



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 05:31 am BST

PDB ID : 2CA4 / pdb_00002ca4
Title : Sulfite dehydrogenase from Starkeya Novella mutant
Authors : Bailey, S.; Kappler, U.
Deposited on : 2005-12-16
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

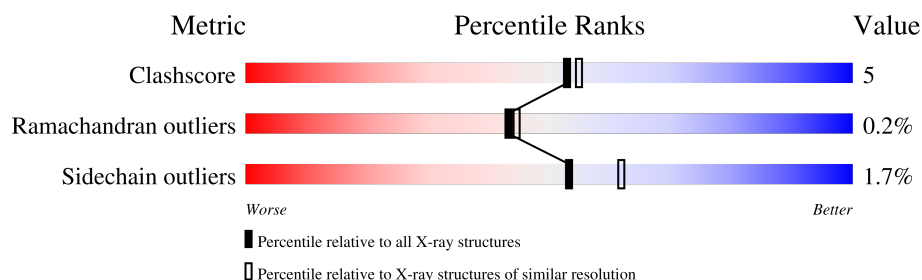
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	373	 89% 10% .
2	B	81	 96% .

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
4	HEC	B	1582[A]	X	-	-	-
4	HEC	B	1582[B]	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3909 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 SULFITE\ :CYTOCHROME C OXIDOREDUCTASE SUB-UNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	1	0
			2834	1808	490	524	12			

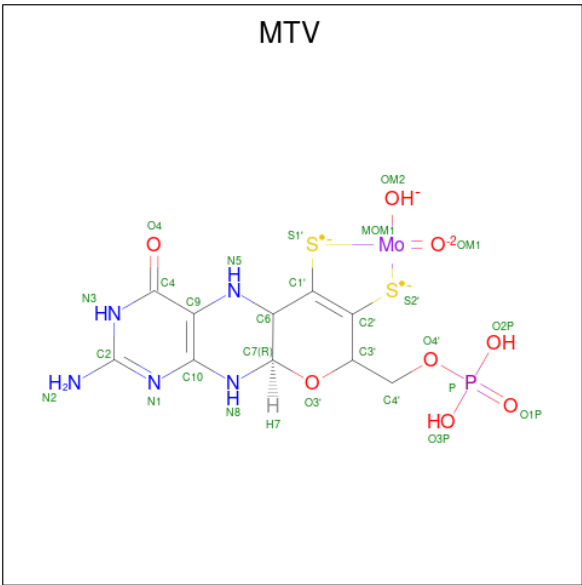
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	HIS	engineered mutation	UNP Q9LA16

- Molecule 2 is a protein called SULFITE\ :CYTOCHROME C OXIDOREDUCTASE SUB-UNIT B.

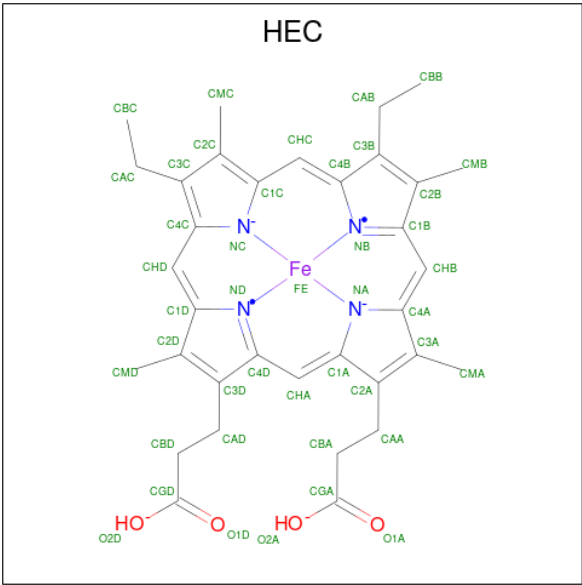
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			623	396	101	123	3			

- Molecule 3 is (MOLYBDOPTERIN-S,S)-DIOXO-THIO-MOLYBDENUM(IV) (CCD ID: MTV) (formula: C₁₀H₁₃MoN₅O₈PS₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total 27	C 10	Mo 1	N 5	O 8	P 1	S 2	0	0

- Molecule 4 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	300	Total 300	O 300	0	0
5	B	78	Total 78	O 78	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. 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: SULFITE\ :CYTOCHROME C OXIDOREDUCTASE SUBUNIT A

Chain A:  89% 10% .



