



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:04 PM UTC

PDB ID : 1QJD / pdb_00001qjd
Title : Flavocytochrome C3 from Shewanella frigidimarina
Authors : Taylor, P.; Pealing, S.L.; Reid, G.A.; Chapman, S.K.; Walkinshaw, M.D.
Deposited on : 1999-06-23
Resolution : 1.80 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)	:	2.49

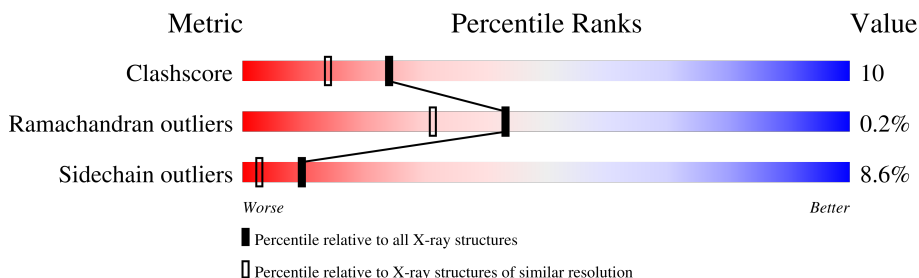
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	571	

2 Entry composition [i](#)

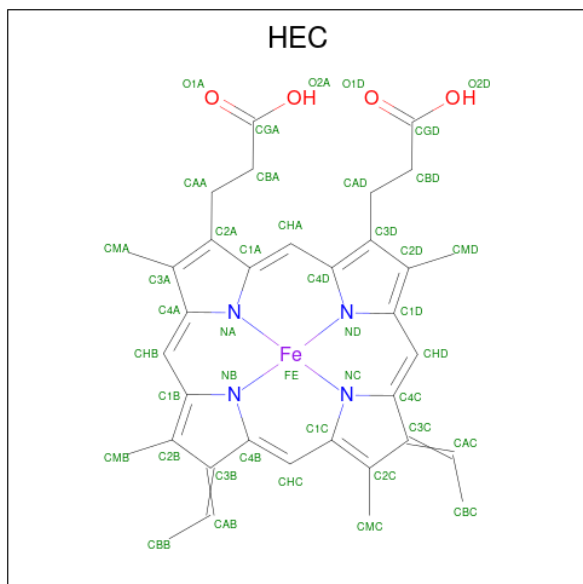
There are 7 unique types of molecules in this entry. The entry contains 5034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME C3.

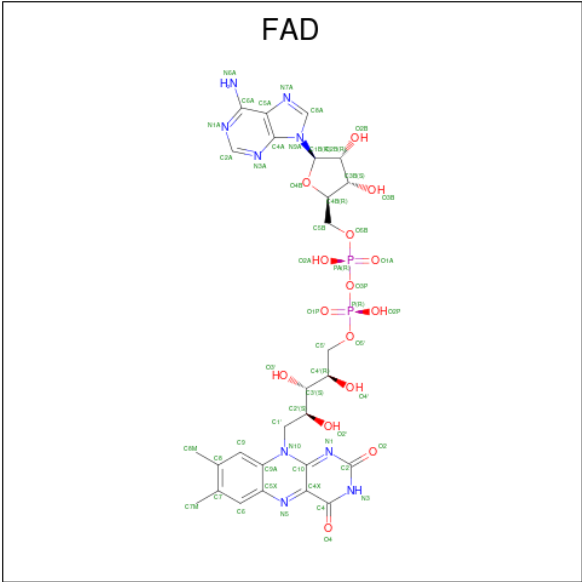
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4217	2615	744	833	25			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



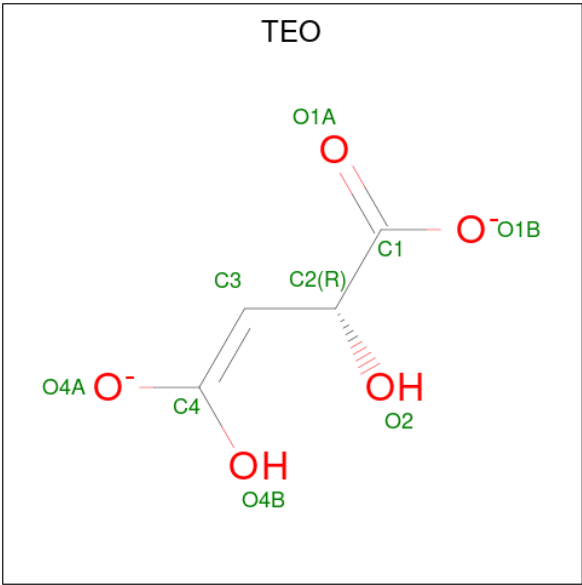
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is MALATE LIKE INTERMEDIATE (CCD ID: TEO) (formula: C₄H₄O₅).

