



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:29 AM EDT

PDB ID : 1FS8 / pdb_00001fs8
Title : CYTOCHROME C NITRITE REDUCTASE FROM WOLINELLA SUCCINOGENES-SULFATE COMPLEX
Authors : Einsle, O.; Stach, P.; Messerschmidt, A.; Simon, J.; Kroeger, A.; Huber, R.; Kroneck, P.M.H.
Deposited on : 2000-09-08
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

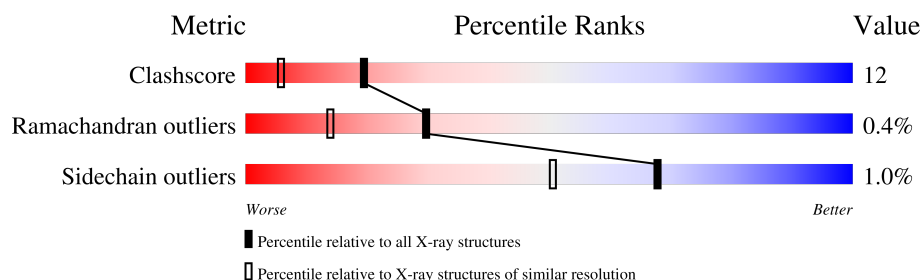
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	485	78%18%..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HEC	A	508	X	-	-	-
6	HEC	A	509	X	-	-	-
6	HEC	A	510	X	-	-	-
6	HEC	A	511	X	-	-	-
6	HEC	A	512	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4661 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 C NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	7	0	0
			3772	2387	648	716	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLU	LYS	conflict	UNP Q9S1E5

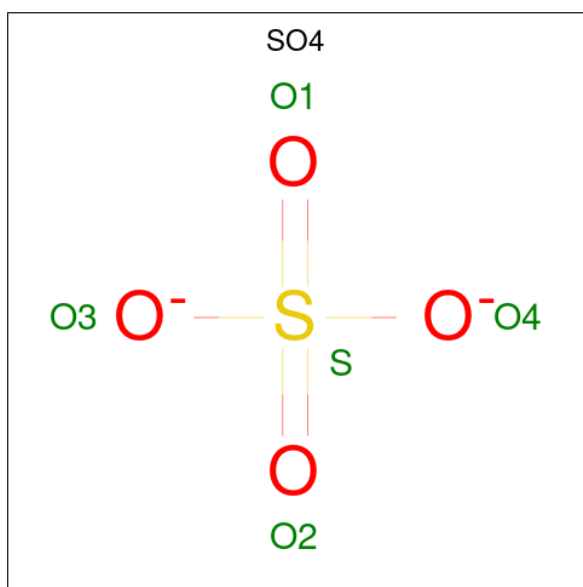
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is YTTRIUM ION (CCD ID: Y1) (formula: Y).

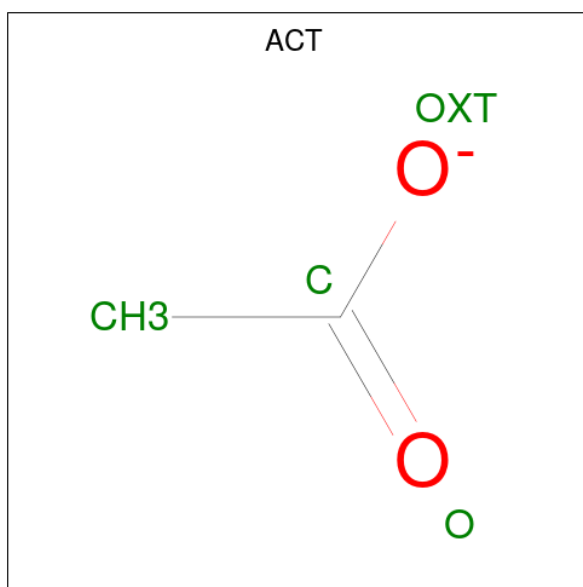
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Y	0	0
			4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



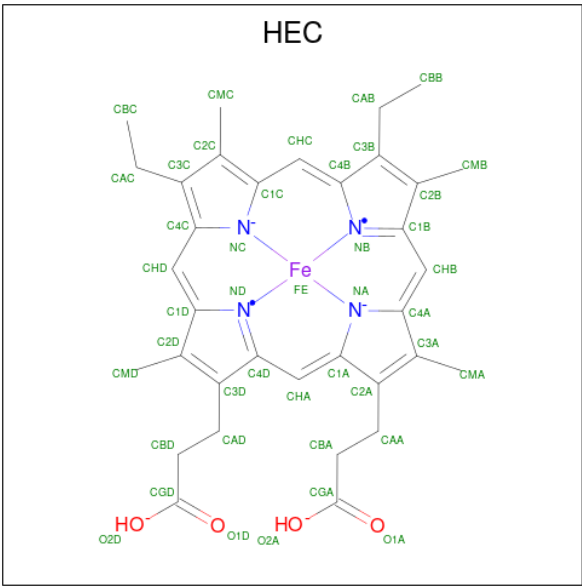
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	650	Total	O	0	0
			650	650		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CYTOCHROME C NITRITE REDUCTASE

