Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 09:49 pm BST

PDB ID	:	6TSI / pdb_00006tsi
Title	:	cd1 nitrite reductase NirS with bound dihydro-heme d1
Authors	:	Kluenemann, T.; Blankenfeldt, W.
Deposited on	:	2019-12-20
Resolution	:	2.38 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 (i) 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 (i)) were used in the production of this report:

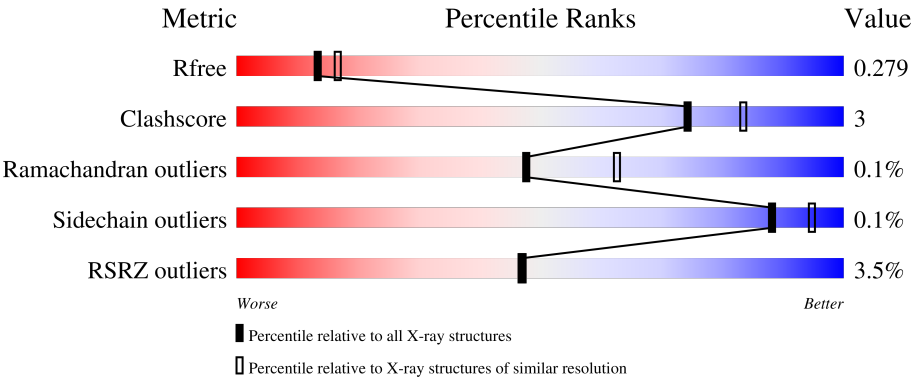
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	543	3% 94% 5%
1	B	543	4% 89% 10%

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
2	HEC	A	601	X	-	-	-
2	HEC	B	601	X	-	-	-

2 Entry composition

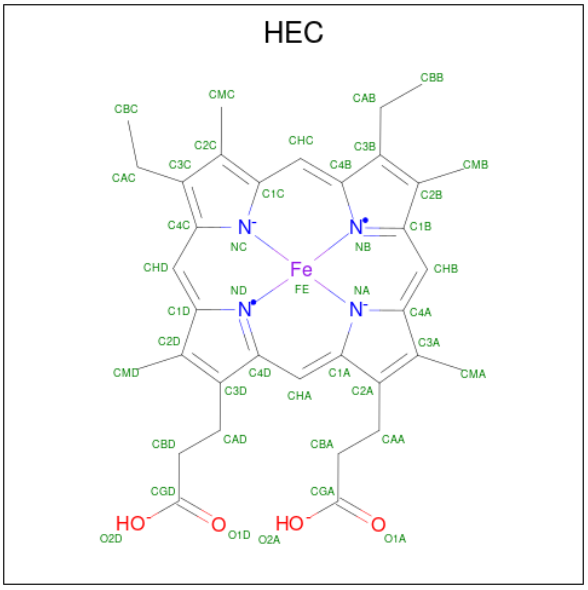
There are 6 unique types of molecules in this entry. The entry contains 17116 atoms, of which 8292 are hydrogens and 0 are deuteriums.

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 Nitrite reductase.

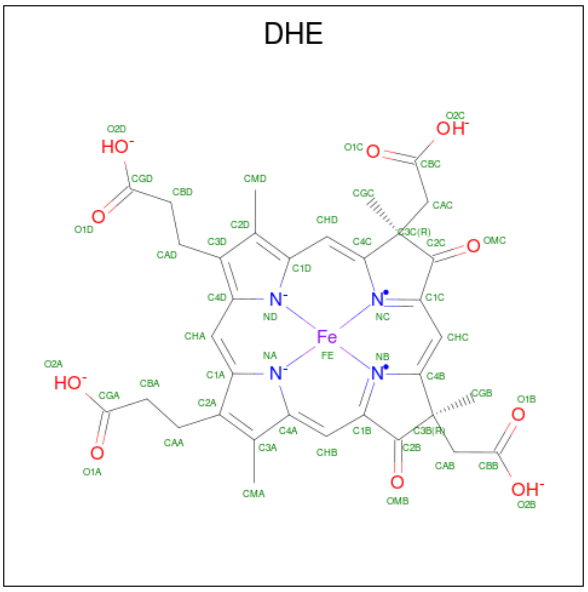
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	540	Total	C	H	N	O	S	0	0	0
			8260	2648	4081	726	793	12			
1	B	540	Total	C	H	N	O	S	0	0	0
			8277	2651	4092	729	793	12			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



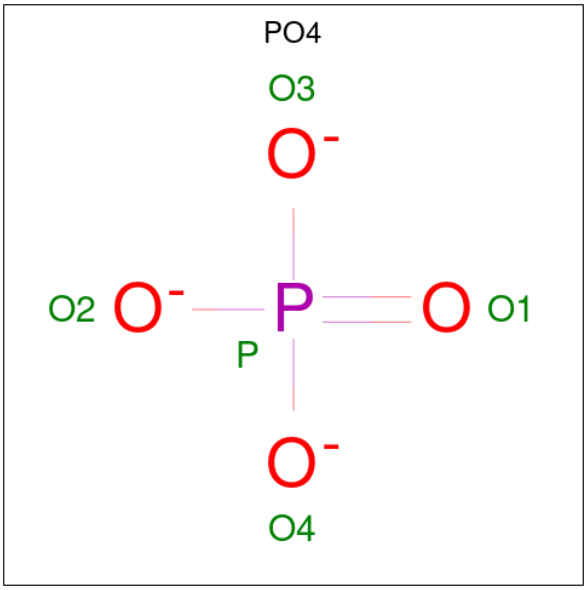
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 3 is HEME D (CCD ID: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			77	34	1	28	4	10		
3	B	1	Total	C	Fe	H	N	O	0	0
			77	34	1	28	4	10		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	3	Total Cl 3 3	0	0

- Molecule 6 is water.

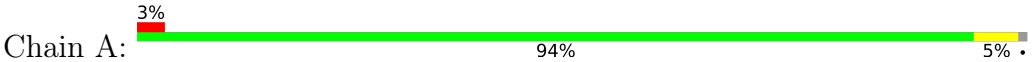
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	121	Total O 121 121	0	0
6	B	125	Total O 125 125	0	0

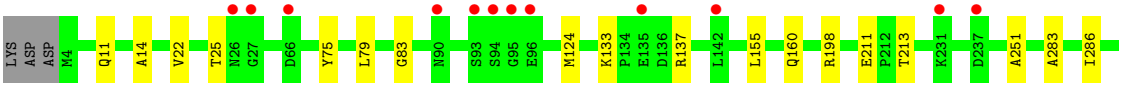
3 Residue-property plots (i)

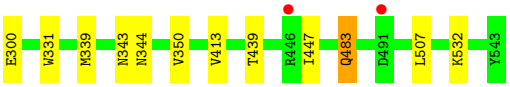
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nitrite reductase

Chain A:

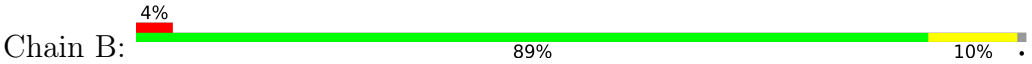


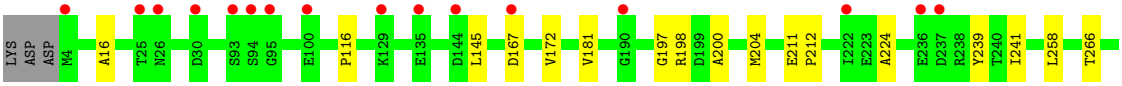


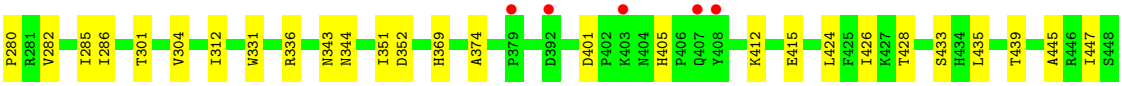


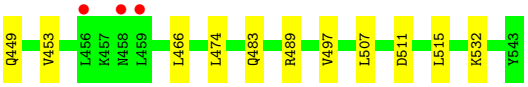
• Molecule 1: Nitrite reductase

Chain B:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.76Å 91.09Å 112.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.61 – 2.38 79.61 – 2.38	Depositor EDS
% Data completeness (in resolution range)	72.8 (79.61-2.38) 73.3 (79.61-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18rc1-3769	Depositor
R, R_{free}	0.238 , 0.280 0.238 , 0.279	Depositor DCC
R_{free} test set	2513 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17116	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2207e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, DHE, PO4, CL

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	0.60	1/4284 (0.0%)	0.39	0/5832
1	B	0.59	0/4290	0.38	0/5839
All	All	0.59	1/8574 (0.0%)	0.39	0/11671

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ALA	N-CA	-7.17	1.41	1.46

There are no bond angle outliers.

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	4179	4081	4081	22	0
1	B	4185	4092	4092	32	0
2	A	43	31	31	1	0
2	B	43	32	31	3	0
3	A	49	28	28	0	0
3	B	49	28	28	1	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	121	0	0	1	0
6	B	125	0	0	0	0
All	All	8824	8292	8291	53	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 3.

All (53) 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:211:GLU:O	1:A:213:THR:HG23	1.94	0.68
1:A:507:LEU:HD22	1:A:532:LYS:HD3	1.82	0.60
1:B:401:ASP:OD2	1:B:405:HIS:ND1	2.34	0.60
1:B:439:THR:OG1	1:B:447:ILE:O	2.19	0.59
1:B:483:GLN:O	1:B:532:LYS:NZ	2.34	0.59
1:B:374:ALA:HB1	1:B:428:THR:HG22	1.86	0.56
1:B:343:ASN:OD1	1:B:344:ASN:N	2.38	0.55
1:A:439:THR:OG1	1:A:447:ILE:O	2.25	0.54
1:B:167:ASP:OD1	1:B:489:ARG:NH2	2.38	0.54
1:B:453:VAL:HG21	1:B:466:LEU:HD11	1.91	0.53
1:A:14:ALA:O	1:B:198:ARG:NH1	2.42	0.53
1:A:339:MET:HE1	1:A:350:VAL:HG22	1.92	0.52
1:A:300:GLU:N	1:A:300:GLU:OE1	2.43	0.52
1:A:25:THR:HG23	1:A:25:THR:O	2.11	0.51
1:A:286:ILE:HD11	1:A:331:TRP:CD1	2.45	0.51
1:A:439:THR:HG23	6:A:724:HOH:O	2.09	0.51
1:A:198:ARG:HG2	1:B:16:ALA:HB2	1.92	0.50
1:B:145:LEU:HD11	1:B:172:VAL:HG11	1.92	0.50
1:A:343:ASN:OD1	1:A:344:ASN:N	2.43	0.50
1:B:266:THR:HG21	1:B:282:VAL:HG22	1.93	0.48
1:B:507:LEU:HD22	1:B:532:LYS:HD3	1.95	0.48
1:B:511:ASP:O	1:B:515:LEU:N	2.43	0.48
1:A:339:MET:CE	1:A:350:VAL:HG22	2.43	0.48
1:A:133:LYS:O	1:A:137:ARG:HG3	2.14	0.47
1:A:79:LEU:O	1:A:83:GLY:N	2.46	0.46
1:A:11:GLN:HB2	2:B:601:HEC:HBC1	1.98	0.46
1:A:79:LEU:HD13	2:A:601:HEC:HAA1	1.97	0.46
1:A:155:LEU:HD12	1:A:160:GLN:HG3	1.98	0.46
1:B:369:HIS:ND1	1:B:424:LEU:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:HD11	1:B:331:TRP:CD1	2.51	0.46
1:A:75:TYR:CE2	1:A:79:LEU:HD12	2.50	0.46
1:B:412:LYS:NZ	1:B:415:GLU:OE2	2.38	0.46
1:B:200:ALA:HA	1:B:224:ALA:HB3	1.99	0.45
1:B:241:ILE:HG21	1:B:285:ILE:HG21	1.99	0.45
1:B:304:VAL:HG11	1:B:351:ILE:HG13	1.99	0.45
1:A:124:MET:HE1	1:A:251:ALA:HB2	1.99	0.44
1:B:239:TYR:CE1	1:B:312:ILE:HD13	2.52	0.44
1:B:433:SER:O	1:B:433:SER:OG	2.29	0.44
1:B:280:PRO:HB3	1:B:301:THR:HG23	1.99	0.44
1:B:426:ILE:HD11	1:B:435:LEU:HD21	1.99	0.44
1:B:204:MET:HE3	1:B:258:LEU:HG	1.99	0.44
1:A:483:GLN:OE1	1:A:532:LYS:N	2.49	0.43
2:B:601:HEC:CBC	2:B:601:HEC:HMC3	2.47	0.43
1:B:445:ALA:O	1:B:449:GLN:HG2	2.18	0.42
1:B:241:ILE:CG2	1:B:285:ILE:HG21	2.49	0.42
2:B:601:HEC:HMC3	2:B:601:HEC:HBC2	2.02	0.42
1:B:181:VAL:HA	1:B:197:GLY:HA2	2.02	0.41
1:B:336:ARG:NH2	1:B:352:ASP:OD2	2.46	0.41
1:A:483:GLN:O	1:A:532:LYS:NZ	2.50	0.41
1:B:474:LEU:CD1	1:B:497:VAL:HG11	2.51	0.41
1:B:198:ARG:NH2	3:B:602:DHE:O1B	2.54	0.40
1:B:211:GLU:O	1:B:212:PRO:C	2.62	0.40
1:A:22:VAL:HG22	1:B:116:PRO:HB3	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	538/543 (99%)	509 (95%)	28 (5%)	1 (0%)	43 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	538/543 (99%)	505 (94%)	33 (6%)	0	100 100
All	All	1076/1086 (99%)	1014 (94%)	61 (6%)	1 (0%)	48 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	GLN