• Molecule 2: SULFITE\ :CYTOCHROME C OXIDOREDUCTASE SUBUNIT B

Chain B:  96% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.44 Å 92.80 Å 55.82 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.5 (20.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.147 , 0.199	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3909	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: MTV, HEC

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	0.75	0/2910	0.84	0/3965
2	B	0.73	0/641	0.86	0/876
All	All	0.75	0/3551	0.84	0/4841

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 [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	2834	0	2814	27	0
2	B	623	0	588	6	0
3	A	27	0	7	2	0
4	B	47	0	8	2	0
5	A	300	0	0	5	1
5	B	78	0	0	1	0
All	All	3909	0	3417	35	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (35) 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)
4:B:1582[B]:HEC:HBD2	5:B:2059:HOH:O	1.79	0.81
1:A:301:ALA:HB2	1:A:328:LEU:HD23	1.66	0.78
1:A:356:ASN:HD21	1:A:360:TYR:H	1.34	0.76
1:A:103:GLN:HE21	1:A:107:ASN:HD22	1.32	0.76
1:A:318:LYS:HB3	5:A:2233:HOH:O	1.87	0.74
1:A:341:ALA:H	1:A:349:GLN:HE21	1.36	0.73
1:A:331:THR:O	1:A:335:HIS:HE1	1.71	0.72
1:A:259:ASN:HD22	1:A:260:ARG:H	1.37	0.70
1:A:33:GLN:OE1	1:A:55[B]:ARG:HD2	1.92	0.69
1:A:259:ASN:ND2	1:A:260:ARG:H	1.90	0.69
1:A:56:TYR:OH	1:A:216:HIS:HE1	1.76	0.69
1:A:291:GLY:O	1:A:318:LYS:HD2	1.94	0.66
1:A:199:TYR:O	1:A:216:HIS:HD2	1.77	0.66
3:A:374:MTV:MOM1	3:A:374:MTV:OM1	1.69	0.63
1:A:260:ARG:NH1	5:A:2213:HOH:O	2.31	0.62
1:A:55[A]:ARG:HD2	3:A:374:MTV:S1'	2.42	0.60
2:B:537:TYR:CE2	4:B:1582[A]:HEC:HBD2	2.40	0.56
1:A:56:TYR:OH	1:A:216:HIS:CE1	2.61	0.51
1:A:2:ASP:HB3	1:A:15:LEU:HD12	1.94	0.49
1:A:181:GLU:OE1	1:A:319:TYR:OH	2.21	0.48
1:A:33:GLN:OE1	1:A:55[A]:ARG:HG2	2.15	0.47
1:A:146:GLN:HG2	5:A:2137:HOH:O	2.16	0.46
1:A:300:SER:O	1:A:337:LEU:HA	2.17	0.45
1:A:132:ARG:HB3	1:A:187:SER:HB3	1.99	0.45
1:A:341:ALA:H	1:A:349:GLN:NE2	2.09	0.45
1:A:170:LYS:HE3	1:A:232:MET:SD	2.57	0.44
1:A:296:GLN:HE21	1:A:342:THR:HG23	1.83	0.43
1:A:158:ASP:O	5:A:2146:HOH:O	2.21	0.42
1:A:12:GLU:HB2	5:A:2018:HOH:O	2.19	0.42
1:A:74:ILE:HD13	1:A:220:ILE:HB	2.02	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2232:HOH:O	5:A:2232:HOH:O[2_655]	2.06	0.14

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	372/373 (100%)	360 (97%)	11 (3%)	1 (0%)	36	36
2	B	79/81 (98%)	79 (100%)	0	0	100	100
All	All	451/454 (99%)	439 (97%)	11 (2%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA

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	295/294 (100%)	289 (98%)	6 (2%)	48	56
2	B	63/63 (100%)	63 (100%)	0	100	100
All	All	358/357 (100%)	352 (98%)	6 (2%)	53	62

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

Mol	Chain	Res	Type
1	A	12	GLU
1	A	45	LEU
1	A	75	LYS
1	A	233	LYS
1	A	305	LYS

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Mol	Chain	Res	Type
1	A	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	216	HIS
1	A	259	ASN
1	A	335	HIS
1	A	349	GLN
1	A	356	ASN
1	A	363	ASN
2	B	528	ASN
2	B	555	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 [i](#)