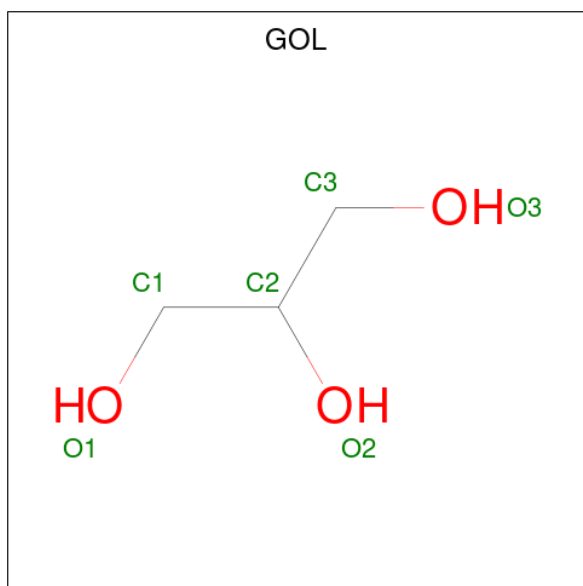


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

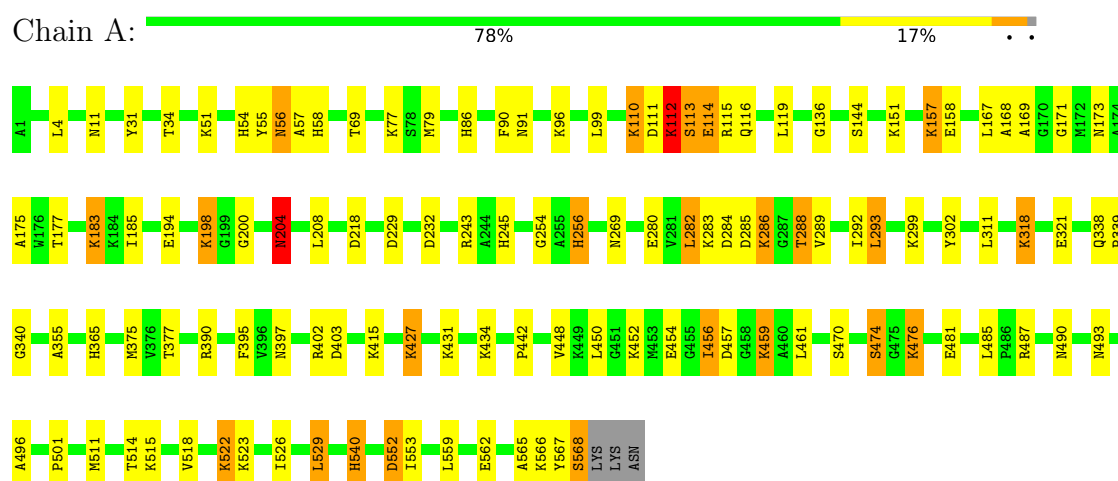
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	576	Total	O	0	0
			576	576		

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: FLAVOCYTOCHROME C3



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.39Å 91.95Å 78.29Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	24.00 – 1.80	Depositor
% Data completeness (in resolution range)	83.1 (24.00-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.192 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: FAD, GOL, TEO, NA, 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	0.47	0/4287	1.40	30/5795 (0.5%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	CA-C-N	14.97	148.65	121.70
1	A	112	LYS	C-N-CA	14.97	148.65	121.70
1	A	487	ARG	CD-NE-CZ	11.66	140.73	124.40
1	A	218	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	86	HIS	CA-CB-CG	6.66	120.46	113.80
1	A	567	TYR	CA-C-N	6.60	133.58	121.70
1	A	567	TYR	C-N-CA	6.60	133.58	121.70
1	A	169	ALA	CA-C-N	6.34	128.07	120.14
1	A	169	ALA	C-N-CA	6.34	128.07	120.14
1	A	377	THR	CA-C-O	6.05	127.85	121.19
1	A	292	ILE	CA-C-N	-6.04	113.65	122.65
1	A	292	ILE	C-N-CA	-6.04	113.65	122.65
1	A	56	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	540	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	288	THR	CA-C-N	-5.71	112.41	120.75
1	A	288	THR	C-N-CA	-5.71	112.41	120.75
1	A	552	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	456	ILE	CA-C-O	-5.58	114.36	120.72
1	A	171	GLY	CA-C-N	5.54	130.98	123.11
1	A	171	GLY	C-N-CA	5.54	130.98	123.11
1	A	204	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	485	LEU	O-C-N	5.49	126.35	121.36
1	A	395	PHE	CA-C-O	5.40	124.46	118.52
1	A	175	ALA	CA-C-N	5.21	131.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	5.21	131.07	121.70
1	A	256	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	285	ASP	CA-C-N	-5.03	114.68	122.67
1	A	285	ASP	C-N-CA	-5.03	114.68	122.67
1	A	232	ASP	CA-C-N	-5.02	116.18	123.11
1	A	232	ASP	C-N-CA	-5.02	116.18	123.11

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	4217	0	4152	87	0
2	A	172	0	120	2	0
3	A	53	0	31	3	0
4	A	9	0	2	1	0
5	A	1	0	0	0	0
6	A	6	0	8	2	0
7	A	576	0	0	13	0
All	All	5034	0	4313	88	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 10.