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	445/458 (97%)	444 (100%)	1 (0%)	87 94
1	B	446/458 (97%)	446 (100%)	0	100 100
All	All	891/916 (97%)	890 (100%)	1 (0%)	88 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	ASN
1	B	69	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)

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	PO4	A	604	-	4,4,4	0.88	0	6,6,6	0.48	0
4	PO4	A	605	-	4,4,4	0.89	0	6,6,6	0.47	0
4	PO4	B	604	-	4,4,4	0.92	0	6,6,6	0.52	0
3	DHE	B	602	1,6	52,56,56	2.74	22 (42%)	53,94,94	1.58	8 (15%)
4	PO4	B	603	-	4,4,4	0.82	0	6,6,6	0.33	0
3	DHE	A	602	1,6	52,56,56	2.71	23 (44%)	53,94,94	1.56	7 (13%)
4	PO4	A	603	-	4,4,4	0.94	0	6,6,6	0.46	0
2	HEC	B	601	1	50,50,50	2.96	26 (52%)	68,82,82	2.18	26 (38%)
2	HEC	A	601	1	50,50,50	2.96	26 (52%)	68,82,82	2.13	22 (32%)

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	DHE	A	602	1,6	-	6/20/108/108	-
2	HEC	A	601	1	1/1/7/7	9/14/54/54	-
3	DHE	B	602	1,6	-	7/20/108/108	-
2	HEC	B	601	1	1/1/7/7	9/14/54/54	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	FE-NB	6.58	2.15	1.94
3	B	602	DHE	FE-NB	6.11	2.13	1.94
3	A	602	DHE	FE-NB	5.99	2.13	1.94
2	B	601	HEC	FE-NB	5.78	2.12	1.94
2	B	601	HEC	CHB-C4A	5.68	1.49	1.38
2	A	601	HEC	CHA-C1A	5.63	1.49	1.38
3	A	602	DHE	CHB-C4A	5.53	1.49	1.38
3	B	602	DHE	CHB-C4A	5.45	1.49	1.38
2	A	601	HEC	CHB-C4A	5.42	1.48	1.38
2	A	601	HEC	CHC-C4B	5.29	1.49	1.38
2	A	601	HEC	FE-NA	5.19	2.12	1.95
3	B	602	DHE	C2A-C3A	5.18	1.47	1.36
2	B	601	HEC	CHA-C1A	5.13	1.48	1.38
3	B	602	DHE	CHA-C4D	5.09	1.50	1.39
2	B	601	HEC	C2A-C3A	5.08	1.47	1.36
3	A	602	DHE	CHA-C1A	5.07	1.48	1.38
2	B	601	HEC	C3D-C2D	4.94	1.47	1.36
3	A	602	DHE	C2A-C3A	4.93	1.47	1.36
2	B	601	HEC	CHC-C4B	4.82	1.48	1.38
2	B	601	HEC	C3B-C2B	4.80	1.46	1.36
2	A	601	HEC	C3D-C2D	4.80	1.46	1.36
2	B	601	HEC	FE-ND	4.75	2.09	1.94
2	B	601	HEC	FE-NA	4.67	2.11	1.95
2	A	601	HEC	C2A-C3A	4.66	1.46	1.36
2	B	601	HEC	CHD-C1D	4.66	1.48	1.38
3	B	602	DHE	CHA-C1A	4.63	1.47	1.38
2	B	601	HEC	FE-NC	4.61	2.10	1.95
3	B	602	DHE	FE-NC	4.53	2.08	1.94
3	A	602	DHE	C3C-C2C	-4.50	1.45	1.52
3	A	602	DHE	CHA-C4D	4.43	1.49	1.39
2	A	601	HEC	C3B-C2B	4.41	1.46	1.36
3	A	602	DHE	CHD-C1D	4.40	1.49	1.39
2	B	601	HEC	CHB-C1B	4.38	1.49	1.39
3	B	602	DHE	C3C-C2C	-4.28	1.46	1.52
3	B	602	DHE	FE-ND	4.22	2.09	1.95
3	A	602	DHE	CHC-C1C	4.22	1.48	1.39
3	B	602	DHE	CHC-C1C	4.18	1.48	1.39
2	A	601	HEC	CHD-C4C	4.14	1.48	1.39
3	A	602	DHE	FE-ND	4.13	2.09	1.95
3	B	602	DHE	CHD-C1D	4.12	1.48	1.39
3	B	602	DHE	OMB-C2B	4.08	1.29	1.22
3	A	602	DHE	CHD-C4C	4.04	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	CHD-C4C	4.00	1.49	1.37
2	B	601	HEC	CHA-C4D	3.99	1.48	1.39
2	A	601	HEC	CHD-C1D	3.94	1.46	1.38
2	A	601	HEC	FE-ND	3.94	2.07	1.94
2	A	601	HEC	C4B-NB	-3.93	1.33	1.40
2	A	601	HEC	FE-NC	3.90	2.08	1.95
2	B	601	HEC	CHC-C1C	3.89	1.48	1.39
2	A	601	HEC	CHB-C1B	3.86	1.48	1.39
3	B	602	DHE	CHB-C1B	3.82	1.47	1.39
3	A	602	DHE	CHB-C1B	3.67	1.47	1.39
3	B	602	DHE	CHC-C4B	3.58	1.47	1.37
2	A	601	HEC	CHC-C1C	3.57	1.47	1.39
3	A	602	DHE	FE-NC	3.53	2.05	1.94
3	A	602	DHE	C3B-C2B	-3.52	1.47	1.52
2	B	601	HEC	CHD-C4C	3.52	1.47	1.39
3	A	602	DHE	CHC-C4B	3.46	1.47	1.37
2	B	601	HEC	C4B-NB	-3.32	1.34	1.40
2	A	601	HEC	CHA-C4D	3.29	1.46	1.39
2	A	601	HEC	C4A-NA	-3.25	1.33	1.39
3	A	602	DHE	C4A-NA	3.20	1.45	1.39
3	A	602	DHE	C3D-C2D	3.12	1.47	1.38
3	B	602	DHE	C4A-NA	3.11	1.45	1.39
3	A	602	DHE	OMB-C2B	3.08	1.27	1.22
3	B	602	DHE	C1A-NA	3.06	1.45	1.39
2	B	601	HEC	C1D-ND	-3.06	1.35	1.40
3	A	602	DHE	OMC-C2C	3.02	1.27	1.22
3	B	602	DHE	C3B-C2B	-3.01	1.48	1.52
3	B	602	DHE	C3D-C2D	3.00	1.46	1.38
3	A	602	DHE	C1A-C2A	2.96	1.50	1.45
3	A	602	DHE	C1A-NA	2.94	1.45	1.39
3	B	602	DHE	OMC-C2C	2.90	1.27	1.22
2	A	601	HEC	C1D-C2D	2.89	1.50	1.44
2	A	601	HEC	C4D-C3D	2.86	1.50	1.45
