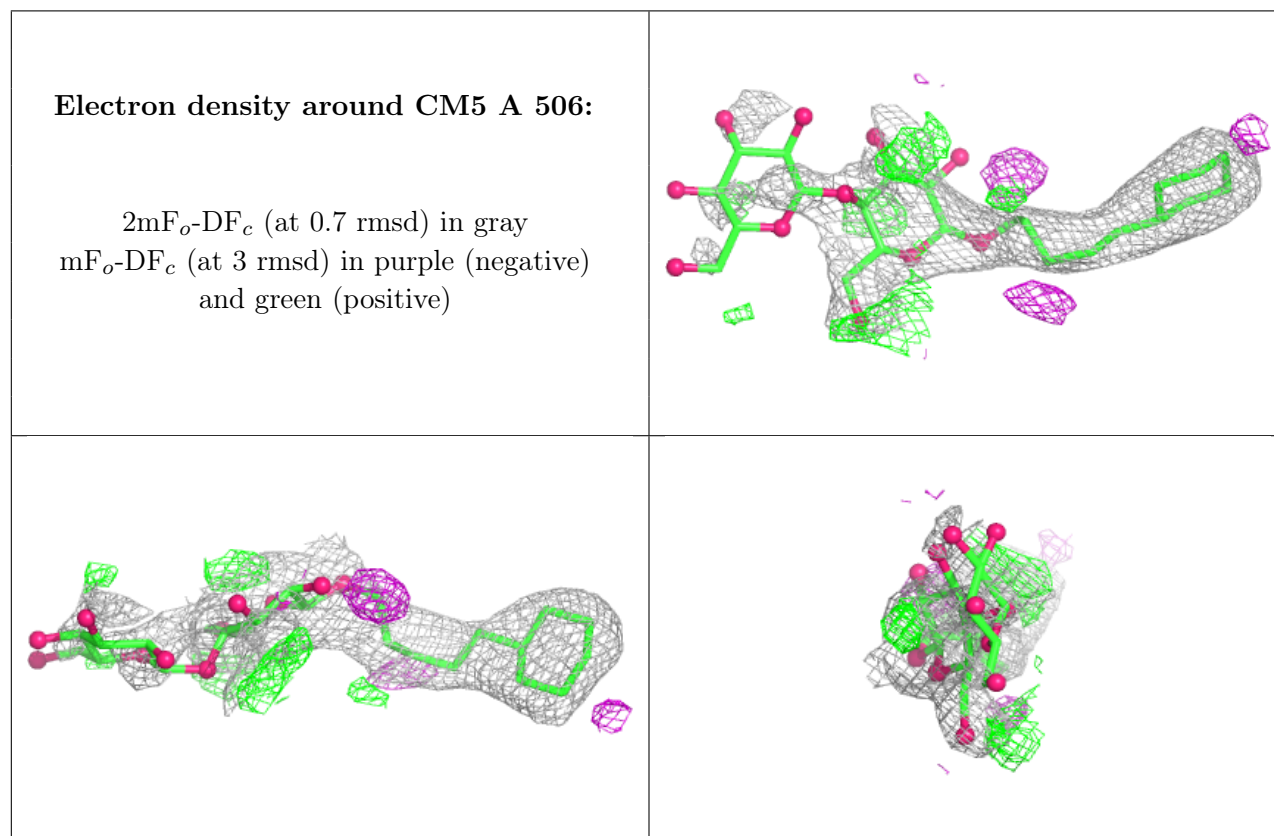
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CM5	A	506	34/34	0.77	0.26	62,163,200,200	0
4	CM5	A	507	34/34	0.79	0.28	71,134,200,200	0
3	TMI	A	503	24/24	0.90	0.15	77,90,123,178	0
4	CM5	A	504	34/34	0.90	0.14	59,68,80,88	0
4	CM5	A	505	34/34	0.92	0.16	60,81,133,139	0