All (88) 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:79:MET:HE2	1:A:96:LYS:HE3	1.55	0.87
1:A:431:LYS:HA	1:A:434:LYS:HD2	1.62	0.80
1:A:204:ASN:HD22	1:A:204:ASN:H	1.28	0.79
1:A:229:ASP:H	1:A:256:HIS:HE1	1.30	0.79
1:A:454:GLU:OE1	6:A:1576:GOL:H2	1.83	0.78
1:A:457:ASP:OD1	1:A:459:LYS:HG3	1.86	0.75
1:A:427:LYS:HE3	1:A:427:LYS:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:OD1	1:A:286:LYS:HD2	1.87	0.74
1:A:397:ASN:HB3	7:A:2438:HOH:O	1.89	0.71
1:A:280:GLU:HB3	1:A:293:LEU:HD11	1.71	0.71
1:A:115:ARG:O	1:A:119:LEU:HD23	1.90	0.71
1:A:431:LYS:HD3	1:A:434:LYS:HD3	1.73	0.70
1:A:526:ILE:HG23	1:A:529:LEU:HB3	1.78	0.66
1:A:302:TYR:HA	7:A:2357:HOH:O	1.96	0.65
1:A:476:LYS:HG2	1:A:476:LYS:O	1.96	0.64
1:A:229:ASP:H	1:A:256:HIS:CE1	2.15	0.64
1:A:69:THR:HB	7:A:2095:HOH:O	2.00	0.62
1:A:183:LYS:O	1:A:185:ILE:HD12	2.01	0.61
1:A:204:ASN:H	1:A:204:ASN:ND2	1.97	0.61
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.66	0.61
1:A:474:SER:HB2	1:A:476:LYS:HE3	1.81	0.60
1:A:402:ARG:HH22	4:A:1574:TEO:C3	2.14	0.60
1:A:168:ALA:HA	3:A:1573:FAD:N5	2.18	0.58
1:A:144:SER:OG	1:A:562:GLU:HG3	2.04	0.57
1:A:286:LYS:HD3	1:A:288:THR:HG23	1.86	0.57
1:A:311:LEU:HD21	1:A:529:LEU:HD21	1.87	0.56
1:A:157:LYS:HZ1	1:A:340:GLY:HA3	1.70	0.56
1:A:318:LYS:HD2	1:A:339:PRO:O	2.06	0.55
1:A:431:LYS:HD3	1:A:434:LYS:CD	2.35	0.55
1:A:434:LYS:HE3	7:A:2468:HOH:O	2.08	0.54
1:A:183:LYS:HD3	7:A:2293:HOH:O	2.09	0.53
1:A:540:HIS:HD2	7:A:2546:HOH:O	1.91	0.53
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.91	0.53
1:A:112:LYS:NZ	1:A:116:GLN:HG3	2.25	0.52
1:A:501:PRO:HD2	7:A:2521:HOH:O	2.10	0.51
1:A:540:HIS:HE1	1:A:552:ASP:OD2	1.93	0.51
1:A:565:ALA:O	1:A:568:SER:HA	2.12	0.50
1:A:522:LYS:O	1:A:523:LYS:HB2	2.11	0.49
1:A:518:VAL:HB	1:A:529:LEU:HD12	1.93	0.49
1:A:113:SER:O	1:A:113:SER:OG	2.28	0.49
1:A:522:LYS:N	1:A:522:LYS:HD2	2.28	0.48
1:A:470:SER:O	1:A:474:SER:OG	2.30	0.48
1:A:112:LYS:O	1:A:116:GLN:HG3	2.12	0.48
1:A:365:HIS:O	1:A:501:PRO:HA	2.14	0.48
1:A:518:VAL:O	1:A:526:ILE:HG22	2.14	0.47
1:A:167:LEU:HD11	2:A:1572:HEC:HBC2	1.96	0.47
1:A:284:ASP:CG	1:A:286:LYS:HD2	2.39	0.47
1:A:112:LYS:HZ2	1:A:116:GLN:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HG21	1:A:461:LEU:HD22	1.96	0.47
1:A:515:LYS:HA	1:A:515:LYS:HD3	1.75	0.47
1:A:518:VAL:CB	1:A:529:LEU:HD12	2.45	0.46
1:A:167:LEU:CD1	2:A:1572:HEC:HBC2	2.44	0.46
1:A:522:LYS:HG2	7:A:2262:HOH:O	2.15	0.46
1:A:91:ASN:HB2	7:A:2137:HOH:O	2.15	0.46
1:A:442:PRO:HD2	1:A:496:ALA:O	2.16	0.45
1:A:111:ASP:HA	1:A:113:SER:OG	2.17	0.45
1:A:198:LYS:NZ	7:A:2270:HOH:O	2.50	0.45
1:A:318:LYS:HD2	1:A:339:PRO:HA	1.99	0.45
1:A:474:SER:HB2	1:A:476:LYS:CE	2.47	0.45
1:A:514:THR:OG1	1:A:515:LYS:NZ	2.50	0.45
1:A:280:GLU:O	1:A:293:LEU:HD12	2.17	0.45
1:A:493:ASN:ND2	7:A:2515:HOH:O	2.50	0.44
1:A:157:LYS:NZ	1:A:158:GLU:OE2	2.49	0.44
1:A:311:LEU:N	1:A:311:LEU:HD22	2.33	0.44
1:A:338:GLN:HB2	1:A:339:PRO:HD2	1.99	0.44
1:A:427:LYS:O	1:A:427:LYS:HG3	2.12	0.44
1:A:151:LYS:NZ	7:A:2214:HOH:O	2.50	0.44
1:A:375:MET:HE2	3:A:1573:FAD:H6	2.00	0.44
1:A:390:ARG:NE	7:A:2427:HOH:O	2.50	0.44
1:A:56:ASN:ND2	1:A:58:HIS:H	2.16	0.43
1:A:31:TYR:O	1:A:34:THR:HB	2.18	0.43
1:A:173:ASN:HA	1:A:243:ARG:O	2.18	0.43
1:A:355:ALA:HB3	1:A:511:MET:HE3	2.00	0.43
1:A:283:LYS:HD3	1:A:526:ILE:HD11	1.98	0.43
1:A:293:LEU:HD12	1:A:293:LEU:H	1.84	0.43
1:A:119:LEU:HD21	1:A:293:LEU:HG	2.01	0.43
1:A:454:GLU:CD	6:A:1576:GOL:H2	2.44	0.42
1:A:136:GLY:HA3	1:A:553:ILE:HD12	2.01	0.42
1:A:168:ALA:HB3	1:A:254:GLY:CA	2.49	0.42
1:A:286:LYS:CD	1:A:288:THR:HG23	2.50	0.42
1:A:57:ALA:HB2	1:A:90:PHE:CE1	2.55	0.42
1:A:110:LYS:HA	1:A:110:LYS:NZ	2.35	0.42
1:A:119:LEU:CD1	1:A:282:LEU:HD21	2.50	0.41
1:A:183:LYS:HE2	1:A:183:LYS:HB3	1.67	0.41
1:A:415:LYS:N	1:A:415:LYS:HD2	2.36	0.41
3:A:1573:FAD:H9	3:A:1573:FAD:H1'1	1.79	0.41
1:A:54:HIS:O	1:A:55:TYR:HB3	2.21	0.41
1:A:375:MET:HE3	1:A:375:MET:HB3	1.95	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	566/571 (99%)	545 (96%)	20 (4%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU

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	442/445 (99%)	404 (91%)	38 (9%)	10	3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	ASN
1	A	51	LYS
1	A	77	LYS
1	A	99	LEU
1	A	110	LYS
1	A	112	LYS
1	A	113	SER
1	A	114	GLU
1	A	157	LYS

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Mol	Chain	Res	Type
1	A	183	LYS
1	A	194	GLU
1	A	198	LYS
1	A	204	ASN
1	A	208	LEU
1	A	269	ASN
1	A	282	LEU
1	A	286	LYS
1	A	289	VAL
1	A	293	LEU
1	A	299	LYS
1	A	318	LYS
1	A	321	GLU
1	A	403	ASP
1	A	427	LYS
1	A	448	VAL
1	A	450	LEU
1	A	452	LYS
1	A	459	LYS
1	A	474	SER
1	A	476	LYS
1	A	481	GLU
1	A	490	ASN
1	A	522	LYS
1	A	529	LEU
1	A	559	LEU
1	A	566	LYS
1	A	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	56	ASN
1	A	91	ASN
1	A	202	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	275	ASN
1	A	484	ASN
1	A	490	ASN

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Mol	Chain	Res	Type
1	A	540	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z > 2$
3	FAD	A	1573	-	58,58,58	1.32	9 (15%)	85,89,89	1.27	5 (5%)
2	HEC	A	1569	1	46,50,50	0.89	0	58,82,82	1.17	4 (6%)
6	GOL	A	1576	-	5,5,5	0.34	0	5,5,5	3.05	1 (20%)
2	HEC	A	1571	1	46,50,50	0.86	0	58,82,82	1.15	3 (5%)
2	HEC	A	1570	1	46,50,50	0.91	0	58,82,82	0.88	2 (3%)
4	TEO	A	1574	-	5,8,8	4.35	3 (60%)	4,10,10	2.68	3 (75%)
2	HEC	A	1572	1	46,50,50	0.95	0	58,82,82	1.12	3 (5%)

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
3	FAD	A	1573	-	-	7/34/50/50	0/6/6/6
2	HEC	A	1569	1	-	9/14/54/54	-
6	GOL	A	1576	-	-	3/4/4/4	-
2	HEC	A	1571	1	-	7/14/54/54	-
2	HEC	A	1570	1	-	7/14/54/54	-
4	TEO	A	1574	-	-	4/6/8/8	-
2	HEC	A	1572	1	-	7/14/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1574	TEO	O2-C2	-8.58	1.32	1.43
3	A	1573	FAD	C2'-C3'	4.33	1.61	1.53
3	A	1573	FAD	C1'-C2'	-3.55	1.47	1.52
4	A	1574	TEO	C2-C1	3.35	1.60	1.54
3	A	1573	FAD	C6-C5X	3.09	1.44	1.40
3	A	1573	FAD	C9-C8	3.06	1.43	1.39
4	A	1574	TEO	O1B-C1	-2.71	1.22	1.30
3	A	1573	FAD	O4-C4	-2.46	1.18	1.23
3	A	1573	FAD	C5'-C4'	2.31	1.54	1.51
3	A	1573	FAD	O4'-C4'	2.27	1.48	1.43
3	A	1573	FAD	C9A-N10	-2.27	1.37	1.41
3	A	1573	FAD	P-O2P	-2.13	1.45	1.55

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1576	GOL	O2-C2-C3	-6.72	81.34	109.18
3	A	1573	FAD	O5'-C5'-C4'	-6.37	92.36	109.36
2	A	1572	HEC	CBB-CAB-C3B	-4.31	118.82	127.43
4	A	1574	TEO	O1B-C1-O1A	3.94	133.01	124.08
2	A	1569	HEC	CBC-CAC-C3C	-3.87	119.71	127.43
2	A	1572	HEC	CBC-CAC-C3C	-3.69	120.06	127.43
2	A	1571	HEC	CBB-CAB-C3B	-3.41	120.62	127.43
3	A	1573	FAD	O4'-C4'-C3'	-3.31	101.50	109.25
2	A	1571	HEC	CBC-CAC-C3C	-3.19	121.05	127.43
2	A	1569	HEC	CBB-CAB-C3B	-3.11	121.21	127.43
2	A	1570	HEC	CBC-CAC-C3C	-2.82	121.81	127.43
3	A	1573	FAD	O4B-C1B-C2B	-2.74	100.75	106.62
3	A	1573	FAD	O4-C4-N3	2.69	125.17	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1570	HEC	CBB-CAB-C3B	-2.58	122.27	127.43
4	A	1574	TEO	O1A-C1-C2	-2.50	116.51	122.52
3	A	1573	FAD	O2'-C2'-C3'	-2.50	103.39	109.25
2	A	1572	HEC	CHC-C4B-NB	-2.37	121.87	124.45
2	A	1569	HEC	CHA-C1A-C2A	-2.30	121.24	124.86
2	A	1571	HEC	C2A-C1A-NA	2.08	112.33	110.32
2	A	1569	HEC	O1A-CGA-CBA	-2.00	116.73	123.09
4	A	1574	TEO	O2-C2-C1	2.00	114.66	109.54