2	B	601	HEC	C3C-C2C	2.80	1.46	1.38
2	A	601	HEC	C3C-C2C	2.78	1.46	1.38
2	A	601	HEC	C1A-NA	-2.70	1.34	1.39
2	B	601	HEC	C1C-C2C	2.59	1.49	1.43
2	B	601	HEC	C1B-C2B	2.56	1.49	1.44
2	B	601	HEC	C1A-NA	-2.54	1.34	1.39
3	A	602	DHE	C4D-ND	-2.49	1.34	1.39
2	B	601	HEC	C4C-NC	-2.43	1.35	1.39
3	B	602	DHE	C4D-ND	-2.42	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	C1D-ND	-2.40	1.36	1.40
2	A	601	HEC	C1C-C2C	2.40	1.48	1.43
3	A	602	DHE	FE-NA	2.39	2.03	1.95
2	B	601	HEC	C4A-NA	-2.37	1.35	1.39
2	B	601	HEC	C1D-C2D	2.25	1.48	1.44
2	A	601	HEC	C4C-NC	-2.23	1.35	1.39
2	A	601	HEC	C1B-C2B	2.23	1.48	1.44
2	B	601	HEC	C4D-C3D	2.19	1.48	1.45
3	B	602	DHE	CGB-C3B	-2.16	1.50	1.54
2	B	601	HEC	C1A-C2A	2.16	1.49	1.45
3	B	602	DHE	C1D-ND	-2.05	1.35	1.39
3	A	602	DHE	C1D-C2D	2.05	1.48	1.43
2	A	601	HEC	C4C-C3C	2.03	1.48	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEC	C1B-C2B-C3B	-5.50	101.17	106.96
2	B	601	HEC	C1B-C2B-C3B	-5.48	101.20	106.96
3	A	602	DHE	C3D-C4D-ND	5.01	115.75	110.15
3	B	602	DHE	C3D-C4D-ND	4.89	115.62	110.15
2	B	601	HEC	C2A-C1A-NA	4.69	114.89	110.32
2	B	601	HEC	C1C-C2C-C3C	-4.57	101.48	106.83
2	A	601	HEC	C2A-C1A-NA	4.53	114.73	110.32
2	A	601	HEC	C2B-C1B-NB	4.35	115.09	109.88
2	A	601	HEC	C3D-C4D-ND	4.21	114.43	110.36
2	B	601	HEC	C3D-C4D-ND	4.21	114.43	110.36
2	B	601	HEC	C2B-C1B-NB	4.18	114.89	109.88
2	A	601	HEC	C1C-C2C-C3C	-4.17	101.95	106.83
2	B	601	HEC	C2D-C1D-ND	4.16	114.76	109.84
2	A	601	HEC	C2D-C1D-ND	3.74	114.27	109.84
2	B	601	HEC	C1D-C2D-C3D	-3.72	103.05	106.96
2	A	601	HEC	C1D-C2D-C3D	-3.67	103.10	106.96
2	A	601	HEC	CBB-CAB-C3B	3.66	122.51	112.43
2	A	601	HEC	C1A-C2A-C3A	-3.41	102.68	107.13
2	B	601	HEC	C1A-C2A-C3A	-3.41	102.68	107.13
2	B	601	HEC	CAA-CBA-CGA	-3.39	106.31	113.60
2	B	601	HEC	CBB-CAB-C3B	3.30	121.53	112.43
2	A	601	HEC	CBC-CAC-C3C	3.18	121.21	112.43
3	B	602	DHE	C4D-C3D-C2D	-3.16	101.92	106.89
3	A	602	DHE	CAA-CBA-CGA	-3.14	106.85	113.60
2	A	601	HEC	CAA-CBA-CGA	-3.05	107.03	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEC	C3A-C4A-NA	3.04	115.29	109.69
2	B	601	HEC	C2C-C1C-NC	2.98	114.62	110.08
2	A	601	HEC	C2C-C1C-NC	2.98	114.61	110.08
3	A	602	DHE	C2D-C1D-ND	2.96	114.59	110.08
3	A	602	DHE	C4D-C3D-C2D	-2.96	102.23	106.89
2	A	601	HEC	CMA-C3A-C4A	2.93	129.87	124.71
3	B	602	DHE	CAA-CBA-CGA	-2.91	107.35	113.60
3	B	602	DHE	C2D-C1D-ND	2.88	114.47	110.08
2	A	601	HEC	C4A-C3A-C2A	-2.87	102.75	106.94
2	B	601	HEC	CMA-C3A-C4A	2.82	129.69	124.71
2	B	601	HEC	CBC-CAC-C3C	2.82	120.20	112.43
2	B	601	HEC	C3B-C4B-NB	2.81	113.30	110.17
3	A	602	DHE	C1D-C2D-C3D	-2.80	103.55	106.83
2	A	601	HEC	C3B-C4B-NB	2.76	113.24	110.17
2	B	601	HEC	CMB-C2B-C1B	2.73	129.20	125.04
2	B	601	HEC	C3A-C4A-NA	2.73	114.72	109.69
2	B	601	HEC	C4A-C3A-C2A	-2.71	102.99	106.94
2	B	601	HEC	C3C-C4C-NC	2.69	113.15	110.15
2	B	601	HEC	C4D-C3D-C2D	-2.61	103.09	106.90
2	B	601	HEC	CAD-C3D-C4D	2.60	129.19	124.66
2	A	601	HEC	C3C-C4C-NC	2.59	113.05	110.15
2	A	601	HEC	CAA-C2A-C1A	2.57	129.73	124.89
2	B	601	HEC	CAD-CBD-CGD	-2.52	108.17	113.60
2	A	601	HEC	C4D-C3D-C2D	-2.48	103.28	106.90
3	B	602	DHE	OMC-C2C-C3C	-2.46	122.85	125.92
3	B	602	DHE	C1D-C2D-C3D	-2.39	104.03	106.83
2	B	601	HEC	CMC-C2C-C1C	2.38	128.99	125.37
2	B	601	HEC	CHA-C1A-C2A	-2.37	121.10	124.94
2	A	601	HEC	CHB-C1B-C2B	-2.34	121.32	124.98
2	B	601	HEC	CMD-C2D-C1D	2.20	128.39	125.04
2	B	601	HEC	CAA-C2A-C1A	2.16	128.97	124.89
2	A	601	HEC	CMD-C2D-C1D	2.15	128.32	125.04
2	B	601	HEC	CHB-C1B-C2B	-2.14	121.63	124.98
3	A	602	DHE	OMC-C2C-C3C	-2.14	123.25	125.92
3	B	602	DHE	C4A-NA-C1A	-2.08	103.31	105.35
2	A	601	HEC	CMC-C2C-C3C	2.07	130.09	125.61
3	A	602	DHE	C4A-NA-C1A	-2.03	103.36	105.35
3	B	602	DHE	O2C-CBC-CAC	2.00	120.78	114.35

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
2	A	601	HEC	NA
2	B	601	HEC	NA