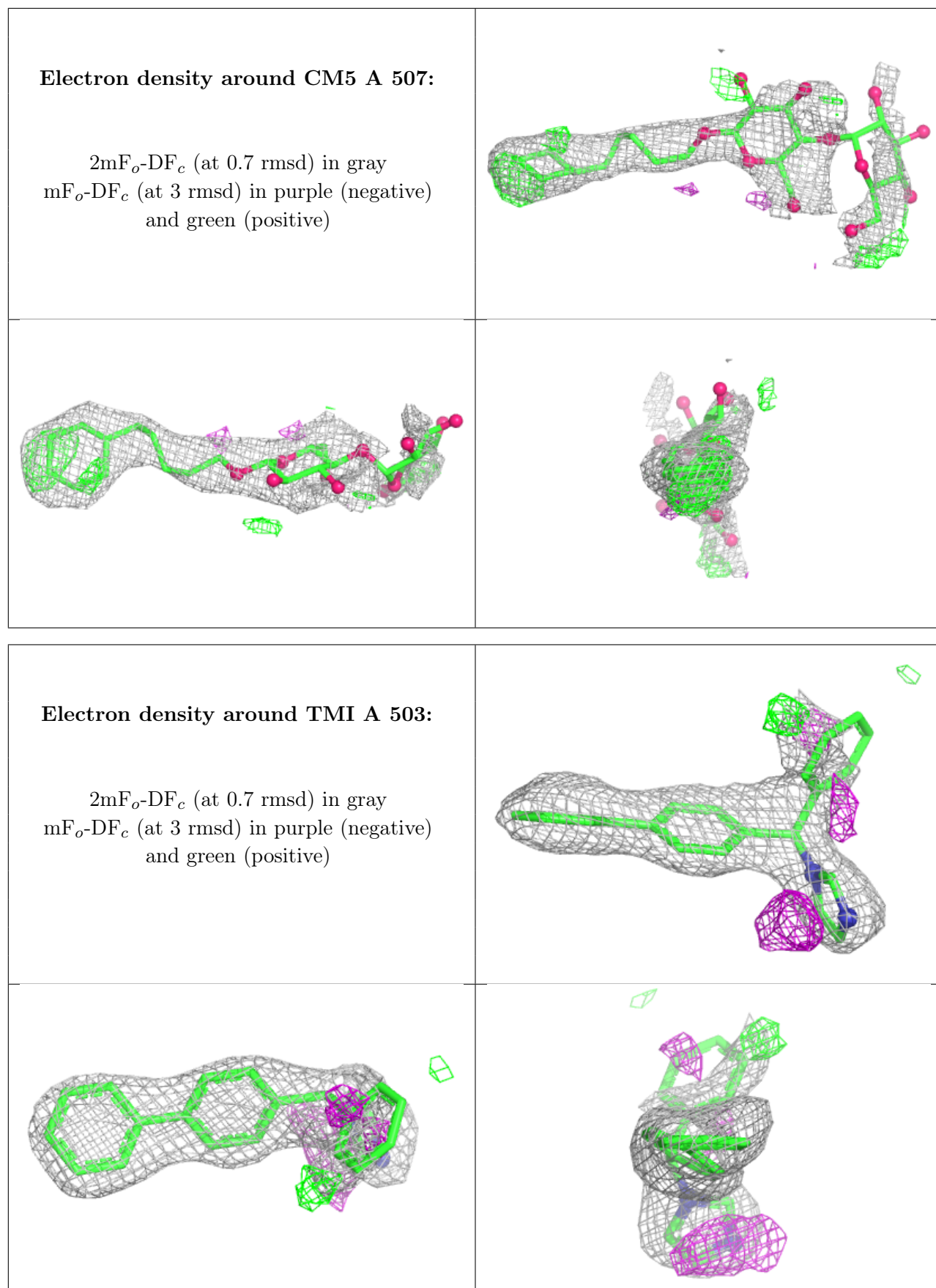
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TMI	A	502	24/24	0.95	0.10	47,56,76,79	0
3	TMI	A	501	24/24	0.97	0.07	38,42,46,49	0
2	HEM	A	500	43/43	0.99	0.07	36,40,50,56	0

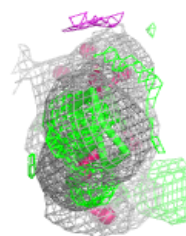
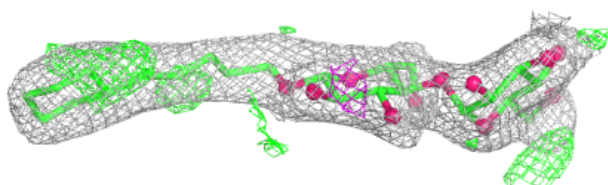
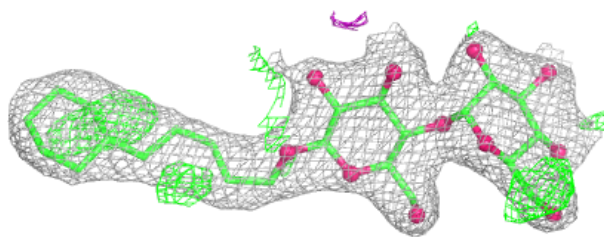
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