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1569	HEC	C2B-C3B-CAB-CBB
2	A	1569	HEC	C4B-C3B-CAB-CBB
2	A	1569	HEC	C2C-C3C-CAC-CBC
2	A	1569	HEC	C4C-C3C-CAC-CBC
2	A	1570	HEC	C2B-C3B-CAB-CBB
2	A	1570	HEC	C4B-C3B-CAB-CBB
2	A	1570	HEC	C2C-C3C-CAC-CBC
2	A	1570	HEC	C4C-C3C-CAC-CBC
2	A	1571	HEC	C2B-C3B-CAB-CBB
2	A	1571	HEC	C4B-C3B-CAB-CBB
2	A	1571	HEC	C2C-C3C-CAC-CBC
2	A	1571	HEC	C4C-C3C-CAC-CBC
2	A	1572	HEC	C2B-C3B-CAB-CBB
2	A	1572	HEC	C4C-C3C-CAC-CBC
3	A	1573	FAD	C2'-C3'-C4'-O4'
4	A	1574	TEO	O1B-C1-C2-O2
4	A	1574	TEO	C1-C2-C3-C4
4	A	1574	TEO	O2-C2-C3-C4
6	A	1576	GOL	O1-C1-C2-O2
6	A	1576	GOL	C1-C2-C3-O3
3	A	1573	FAD	C2'-C3'-C4'-C5'
4	A	1574	TEO	O1A-C1-C2-O2
3	A	1573	FAD	O3'-C3'-C4'-O4'
3	A	1573	FAD	O3'-C3'-C4'-C5'
3	A	1573	FAD	P-O3P-PA-O1A
3	A	1573	FAD	PA-O3P-P-O5'
6	A	1576	GOL	O2-C2-C3-O3
2	A	1569	HEC	C4D-C3D-CAD-CBD
2	A	1572	HEC	C4B-C3B-CAB-CBB

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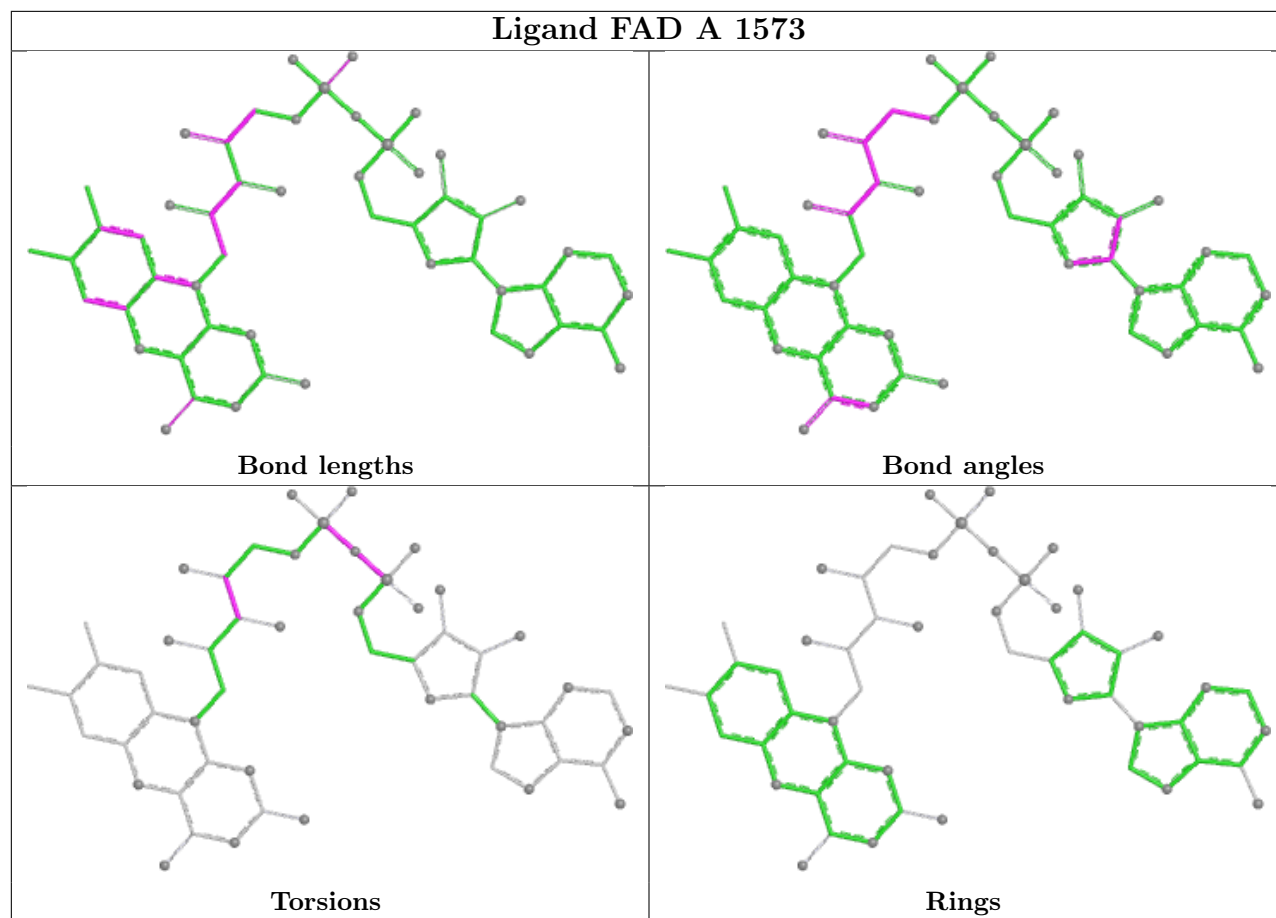
Mol	Chain	Res	Type	Atoms
2	A	1572	HEC	C2C-C3C-CAC-CBC
3	A	1573	FAD	P-O3P-PA-O2A
2	A	1570	HEC	CAD-CBD-CGD-O2D
2	A	1570	HEC	CAD-CBD-CGD-O1D
2	A	1572	HEC	CAA-CBA-CGA-O1A
2	A	1571	HEC	C3D-CAD-CBD-CGD
2	A	1572	HEC	CAA-CBA-CGA-O2A
2	A	1569	HEC	CAD-CBD-CGD-O1D
2	A	1569	HEC	CAD-CBD-CGD-O2D
2	A	1571	HEC	CAA-CBA-CGA-O2A
2	A	1571	HEC	CAA-CBA-CGA-O1A
2	A	1569	HEC	C3A-C2A-CAA-CBA
2	A	1569	HEC	CAA-CBA-CGA-O2A
2	A	1570	HEC	CAA-CBA-CGA-O1A
2	A	1572	HEC	C2A-CAA-CBA-CGA