Chain A:  78% 18% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.01Å 119.01Å 186.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-1.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, Y1, CA, ACT, SO4

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	0.34	0/3863	0.89	6/5202 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	SER	N-CA-C	7.74	118.09	108.11
1	A	237	VAL	N-CA-C	5.88	117.04	108.58
1	A	126	LEU	N-CA-C	5.57	117.70	110.40
1	A	272	MET	N-CA-C	5.51	118.67	110.52
1	A	286	GLY	N-CA-C	-5.28	104.34	112.85
1	A	67	THR	N-CA-C	-5.06	106.93	113.01

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	3772	0	3682	91	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	15	0	0	0	0
5	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	215	0	150	5	0
7	A	650	0	0	10	0
All	All	4661	0	3835	91	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 12.

All (91) 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:498:LYS:HE3	1:A:506:LYS:HA	1.26	1.09
1:A:100:ARG:HH22	1:A:507:LYS:HD2	1.33	0.94
1:A:100:ARG:NH2	1:A:507:LYS:HD2	1.94	0.82
1:A:333:SER:HB3	1:A:336:LYS:HG3	1.62	0.79
1:A:498:LYS:O	1:A:507:LYS:HE3	1.83	0.79
1:A:488:ASN:HB3	7:A:1298:HOH:O	1.85	0.77
1:A:117:ALA:HB3	1:A:465:GLU:HG2	1.69	0.74
1:A:100:ARG:HH22	1:A:507:LYS:CD	2.00	0.73
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.54	0.73
1:A:497:GLU:HG3	1:A:507:LYS:HA	1.72	0.72
1:A:139:PRO:O	1:A:143:GLU:HG3	1.90	0.70
1:A:467:LEU:O	1:A:471:GLN:HG3	1.94	0.68
1:A:498:LYS:H	1:A:507:LYS:CE	2.07	0.67
1:A:51:GLU:HB2	7:A:1035:HOH:O	1.96	0.66
1:A:497:GLU:H	1:A:507:LYS:HG2	1.60	0.66
1:A:117:ALA:CB	1:A:465:GLU:HG2	2.27	0.65
1:A:496:ASP:HA	1:A:507:LYS:HE2	1.79	0.64
1:A:498:LYS:H	1:A:507:LYS:HE3	1.63	0.64
1:A:503:ASP:C	1:A:505:THR:H	2.04	0.64
1:A:106:LEU:HD21	1:A:163:VAL:HA	1.82	0.62
1:A:497:GLU:HB2	1:A:507:LYS:HG2	1.81	0.62
1:A:497:GLU:N	1:A:507:LYS:HE2	2.15	0.62
1:A:228:ASP:OD1	1:A:229:LYS:HG3	1.99	0.62
1:A:204:GLN:HE21	1:A:204:GLN:HA	1.66	0.61
1:A:62:ASP:HB3	7:A:1272:HOH:O	2.02	0.59
1:A:100:ARG:HH22	1:A:507:LYS:CE	2.17	0.58
1:A:330:HIS:HB3	1:A:332:GLU:OE2	2.05	0.55
1:A:497:GLU:HB2	1:A:507:LYS:HA	1.88	0.55
1:A:328:ASN:HB2	7:A:1122:HOH:O	2.07	0.55
1:A:100:ARG:CZ	1:A:507:LYS:HD2	2.37	0.54
1:A:228:ASP:HB3	7:A:1304:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:CG	1:A:507:LYS:HA	2.38	0.54
1:A:100:ARG:NH1	1:A:507:LYS:HD2	2.24	0.53
1:A:495:VAL:O	1:A:507:LYS:NZ	2.42	0.53
1:A:215:HIS:HB3	1:A:279:ASP:HB2	1.91	0.53
1:A:490:GLU:HB2	7:A:1298:HOH:O	2.09	0.53