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C2B-C3B-CAB-CBB
3	A	602	DHE	CGB-C3B-CAB-CBB
3	A	602	DHE	C4B-C3B-CAB-CBB
3	B	602	DHE	C2B-C3B-CAB-CBB
3	B	602	DHE	C4B-C3B-CAB-CBB
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4B-C3B-CAB-CBB
2	B	601	HEC	C2B-C3B-CAB-CBB
2	B	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C4C-C3C-CAC-CBC
2	B	601	HEC	C4C-C3C-CAC-CBC
2	A	601	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	C3D-CAD-CBD-CGD
2	A	601	HEC	C3D-CAD-CBD-CGD
3	B	602	DHE	C3C-CAC-CBC-O2C
3	B	602	DHE	C2D-C3D-CAD-CBD
3	B	602	DHE	C3C-CAC-CBC-O1C
3	B	602	DHE	CGB-C3B-CAB-CBB
3	A	602	DHE	C3D-CAD-CBD-CGD
2	B	601	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O1A
2	B	601	HEC	CAA-CBA-CGA-O1A
2	B	601	HEC	CAD-CBD-CGD-O1D
3	A	602	DHE	C2D-C3D-CAD-CBD
2	B	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAA-CBA-CGA-O2A
3	B	602	DHE	C4D-C3D-CAD-CBD
2	A	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O1D
3	A	602	DHE	CAD-CBD-CGD-O2D

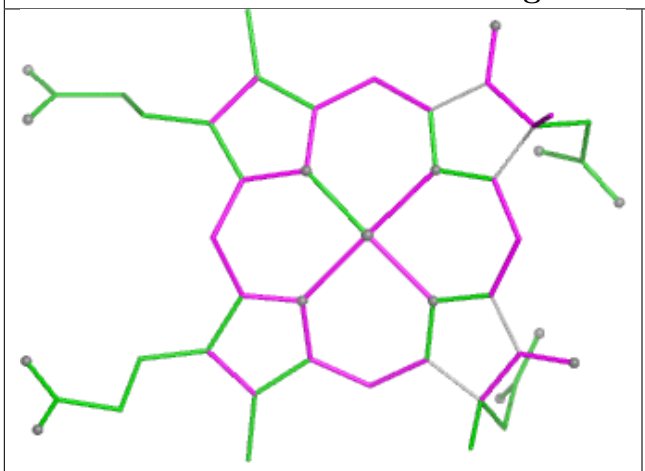
There are no ring outliers.

3 monomers are involved in 5 short contacts:

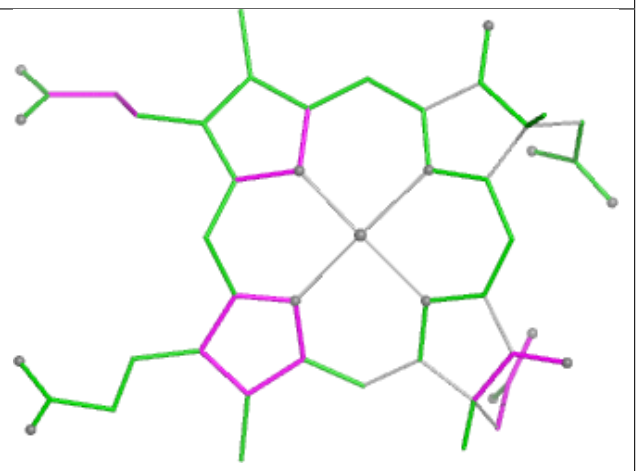
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	DHE	1	0
2	B	601	HEC	3	0
2	A	601	HEC	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