There are no ring outliers.

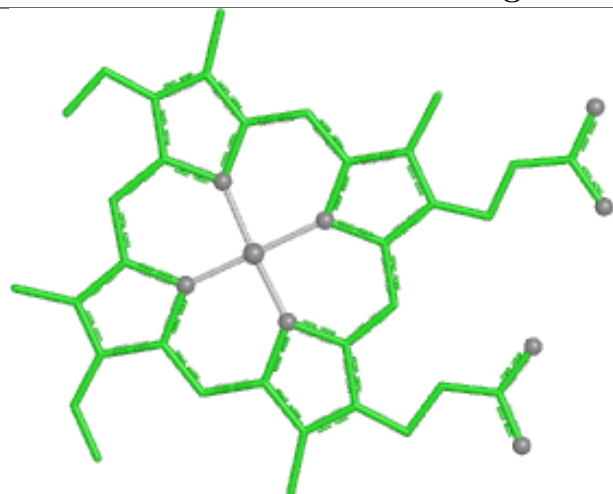
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1573	FAD	3	0
6	A	1576	GOL	2	0
4	A	1574	TEO	1	0
2	A	1572	HEC	2	0

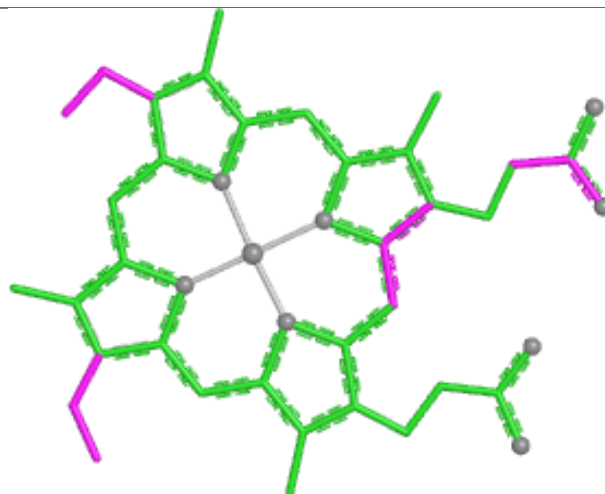
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