1:A:242:TRP:CD1	1:A:251:MET:HE2	2.44	0.52
1:A:497:GLU:HA	1:A:504:LYS:HD2	1.91	0.52
1:A:100:ARG:HH12	1:A:507:LYS:HD2	1.74	0.52
1:A:159:GLY:HA3	1:A:477:TRP:CE2	2.45	0.52
1:A:503:ASP:C	1:A:505:THR:N	2.68	0.52
1:A:202:THR:OG1	1:A:205:GLU:HG3	2.10	0.51
1:A:179:LEU:HD11	6:A:509:HEC:HBD1	1.92	0.51
1:A:496:ASP:CA	1:A:507:LYS:HE2	2.40	0.51
1:A:476:GLU:HG2	7:A:1264:HOH:O	2.11	0.51
1:A:422:GLN:HA	1:A:422:GLN:NE2	2.26	0.50
1:A:342:LYS:O	1:A:346:GLU:HG3	2.12	0.50
1:A:504:LYS:O	1:A:505:THR:CB	2.59	0.50
1:A:196:LYS:HB2	1:A:196:LYS:NZ	2.27	0.50
1:A:290:GLN:NE2	7:A:1219:HOH:O	2.45	0.50
1:A:165:THR:O	1:A:166:ILE:C	2.55	0.49
1:A:99:PRO:HG3	6:A:508:HEC:CGD	2.41	0.49
1:A:498:LYS:H	1:A:507:LYS:CG	2.24	0.49
1:A:497:GLU:N	1:A:507:LYS:HG2	2.27	0.49
1:A:497:GLU:CB	1:A:507:LYS:HG2	2.42	0.49
1:A:59:ARG:HD2	1:A:305:GLU:OE2	2.12	0.48
1:A:287:ILE:HA	1:A:290:GLN:HE21	1.78	0.48
1:A:291:LYS:HG2	6:A:512:HEC:CMD	2.43	0.48
1:A:204:GLN:HA	1:A:204:GLN:NE2	2.29	0.48
1:A:207:ARG:NH1	6:A:509:HEC:O1D	2.46	0.48
1:A:472:THR:O	1:A:476:GLU:HG3	2.13	0.48
1:A:227:ASP:OD2	1:A:233:LYS:HE3	2.15	0.47
1:A:488:ASN:ND2	7:A:1035:HOH:O	2.47	0.47
1:A:321:ASN:OD1	1:A:324:LYS:HG2	2.15	0.46
1:A:496:ASP:C	1:A:507:LYS:HE2	2.41	0.46
1:A:247:SER:OG	1:A:250:GLN:HG3	2.16	0.45
1:A:475:GLN:O	1:A:479:LYS:HG3	2.17	0.45
1:A:497:GLU:HB2	1:A:507:LYS:CA	2.46	0.45
1:A:84:VAL:HB	1:A:451:ALA:HB1	1.99	0.44
1:A:504:LYS:O	1:A:505:THR:HB	2.18	0.44
1:A:338:LYS:HZ2	1:A:338:LYS:HB2	1.82	0.44
1:A:498:LYS:N	1:A:507:LYS:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASP:HA	1:A:507:LYS:CE	2.48	0.43
1:A:133:CYS:HB3	1:A:214:CYS:HB3	1.99	0.43
1:A:328:ASN:ND2	7:A:1127:HOH:O	2.52	0.42
1:A:128:SER:HA	1:A:155:TRP:HA	2.01	0.42
1:A:176:SER:O	1:A:177:ALA:HB3	2.19	0.42
1:A:498:LYS:HG2	1:A:503:ASP:OD1	2.19	0.42
1:A:375:THR:OG1	1:A:378:GLU:HG3	2.20	0.42
1:A:490:GLU:O	1:A:493:LYS:HG3	2.19	0.42
1:A:66:LYS:C	1:A:68:LYS:H	2.28	0.41
1:A:100:ARG:HH22	1:A:507:LYS:NZ	2.19	0.41
1:A:227:ASP:OD2	1:A:231:VAL:HB	2.21	0.41
1:A:304:GLN:HA	1:A:308:VAL:O	2.21	0.41
1:A:66:LYS:C	1:A:68:LYS:N	2.76	0.41
1:A:126:LEU:HB3	1:A:127:PRO:HD2	2.03	0.40
1:A:133:CYS:HB3	1:A:214:CYS:SG	2.61	0.40
1:A:348:LYS:HD2	1:A:348:LYS:C	2.46	0.40
1:A:339:ASP:O	1:A:343:GLN:HG3	2.22	0.40
1:A:291:LYS:HG2	6:A:512:HEC:HMD3	2.03	0.40
1:A:163:VAL:HG21	1:A:487:LEU:HB2	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	469/485 (97%)	453 (97%)	14 (3%)	2 (0%)	30 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	THR
1	A	166	ILE