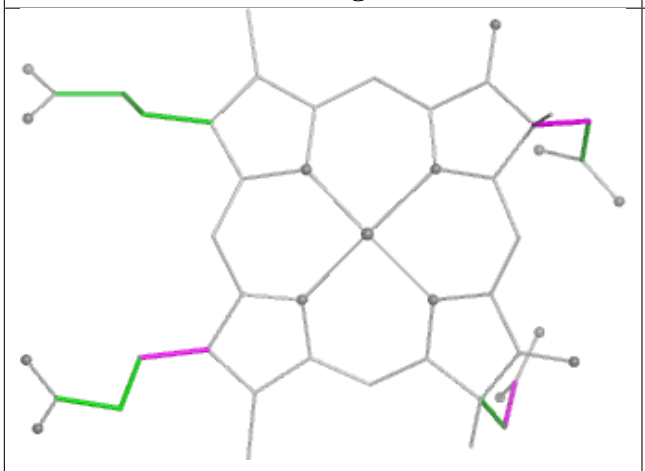
Ligand DHE B 602



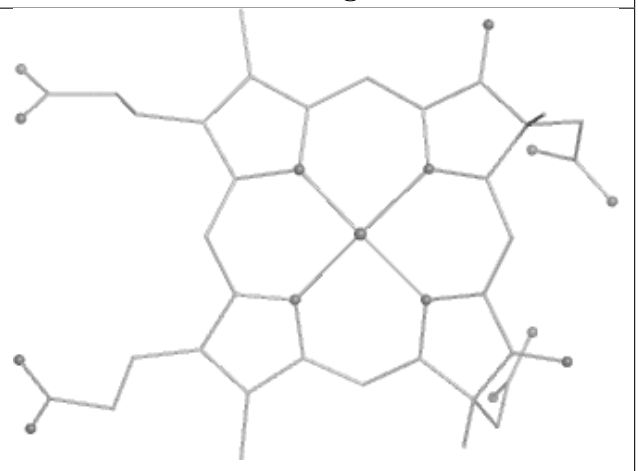
Bond lengths



Bond angles

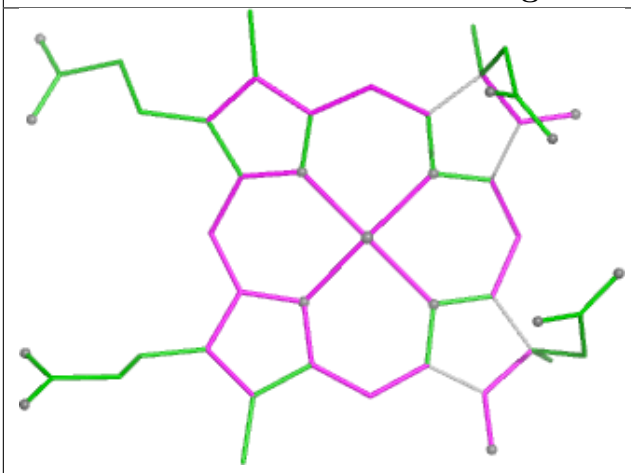


Torsions

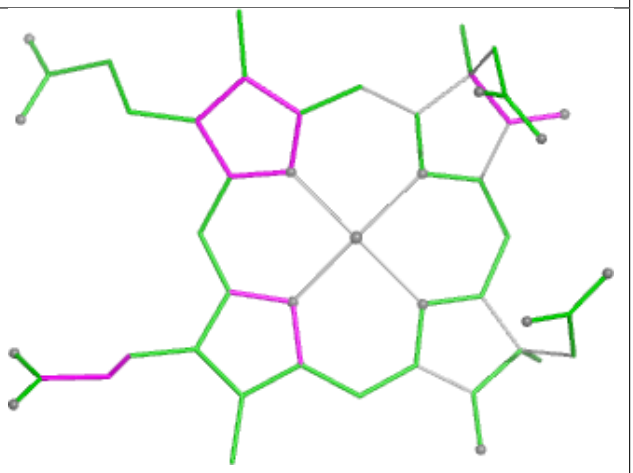


Rings

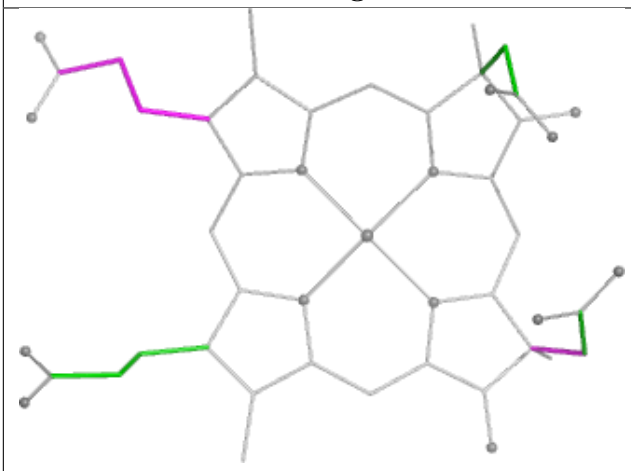
Ligand DHE A 602



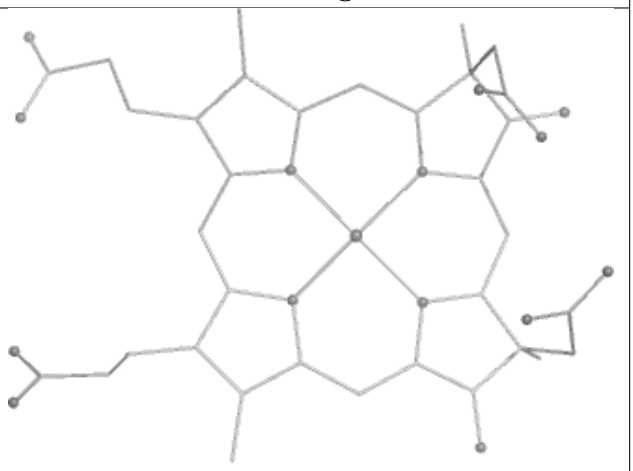
Bond lengths



Bond angles

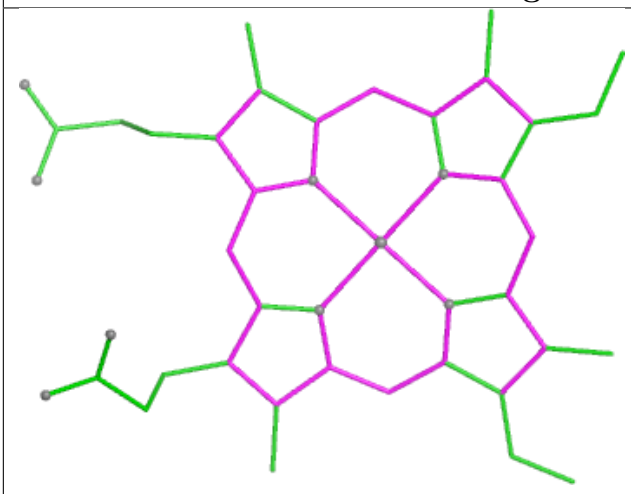


Torsions

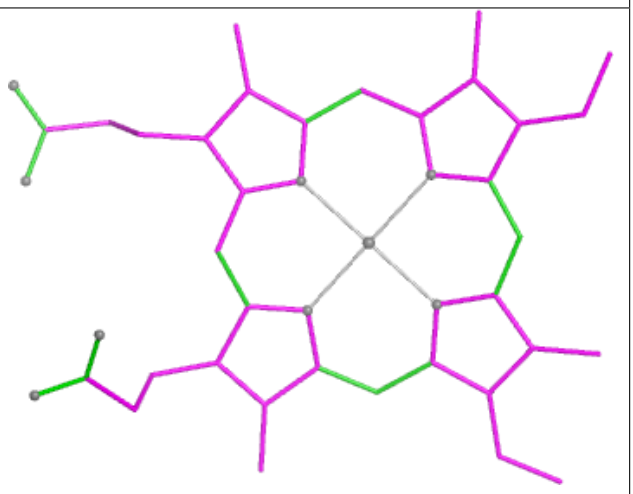


Rings

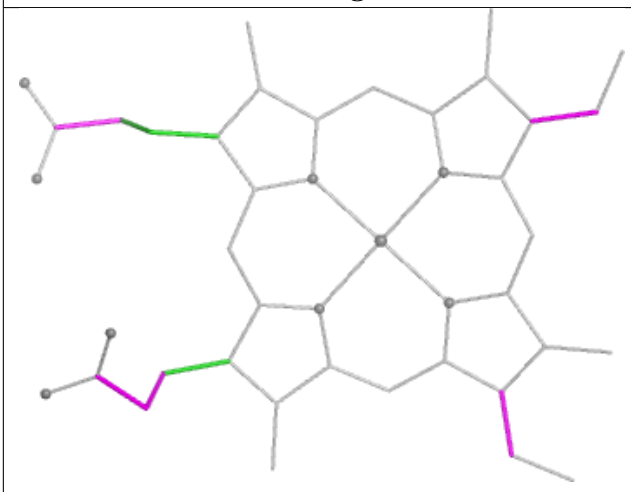
Ligand HEC B 601



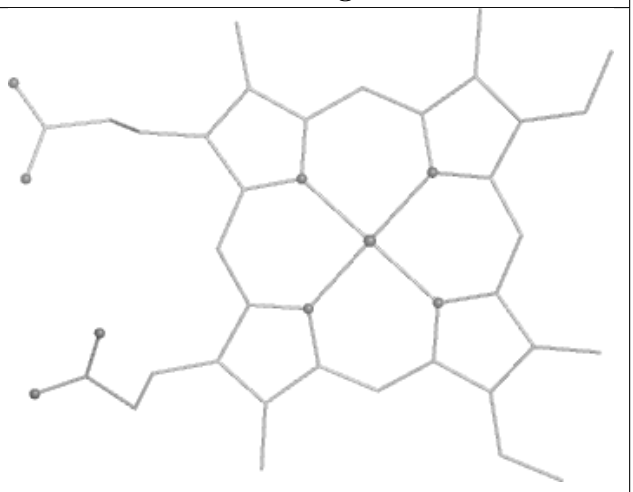
Bond lengths



Bond angles

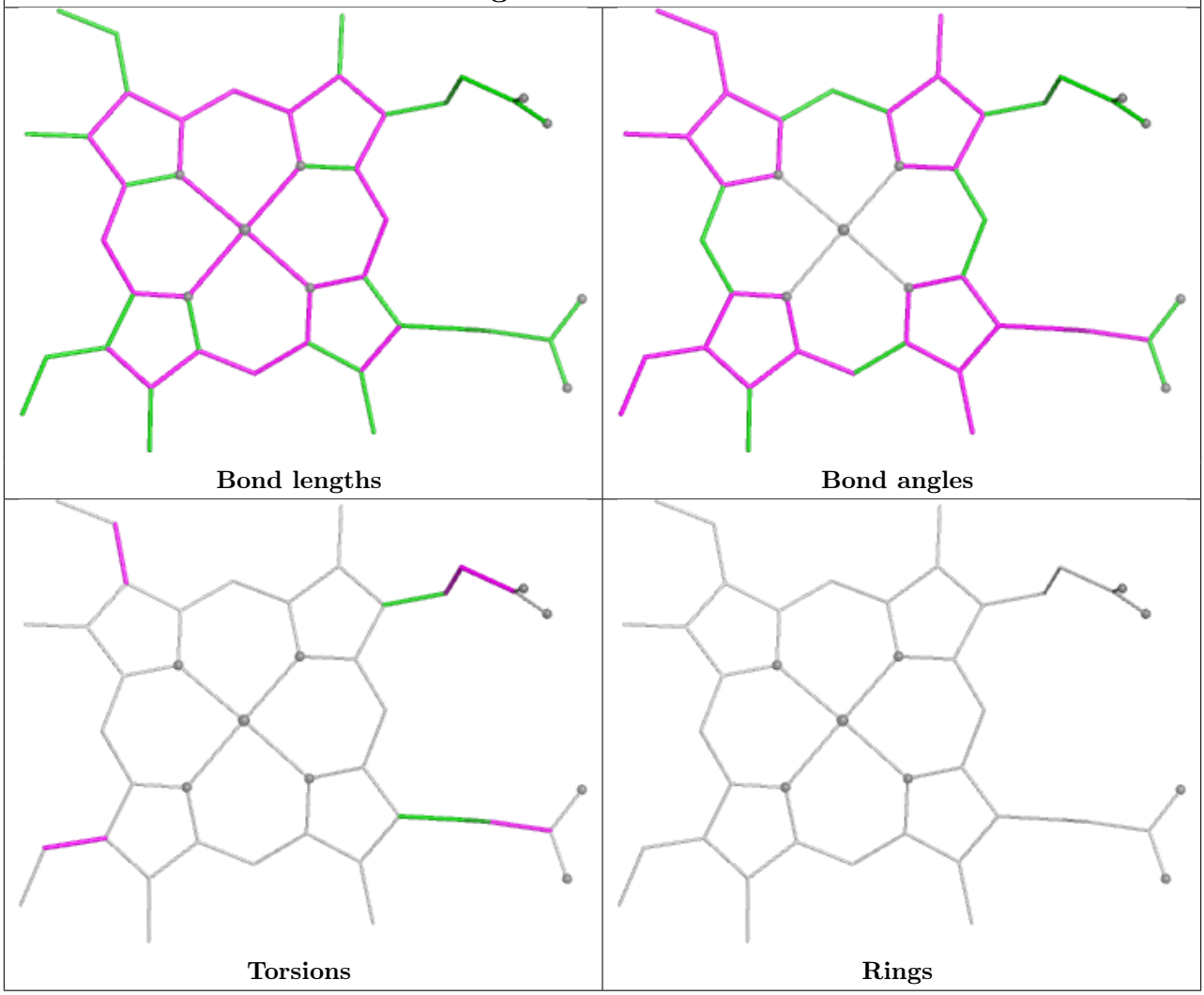


Torsions



Rings

Ligand HEC A 601



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, 95^{th} 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	540/543 (99%)	0.44	14 (2%)	57	56	12, 24, 38, 58	0
1	B	540/543 (99%)	0.55	24 (4%)	39	38	13, 25, 41, 62	0
All	All	1080/1086 (99%)	0.49	38 (3%)	47	47	12, 25, 40, 62	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASN	6.1
1	A	94	SER	5.5
1	B	26	ASN	5.2
1	B	4	MET	4.4
1	B	458	ASN	4.3
1	A	93	SER	4.0
1	B	95	GLY	3.9
1	A	95	GLY	3.5
1	B	135	GLU	3.3
1	A	231	LYS	3.3
1	B	93	SER	3.3
1	B	408	TYR	3.3
1	B	30	ASP	3.2
1	A	446	ARG	3.0
1	B	407	GLN	2.8