3 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	HEC	B	1582[B]	-	50,50,50	1.92	11 (22%)	68,82,82	1.61	10 (14%)
3	MTV	A	374	1	21,30,30	1.61	2 (9%)	20,48,48	2.15	6 (30%)
4	HEC	B	1582[A]	-	50,50,50	1.92	11 (22%)	68,82,82	1.61	10 (14%)

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	HEC	B	1582[B]	-	1/1/3/7	6/14/54/54	-
3	MTV	A	374	1	-	0/6/44/44	0/4/4/4
4	HEC	B	1582[A]	-	1/1/3/7	2/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1582[A]	HEC	C3D-C2D	7.86	1.53	1.36
4	B	1582[B]	HEC	C3D-C2D	7.86	1.53	1.36
3	A	374	MTV	C9-C10	5.99	1.48	1.38
4	B	1582[A]	HEC	FE-NA	4.53	2.10	1.95
4	B	1582[B]	HEC	FE-NA	4.53	2.10	1.95
4	B	1582[A]	HEC	FE-NB	4.37	2.08	1.94
4	B	1582[B]	HEC	FE-NB	4.37	2.08	1.94
4	B	1582[A]	HEC	FE-ND	4.05	2.07	1.94
4	B	1582[B]	HEC	FE-ND	4.05	2.07	1.94
4	B	1582[A]	HEC	FE-NC	3.75	2.07	1.95
4	B	1582[B]	HEC	FE-NC	3.75	2.07	1.95
3	A	374	MTV	C9-C4	2.79	1.49	1.42
4	B	1582[A]	HEC	CMA-C3A	2.57	1.56	1.50
4	B	1582[B]	HEC	CMA-C3A	2.57	1.56	1.50
4	B	1582[A]	HEC	CMC-C2C	2.44	1.56	1.50
4	B	1582[B]	HEC	CMC-C2C	2.44	1.56	1.50
4	B	1582[A]	HEC	CAB-C3B	2.28	1.57	1.51
4	B	1582[B]	HEC	CAB-C3B	2.28	1.57	1.51
4	B	1582[A]	HEC	CAA-C2A	2.16	1.56	1.51
4	B	1582[B]	HEC	CAA-C2A	2.16	1.56	1.51
4	B	1582[A]	HEC	CMB-C2B	2.15	1.55	1.50
4	B	1582[B]	HEC	CMB-C2B	2.15	1.55	1.50
4	B	1582[A]	HEC	CMD-C2D	2.12	1.55	1.50
4	B	1582[B]	HEC	CMD-C2D	2.12	1.55	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1582[A]	HEC	C1D-ND-C4D	7.03	112.34	105.07
4	B	1582[B]	HEC	C1D-ND-C4D	7.03	112.34	105.07
3	A	374	MTV	C2-N1-C10	5.07	122.58	113.43
3	A	374	MTV	C1'-C2'-S2'	3.91	122.37	120.15
3	A	374	MTV	C2'-C1'-S1'	3.49	122.13	120.15
4	B	1582[A]	HEC	C4C-NC-C1C	3.37	108.65	105.35
4	B	1582[B]	HEC	C4C-NC-C1C	3.37	108.65	105.35
4	B	1582[A]	HEC	CAD-C3D-C4D	3.07	130.02	124.66
4	B	1582[B]	HEC	CAD-C3D-C4D	3.07	130.02	124.66
3	A	374	MTV	C4-C9-N5	2.99	124.78	116.76
4	B	1582[A]	HEC	C3C-C4C-NC	-2.91	106.89	110.15
4	B	1582[B]	HEC	C3C-C4C-NC	-2.91	106.89	110.15
4	B	1582[A]	HEC	C4A-NA-C1A	2.89	108.18	105.35
4	B	1582[B]	HEC	C4A-NA-C1A	2.89	108.18	105.35
4	B	1582[A]	HEC	C4B-NB-C1B	2.81	107.97	105.07
4	B	1582[B]	HEC	C4B-NB-C1B	2.81	107.97	105.07
4	B	1582[A]	HEC	CHB-C1B-NB	2.68	127.33	124.42
4	B	1582[B]	HEC	CHB-C1B-NB	2.68	127.33	124.42
3	A	374	MTV	O4-C4-C9	-2.48	121.56	127.24
4	B	1582[A]	HEC	C2A-C1A-NA	-2.30	108.08	110.32
4	B	1582[B]	HEC	C2A-C1A-NA	-2.30	108.08	110.32
4	B	1582[A]	HEC	C3D-C4D-ND	-2.24	108.19	110.36
4	B	1582[B]	HEC	C3D-C4D-ND	-2.24	108.19	110.36
4	B	1582[A]	HEC	O2A-CGA-CBA	2.01	120.48	114.03
4	B	1582[B]	HEC	O2A-CGA-CBA	2.01	120.48	114.03
3	A	374	MTV	C9-C4-N3	2.00	118.27	112.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1582[A]	HEC	NA
4	B	1582[B]	HEC	NA