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	397/410 (97%)	393 (99%)	4 (1%)	68	50

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	TYR
1	A	332	GLU
1	A	338	LYS
1	A	422	GLN

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	72	ASN
1	A	204	GLN
1	A	290	GLN
1	A	328	ASN
1	A	335	GLN
1	A	422	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	SO4	A	658	3	4,4,4	0.36	0	6,6,6	0.12	0
5	ACT	A	659	-	3,3,3	0.92	0	3,3,3	0.64	0
6	HEC	A	509	1	50,50,50	1.19	4 (8%)	68,82,82	0.90	3 (4%)
4	SO4	A	657	3	4,4,4	0.36	0	6,6,6	0.10	0
6	HEC	A	510	1,3	50,50,50	1.15	4 (8%)	68,82,82	1.12	4 (5%)
6	HEC	A	512	1,3	50,50,50	1.20	5 (10%)	68,82,82	1.11	2 (2%)
6	HEC	A	508	1,4	50,50,50	1.15	3 (6%)	68,82,82	1.11	5 (7%)
4	SO4	A	656	6	4,4,4	0.35	0	6,6,6	0.10	0
6	HEC	A	511	1,3	50,50,50	1.16	4 (8%)	68,82,82	0.98	2 (2%)

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
6	HEC	A	509	1	1/1/3/7	7/14/54/54	-
6	HEC	A	510	1,3	1/1/3/7	5/14/54/54	-
6	HEC	A	512	1,3	1/1/3/7	7/14/54/54	-
6	HEC	A	508	1,4	1/1/3/7	4/14/54/54	-
6	HEC	A	511	1,3	1/1/3/7	7/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	HEC	CAB-C3B	-4.13	1.40	1.51
6	A	508	HEC	CAB-C3B	-4.06	1.40	1.51
6	A	512	HEC	CAB-C3B	-4.06	1.40	1.51
6	A	509	HEC	CAC-C3C	-3.94	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	510	HEC	CAB-C3B	-3.92	1.41	1.51
6	A	511	HEC	CAC-C3C	-3.91	1.41	1.51
6	A	512	HEC	CAC-C3C	-3.90	1.41	1.51
6	A	510	HEC	CAC-C3C	-3.78	1.41	1.51
6	A	511	HEC	CAB-C3B	-3.73	1.41	1.51
6	A	508	HEC	CAC-C3C	-3.66	1.41	1.51
6	A	509	HEC	CBB-CAB	-2.41	1.41	1.51
6	A	509	HEC	CBC-CAC	-2.34	1.41	1.51
6	A	511	HEC	CBC-CAC	-2.32	1.41	1.51
6	A	510	HEC	CBB-CAB	-2.32	1.41	1.51
6	A	512	HEC	CBC-CAC	-2.31	1.41	1.51
6	A	512	HEC	CBB-CAB	-2.25	1.42	1.51
6	A	512	HEC	O2A-CGA	-2.09	1.23	1.30
6	A	511	HEC	CBB-CAB	-2.08	1.42	1.51
6	A	508	HEC	CBC-CAC	-2.06	1.42	1.51
6	A	510	HEC	CBC-CAC	-2.01	1.43	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	508	HEC	CBC-CAC-C3C	4.08	123.47	112.42
6	A	510	HEC	CBB-CAB-C3B	4.06	123.42	112.42
6	A	512	HEC	CBC-CAC-C3C	3.77	122.63	112.42
6	A	512	HEC	CBB-CAB-C3B	3.57	122.10	112.42
6	A	511	HEC	CBC-CAC-C3C	3.27	121.28	112.42
6	A	510	HEC	CBC-CAC-C3C	3.25	121.23	112.42
6	A	509	HEC	CBC-CAC-C3C	2.94	120.39	112.42
6	A	509	HEC	CBB-CAB-C3B	2.86	120.17	112.42
6	A	511	HEC	CBB-CAB-C3B	2.77	119.92	112.42
6	A	510	HEC	CAC-C3C-C4C	2.72	128.65	124.91
6	A	508	HEC	CBB-CAB-C3B	2.44	119.05	112.42
6	A	508	HEC	CAB-C3B-C4B	2.33	127.82	124.79
6	A	508	HEC	CBD-CAD-C3D	2.29	118.87	112.53
6	A	510	HEC	CAD-C3D-C4D	2.24	128.60	124.70
6	A	509	HEC	CAB-C3B-C4B	2.06	127.47	124.79
6	A	508	HEC	CAD-C3D-C2D	-2.04	124.05	127.87

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	508	HEC	NA
6	A	509	HEC	NA

Continued on next page...

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Mol	Chain	Res	Type	Atom
6	A	510	HEC	NA
6	A	511	HEC	NA
6	A	512	HEC	NA

All (30) torsion outliers are listed below:

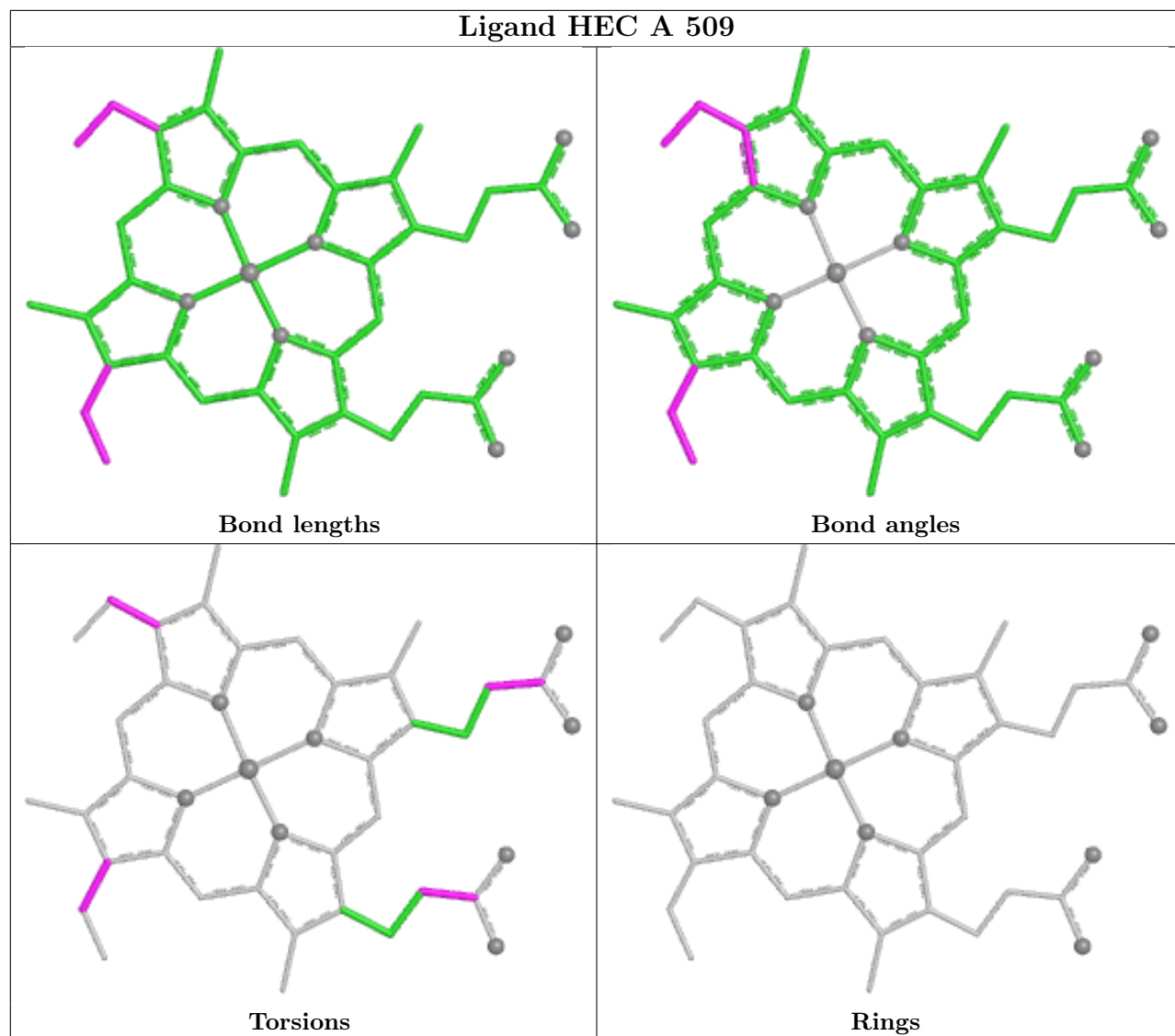
Mol	Chain	Res	Type	Atoms
6	A	511	HEC	C2B-C3B-CAB-CBB
6	A	508	HEC	C4C-C3C-CAC-CBC
6	A	508	HEC	C2C-C3C-CAC-CBC
6	A	511	HEC	C4C-C3C-CAC-CBC
6	A	512	HEC	C2A-CAA-CBA-CGA
6	A	511	HEC	C2C-C3C-CAC-CBC
6	A	512	HEC	C4C-C3C-CAC-CBC
6	A	510	HEC	C4C-C3C-CAC-CBC
6	A	510	HEC	C2B-C3B-CAB-CBB
6	A	510	HEC	C2C-C3C-CAC-CBC
6	A	509	HEC	C2B-C3B-CAB-CBB
6	A	511	HEC	C4B-C3B-CAB-CBB
6	A	509	HEC	C4C-C3C-CAC-CBC
6	A	512	HEC	C2B-C3B-CAB-CBB
6	A	509	HEC	C4B-C3B-CAB-CBB
6	A	510	HEC	C4B-C3B-CAB-CBB
6	A	512	HEC	C2C-C3C-CAC-CBC
6	A	508	HEC	CAA-CBA-CGA-O1A
6	A	509	HEC	CAA-CBA-CGA-O1A
6	A	509	HEC	CAA-CBA-CGA-O2A
6	A	508	HEC	CAA-CBA-CGA-O2A
6	A	511	HEC	CAD-CBD-CGD-O2D
6	A	511	HEC	CAD-CBD-CGD-O1D
6	A	512	HEC	CAD-CBD-CGD-O2D
6	A	512	HEC	C4B-C3B-CAB-CBB
6	A	512	HEC	CAD-CBD-CGD-O1D
6	A	509	HEC	CAD-CBD-CGD-O2D
6	A	510	HEC	C3A-C2A-CAA-CBA
6	A	509	HEC	CAD-CBD-CGD-O1D
6	A	511	HEC	CAA-CBA-CGA-O2A