1	A	237	ASP	2.7
1	B	144	ASP	2.7
1	A	96	GLU	2.6
1	A	27	GLY	2.5
1	B	237	ASP	2.5
1	A	491	ASP	2.5
1	B	94	SER	2.4
1	B	25	THR	2.4
1	A	142	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	459	LEU	2.3
1	B	167	ASP	2.3
1	B	236	GLU	2.3
1	A	66	ASP	2.3
1	B	190	GLY	2.3
1	B	456	LEU	2.2
1	B	100	GLU	2.2
1	B	379	PRO	2.2
1	A	135	GLU	2.2
1	B	403	LYS	2.2
1	A	90	ASN	2.1
1	B	222	ILE	2.1
1	B	392	ASP	2.1
1	B	129	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
3	DHE	B	602	49/49	0.90	0.13	12,18,25,33	0
5	CL	A	607	1/1	0.90	0.19	40,40,40,40	0
3	DHE	A	602	49/49	0.92	0.12	11,18,27,34	0
2	HEC	A	601	43/43	0.92	0.14	11,19,33,35	0
2	HEC	B	601	43/43	0.92	0.12	13,21,35,40	0
4	PO4	A	603	5/5	0.93	0.09	30,33,44,45	0
5	CL	B	606	1/1	0.96	0.11	22,22,22,22	0
5	CL	B	605	1/1	0.97	0.09	23,23,23,23	0
4	PO4	A	604	5/5	0.97	0.08	19,23,25,34	0

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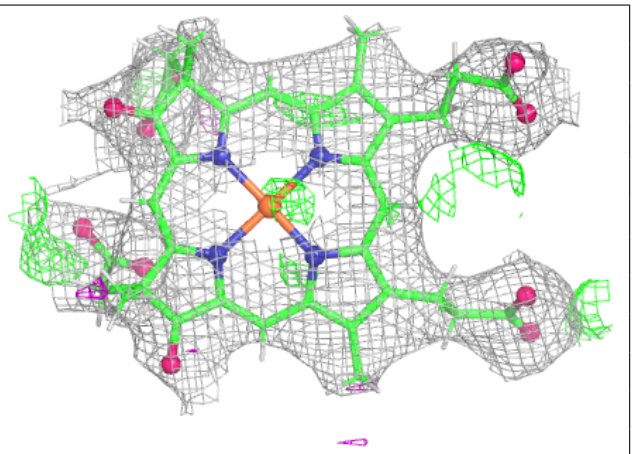
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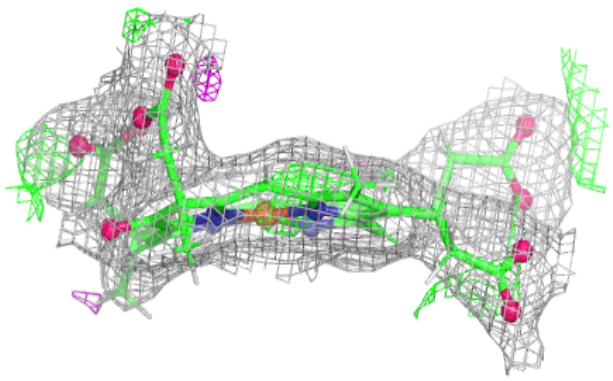
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	607	1/1	0.97	0.11	24,24,24,24	0
4	PO4	B	603	5/5	0.98	0.07	18,18,28,34	0
5	CL	A	606	1/1	0.98	0.06	20,20,20,20	0
4	PO4	A	605	5/5	0.98	0.06	18,18,23,23	0
4	PO4	B	604	5/5	0.99	0.05	17,20,22,22	0