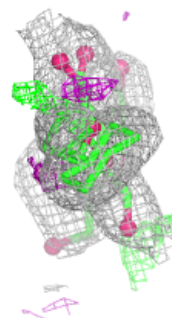
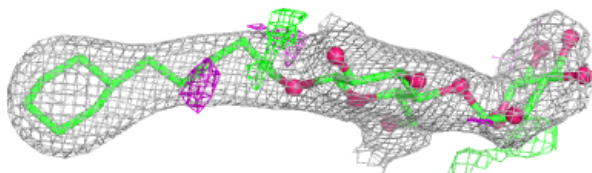
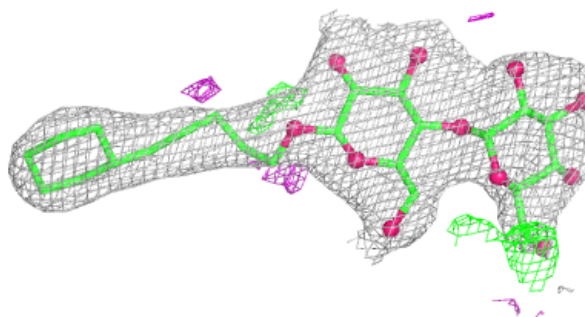


Electron density around CM5 A 504:

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

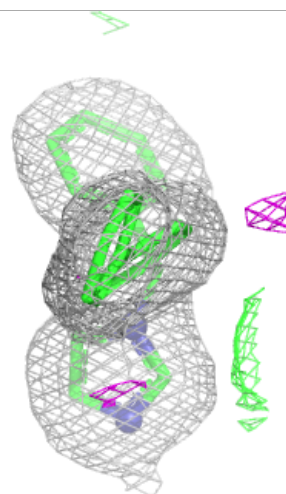
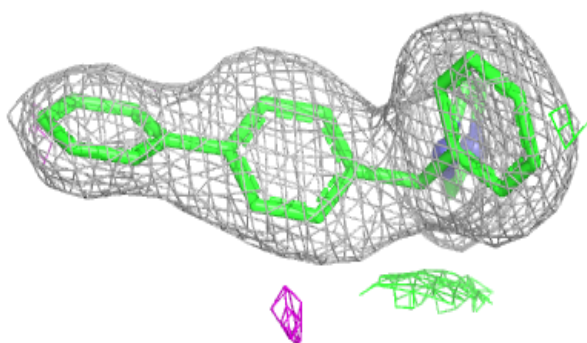
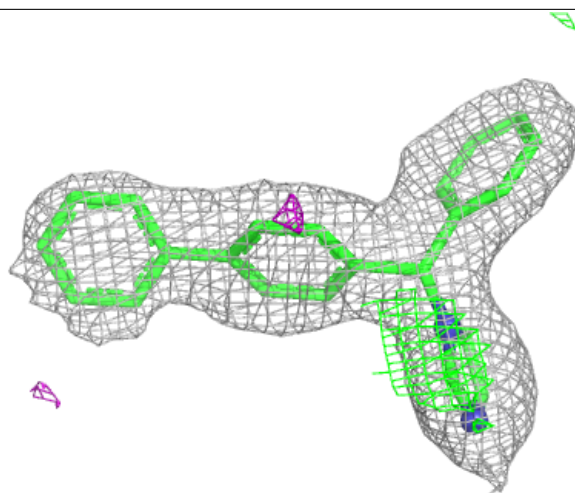
**Electron density around CM5 A 505:**

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



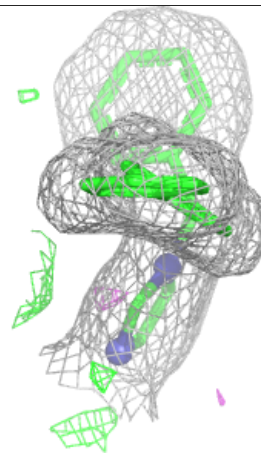
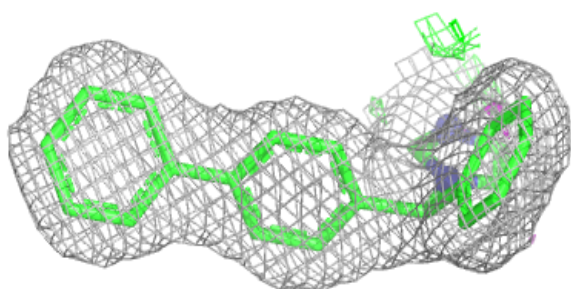
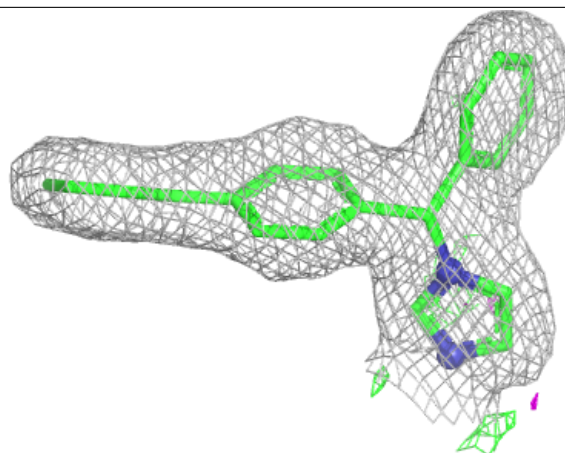
Electron density around TMI A 502:

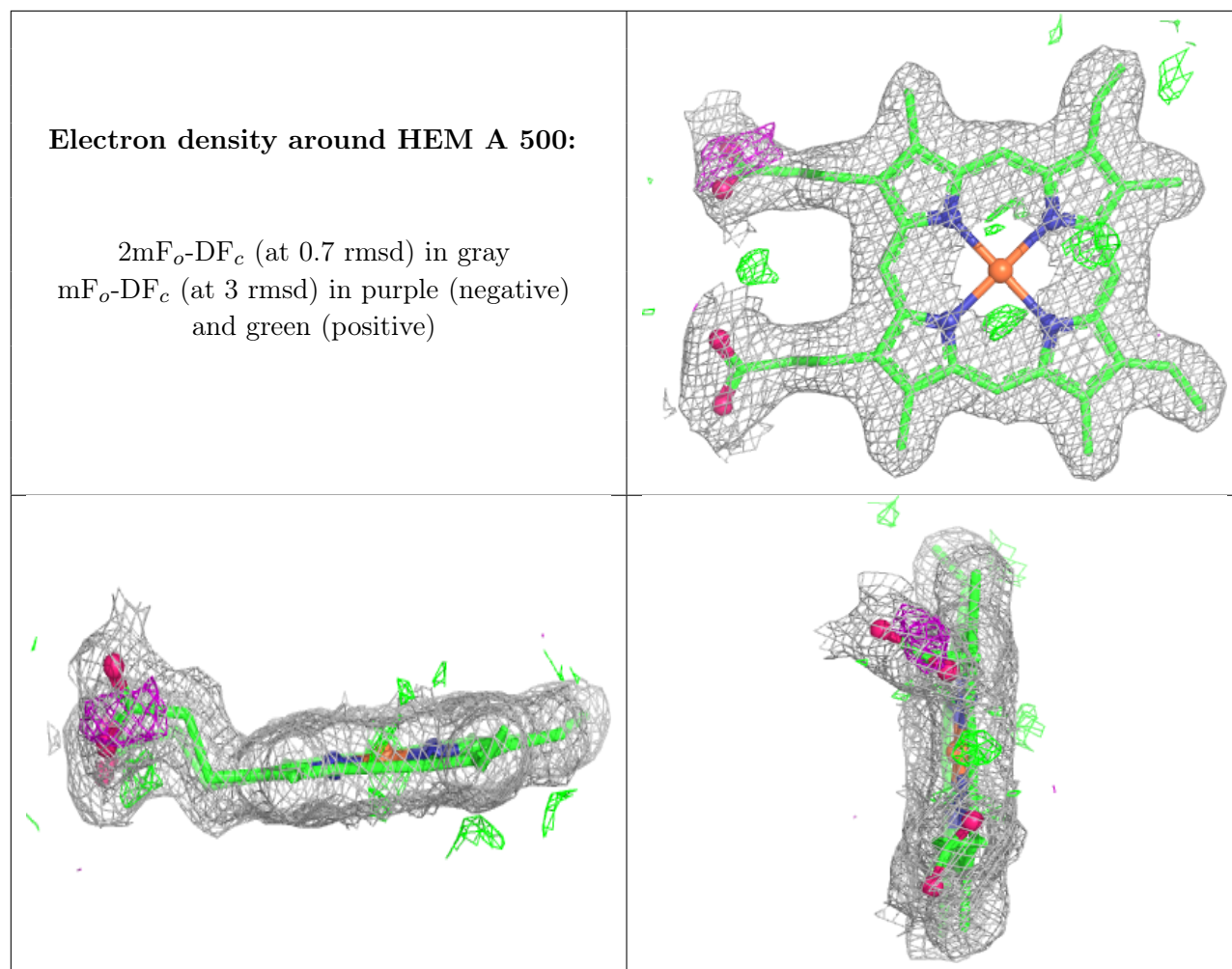
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TMI 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.