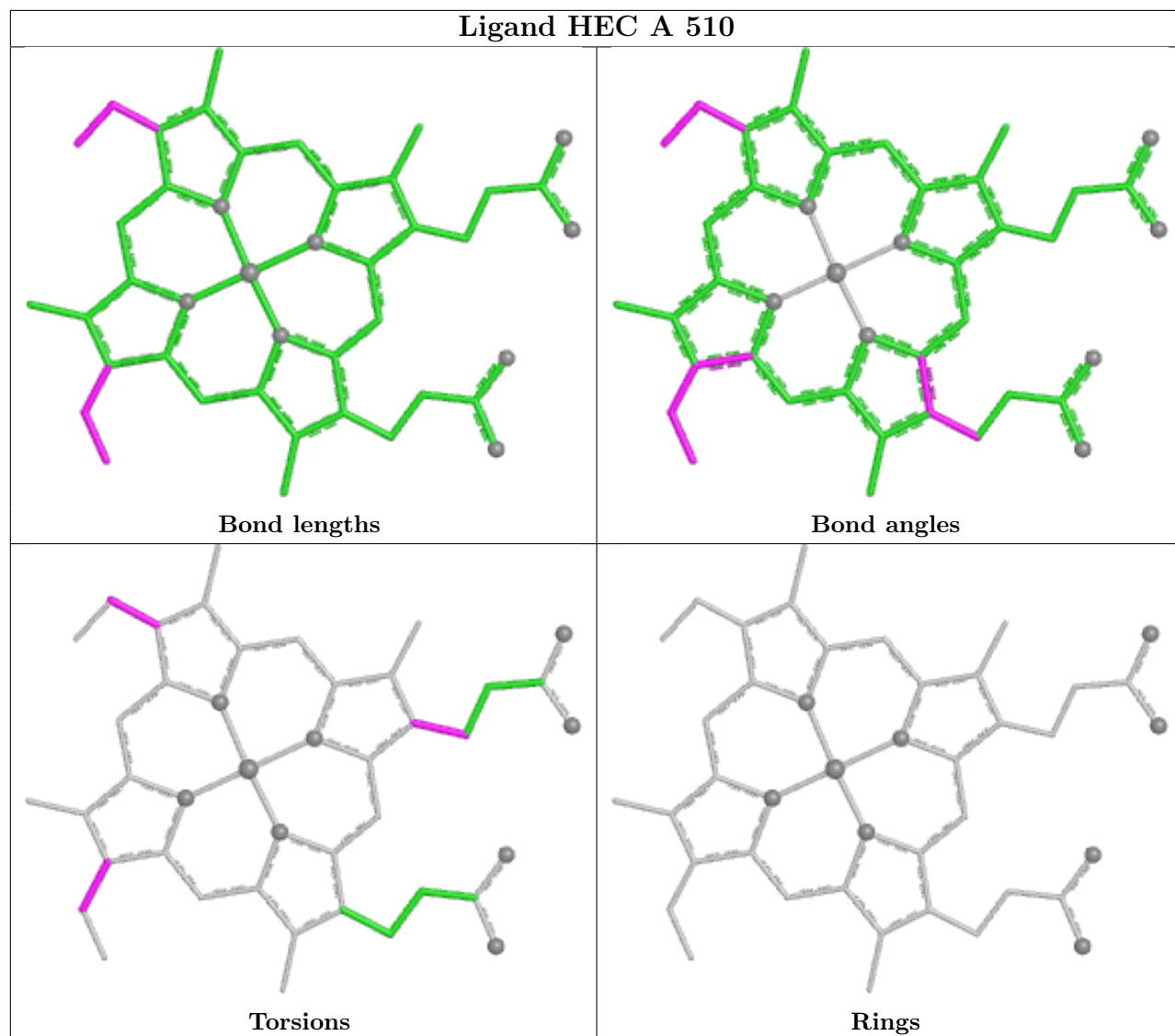
There are no ring outliers.