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1582[B]	HEC	C4D-C3D-CAD-CBD
4	B	1582[B]	HEC	C2D-C3D-CAD-CBD
4	B	1582[A]	HEC	CAA-CBA-CGA-O2A
4	B	1582[B]	HEC	CAA-CBA-CGA-O2A
4	B	1582[A]	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
4	B	1582[B]	HEC	CAA-CBA-CGA-O1A
4	B	1582[B]	HEC	CAD-CBD-CGD-O1D
4	B	1582[B]	HEC	CAD-CBD-CGD-O2D

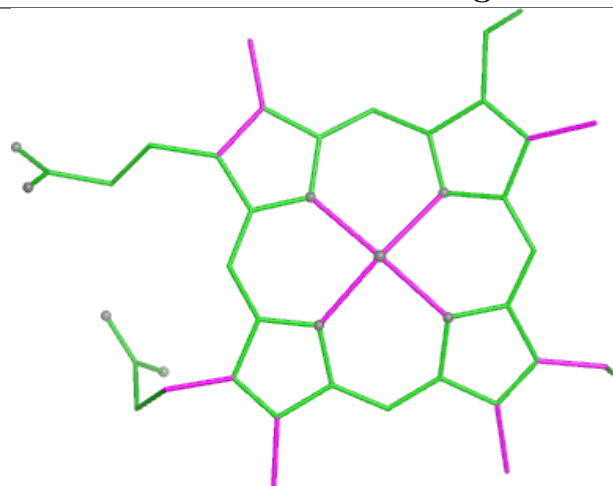
There are no ring outliers.

3 monomers are involved in 4 short contacts:

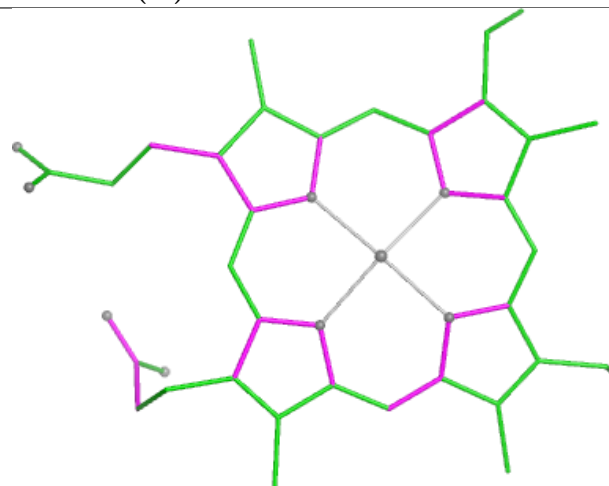
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1582[B]	HEC	1	0
3	A	374	MTV	2	0
4	B	1582[A]	HEC	1	0

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.

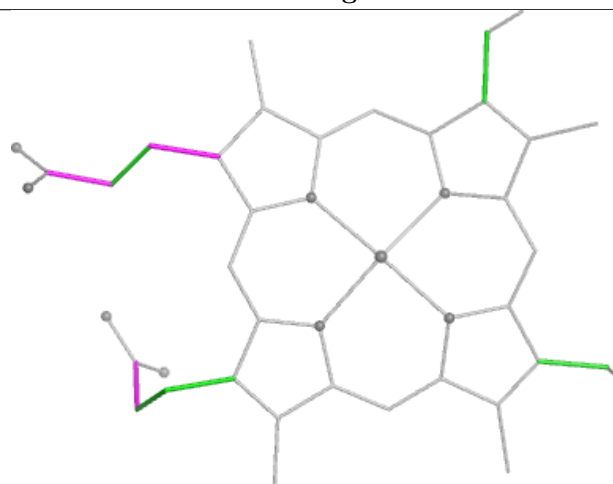
Ligand HEC B 1582 (B)