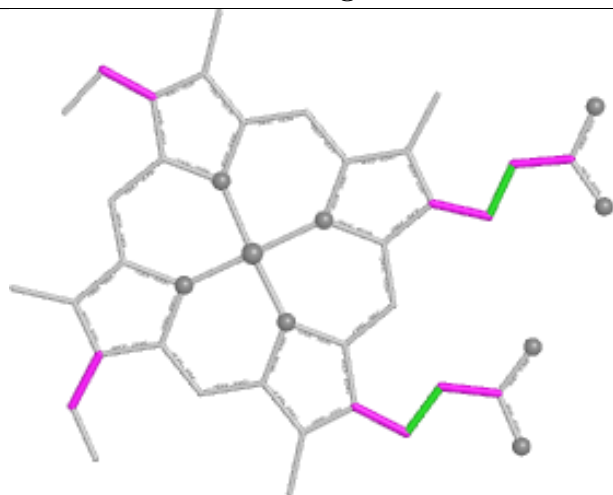
Ligand HEC A 1569



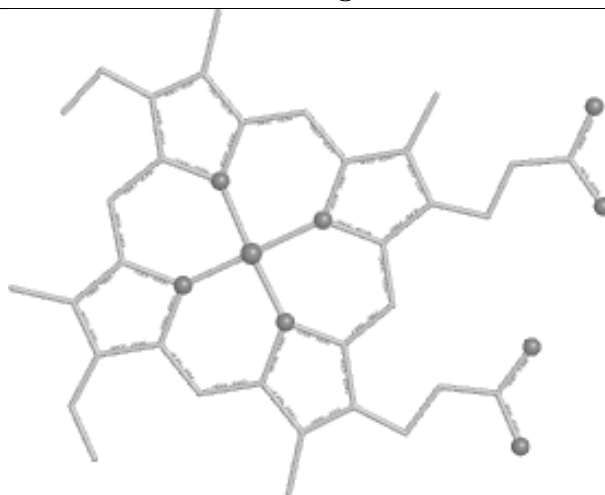
Bond lengths



Bond angles

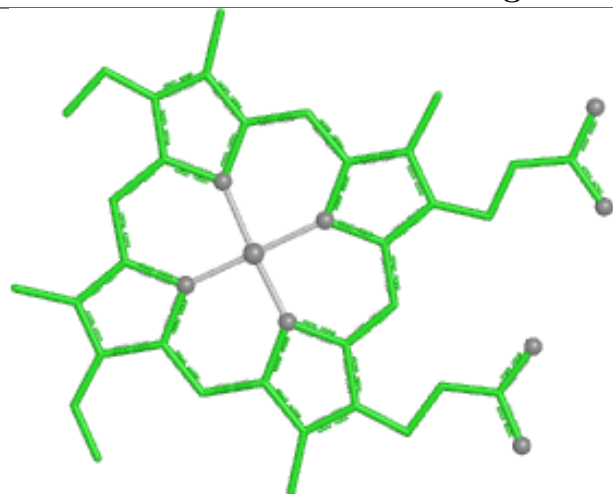


Torsions

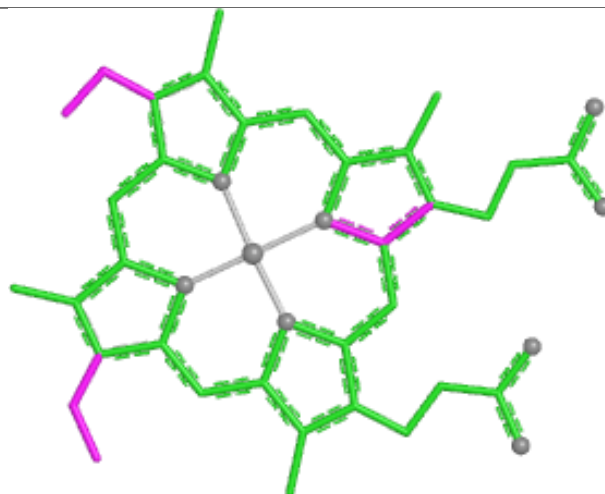


Rings

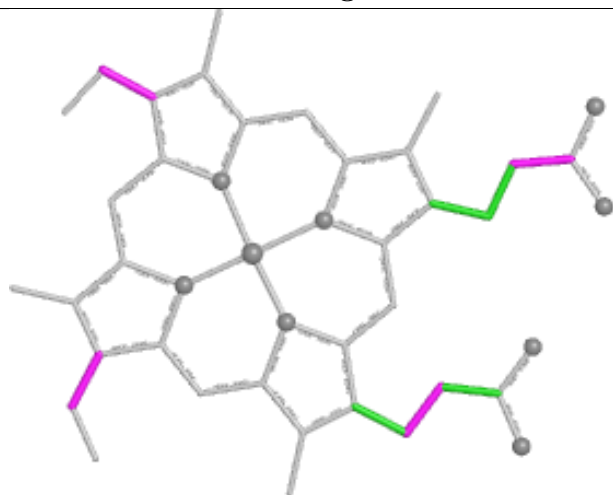
Ligand HEC A 1571



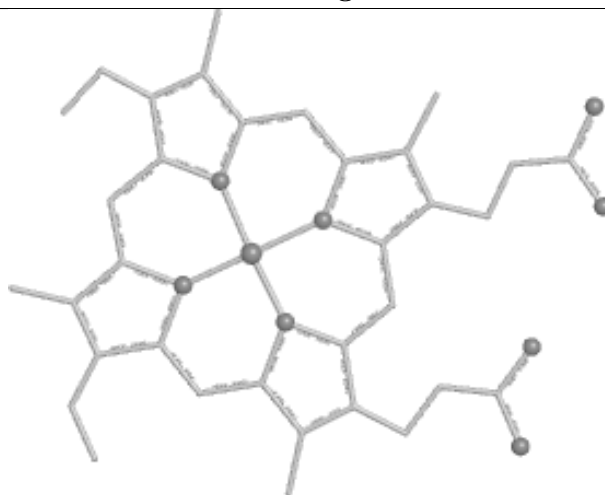
Bond lengths