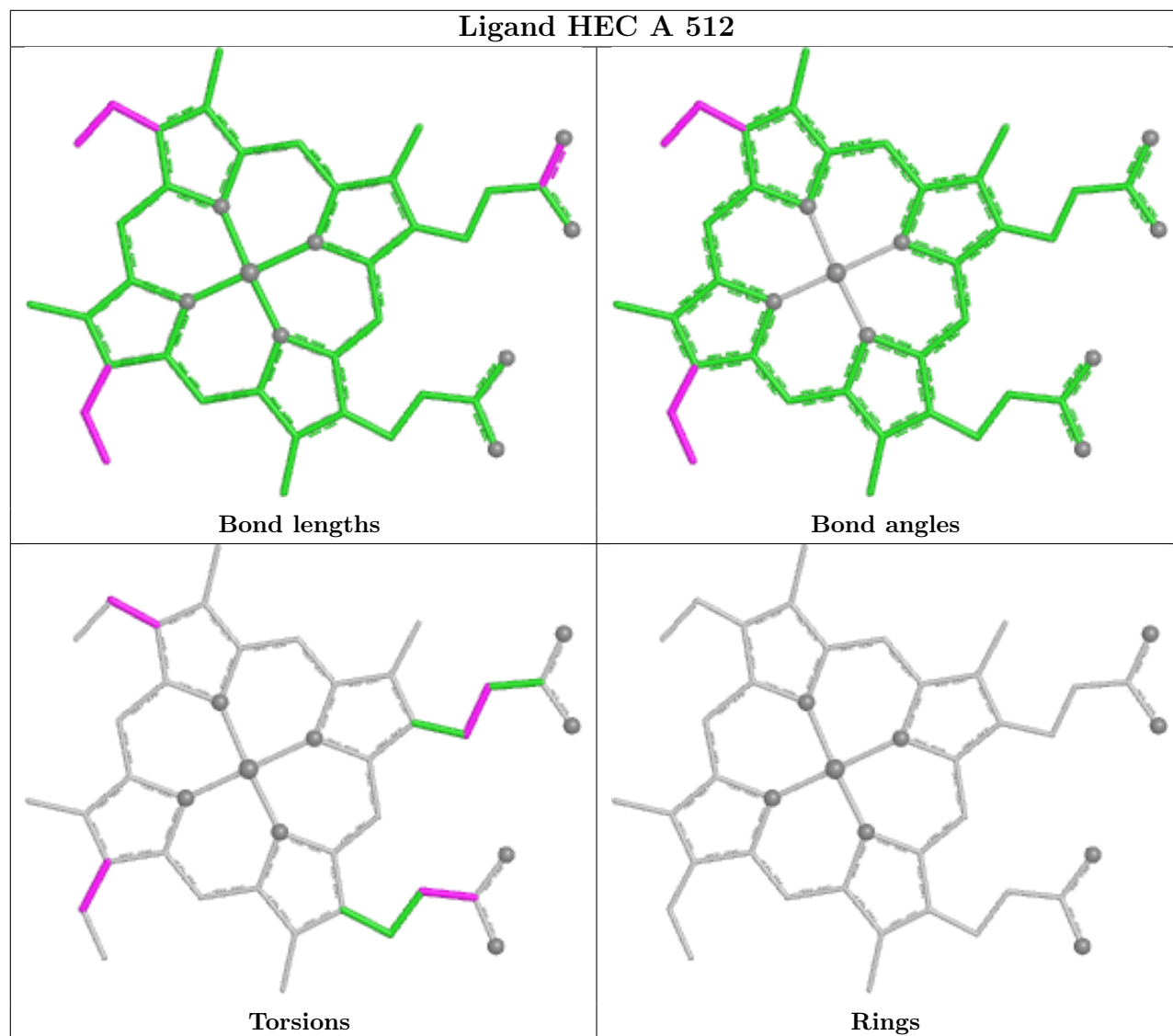
3 monomers are involved in 5 short contacts:

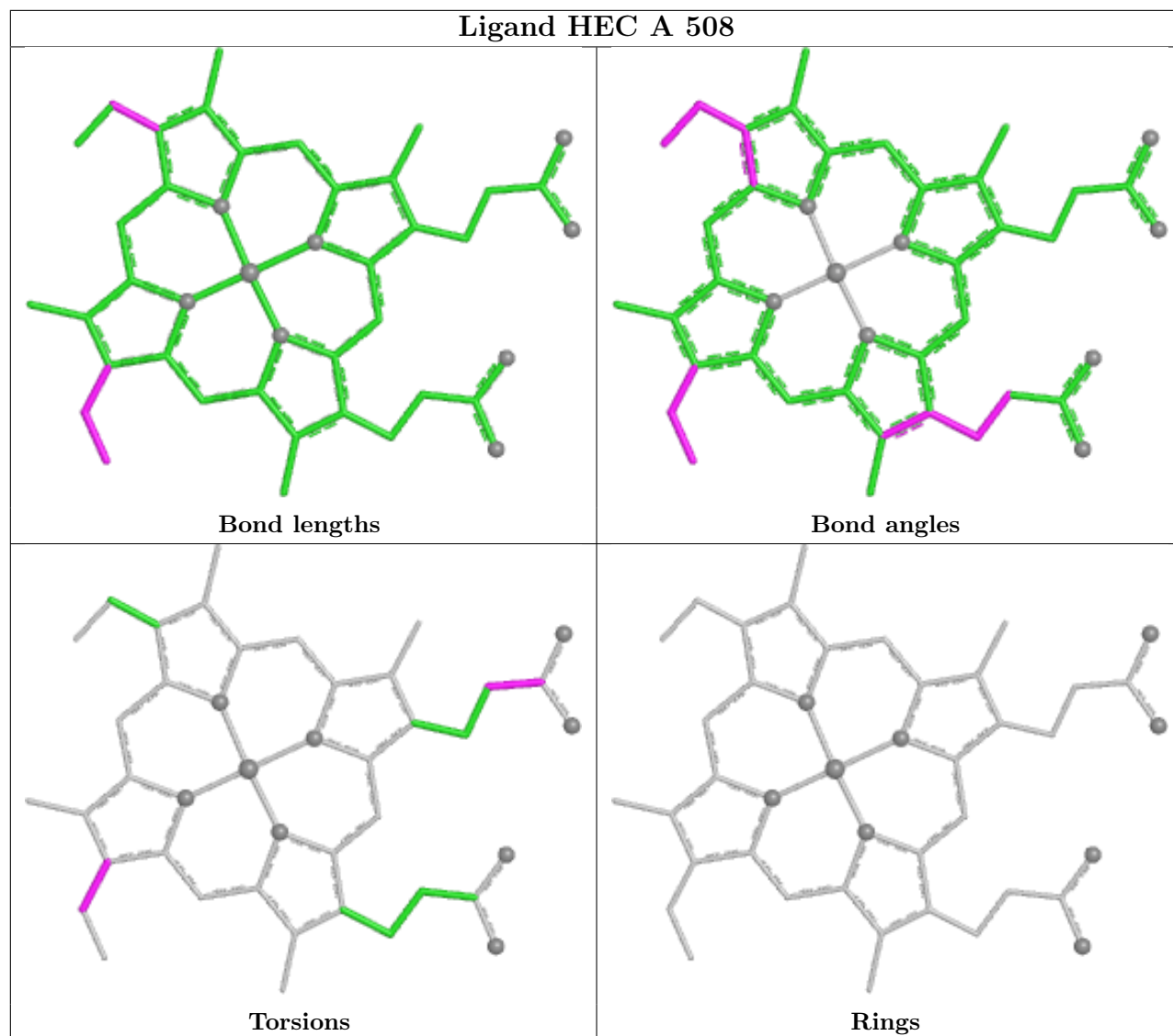
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509	HEC	2	0
6	A	512	HEC	2	0
6	A	508	HEC	1	0