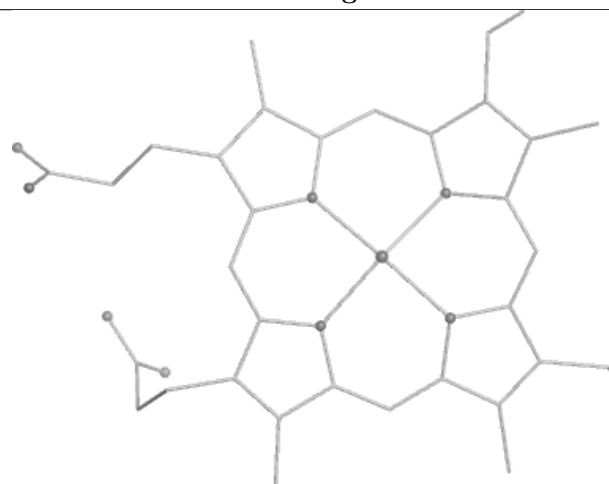
Bond lengths



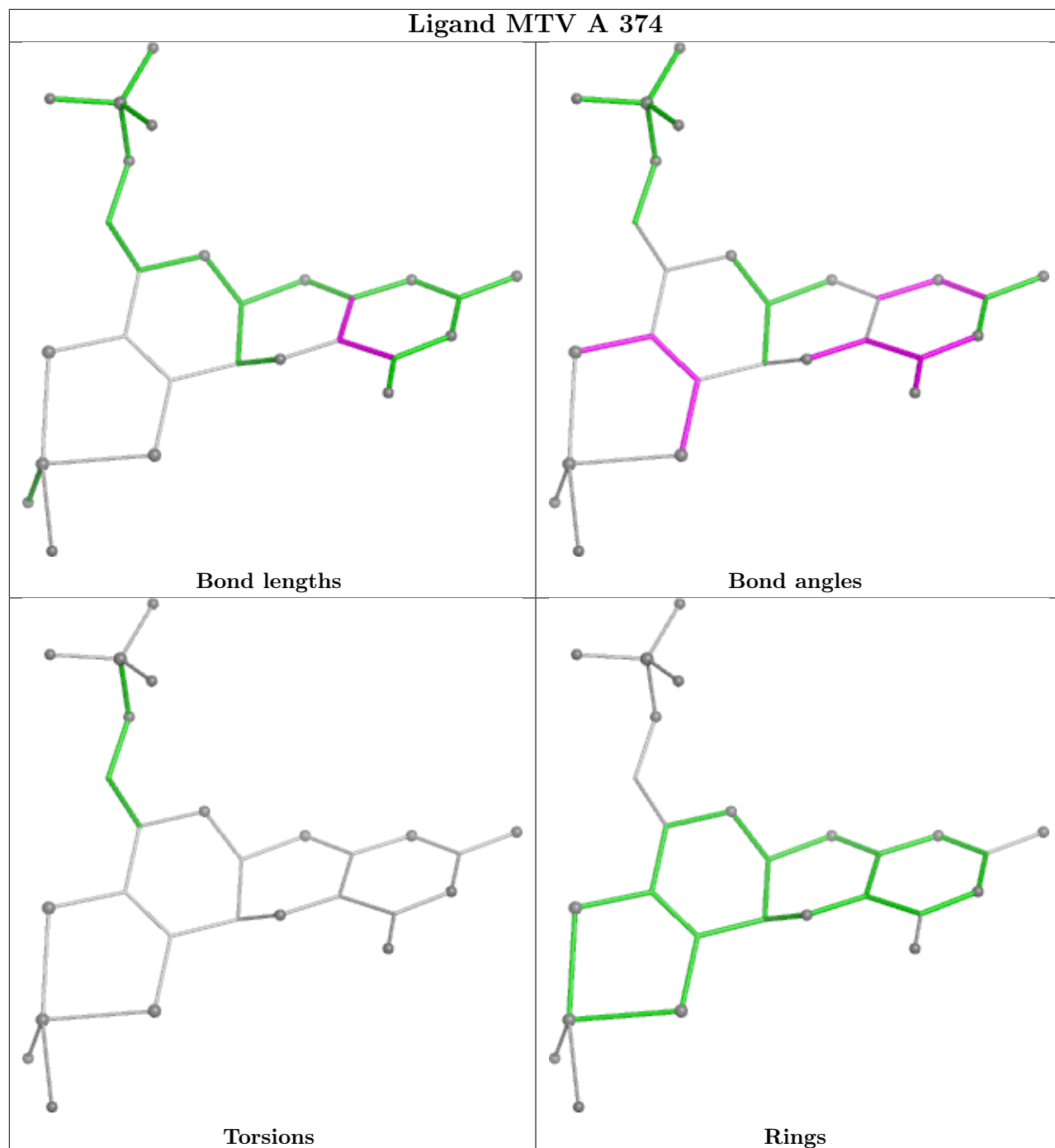
Bond angles

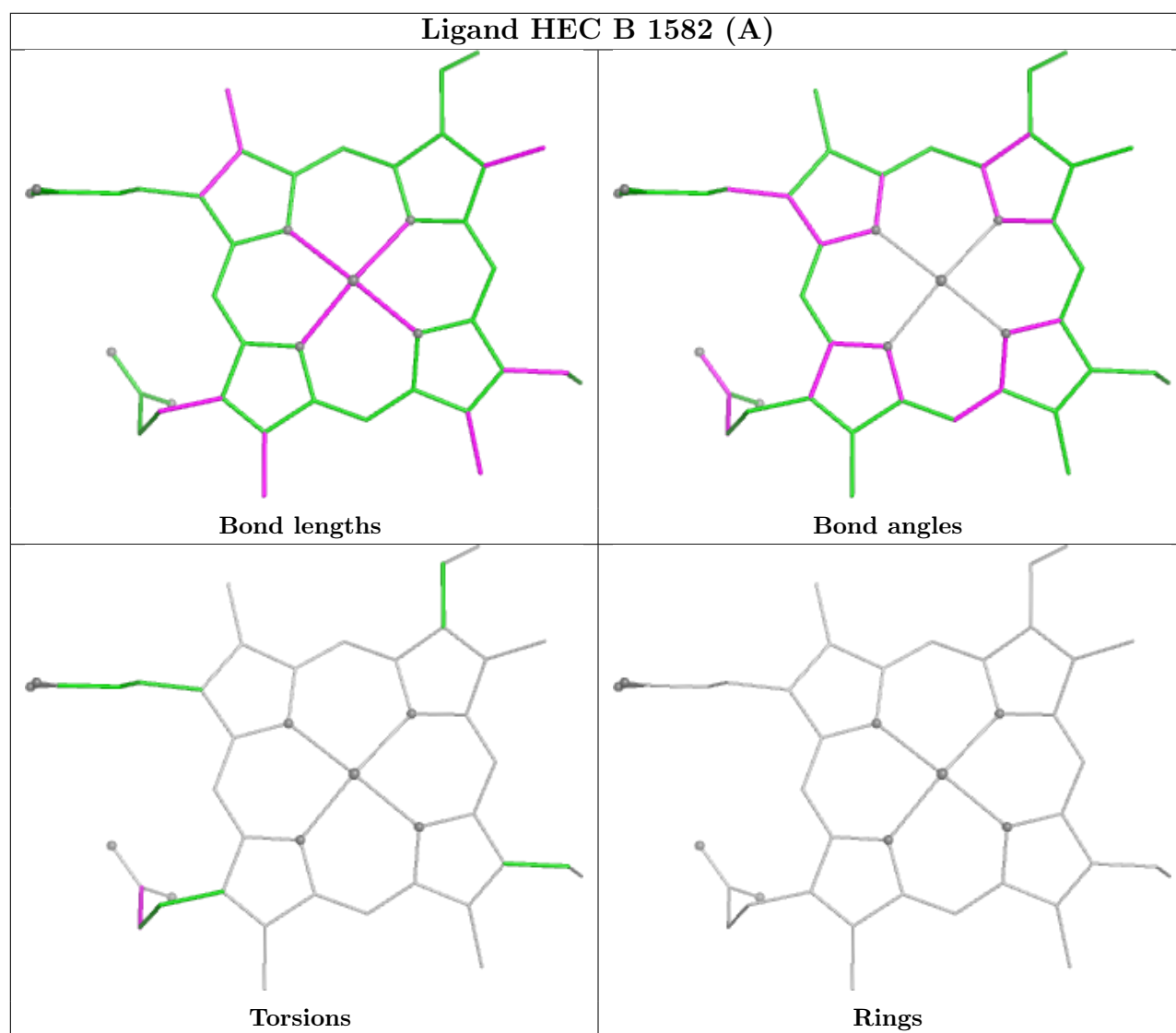


Torsions



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

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.