Bond angles

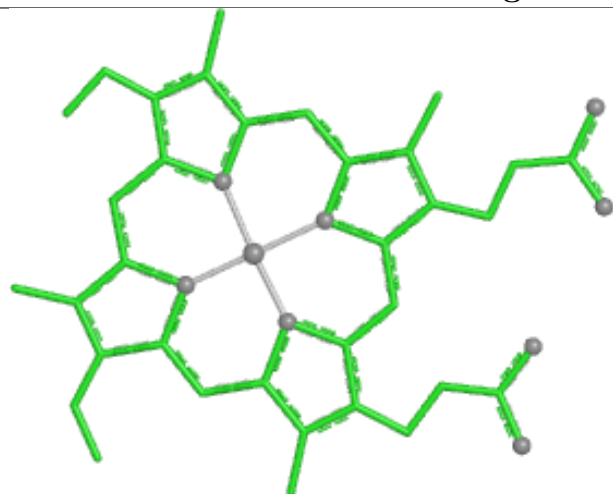


Torsions

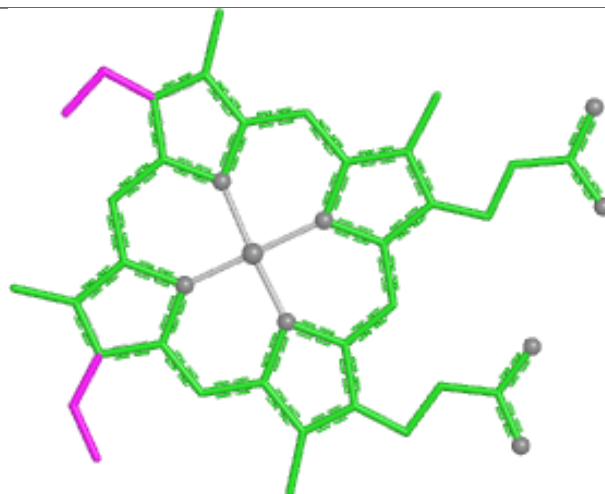


Rings

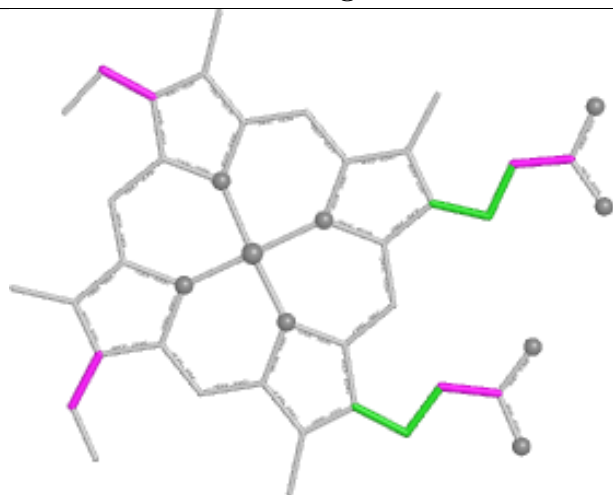
Ligand HEC A 1570



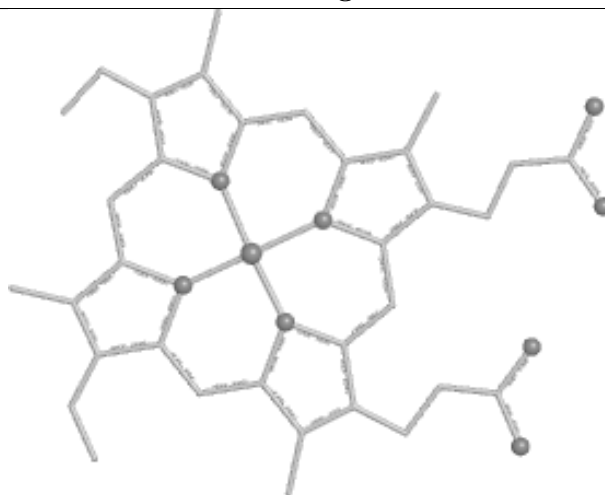
Bond lengths



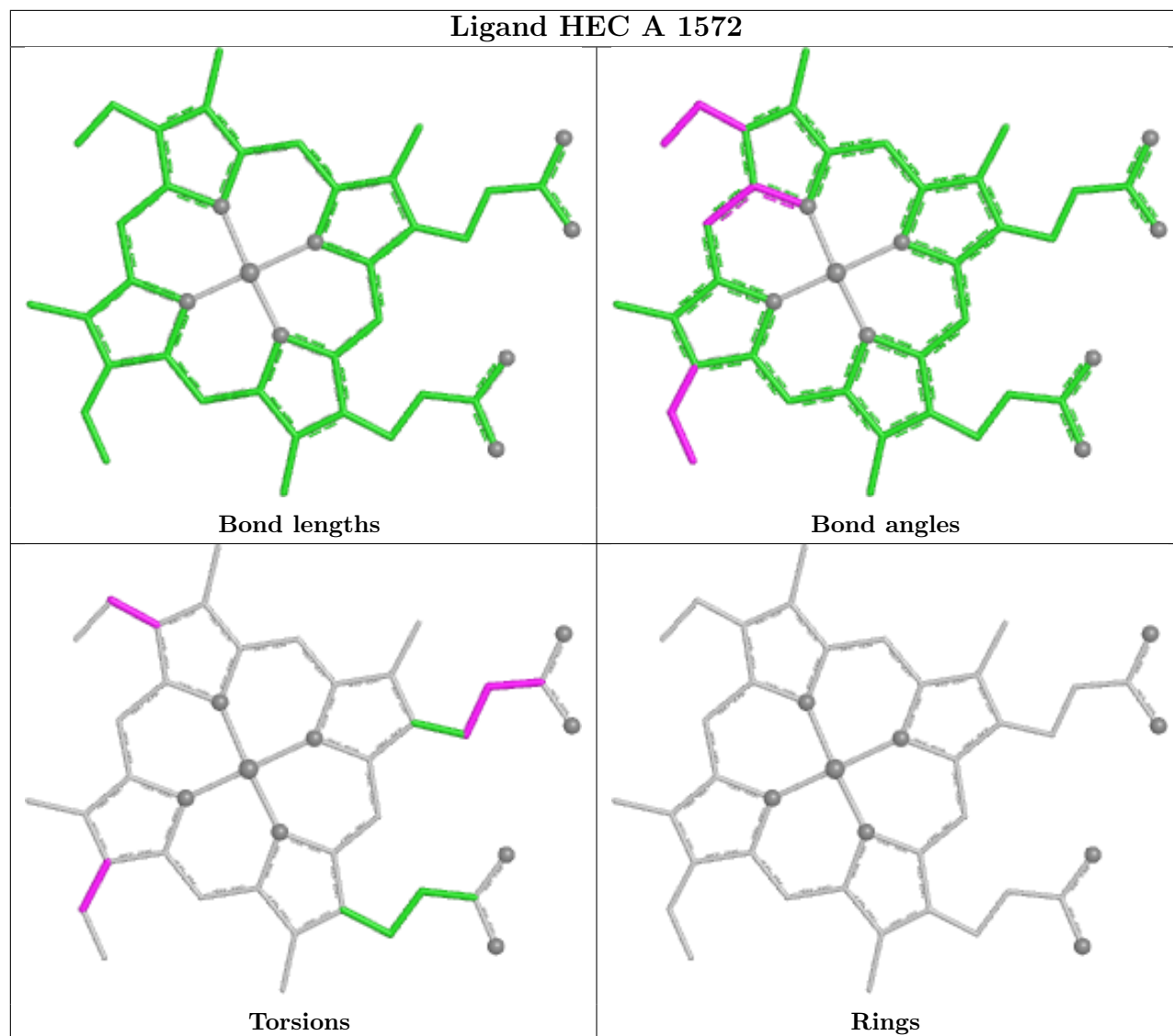
Bond angles



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.