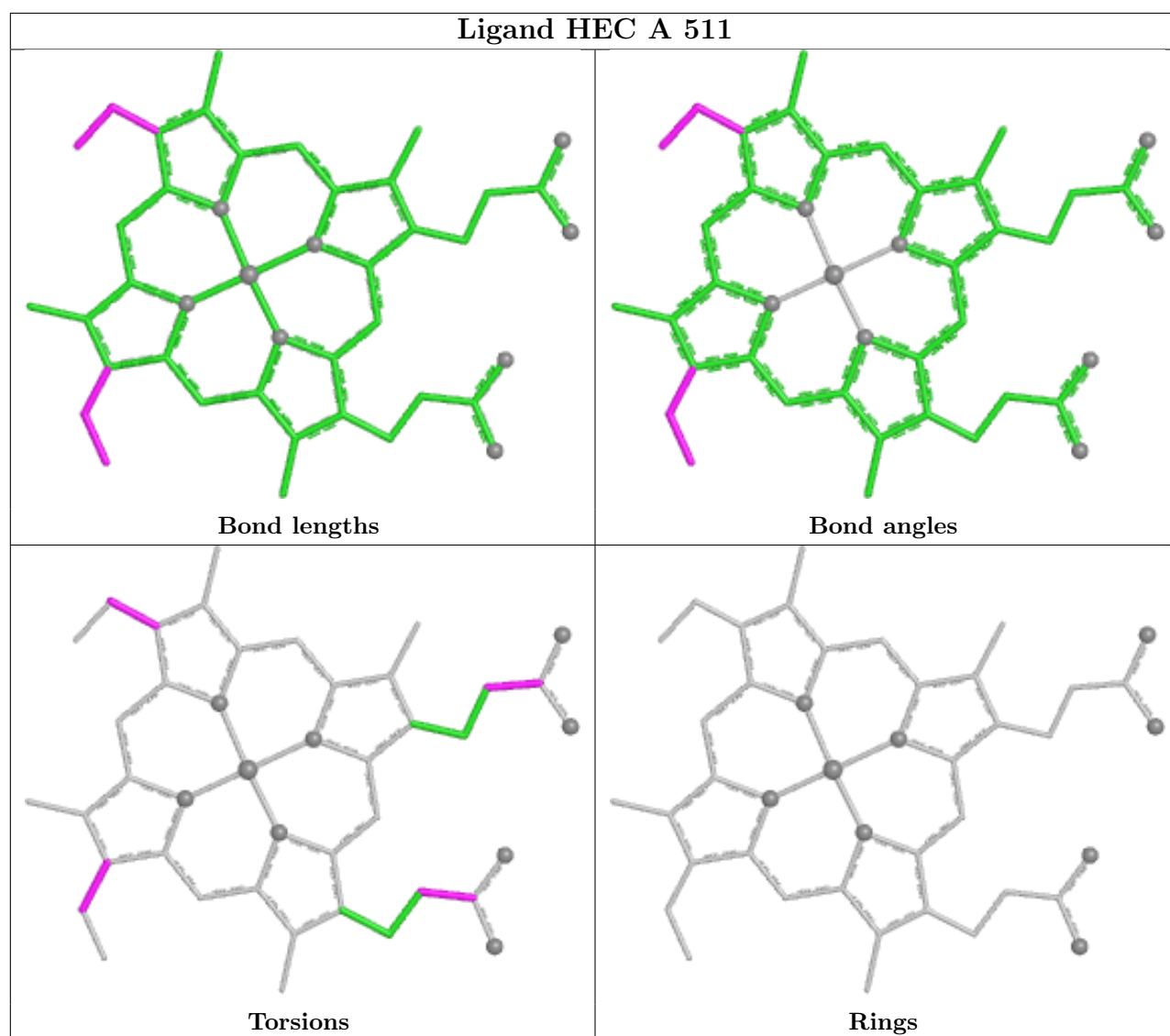
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.