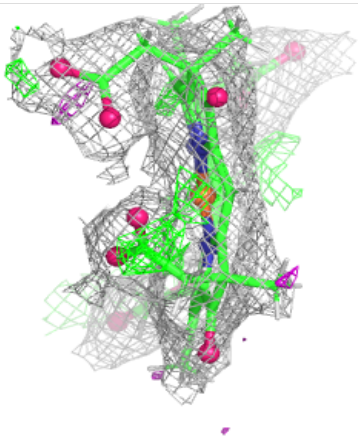
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DHE B 602:

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

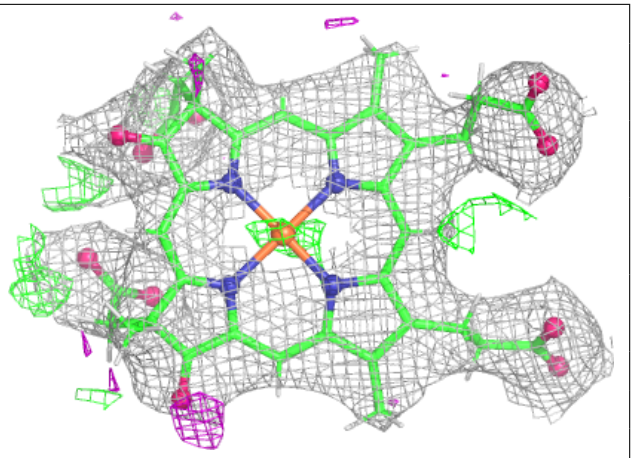


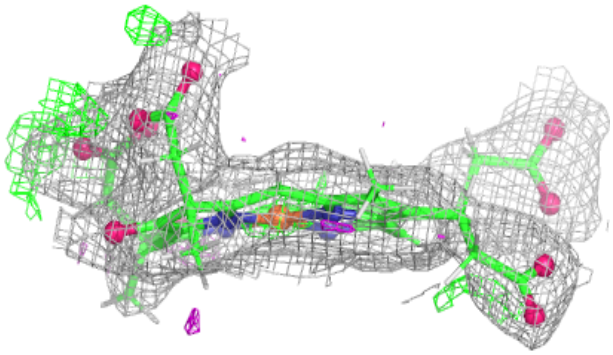




Electron density around DHE A 602:

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

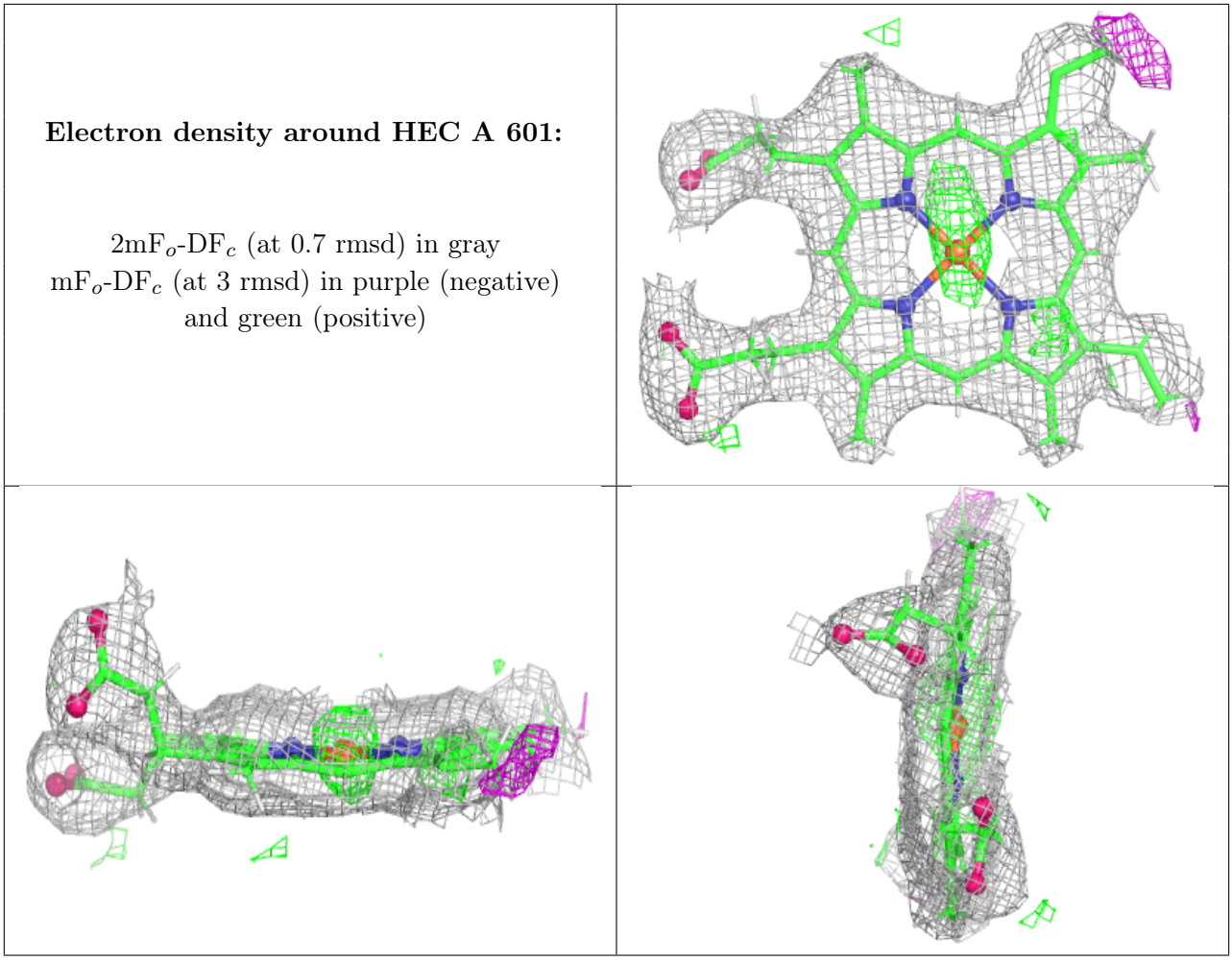






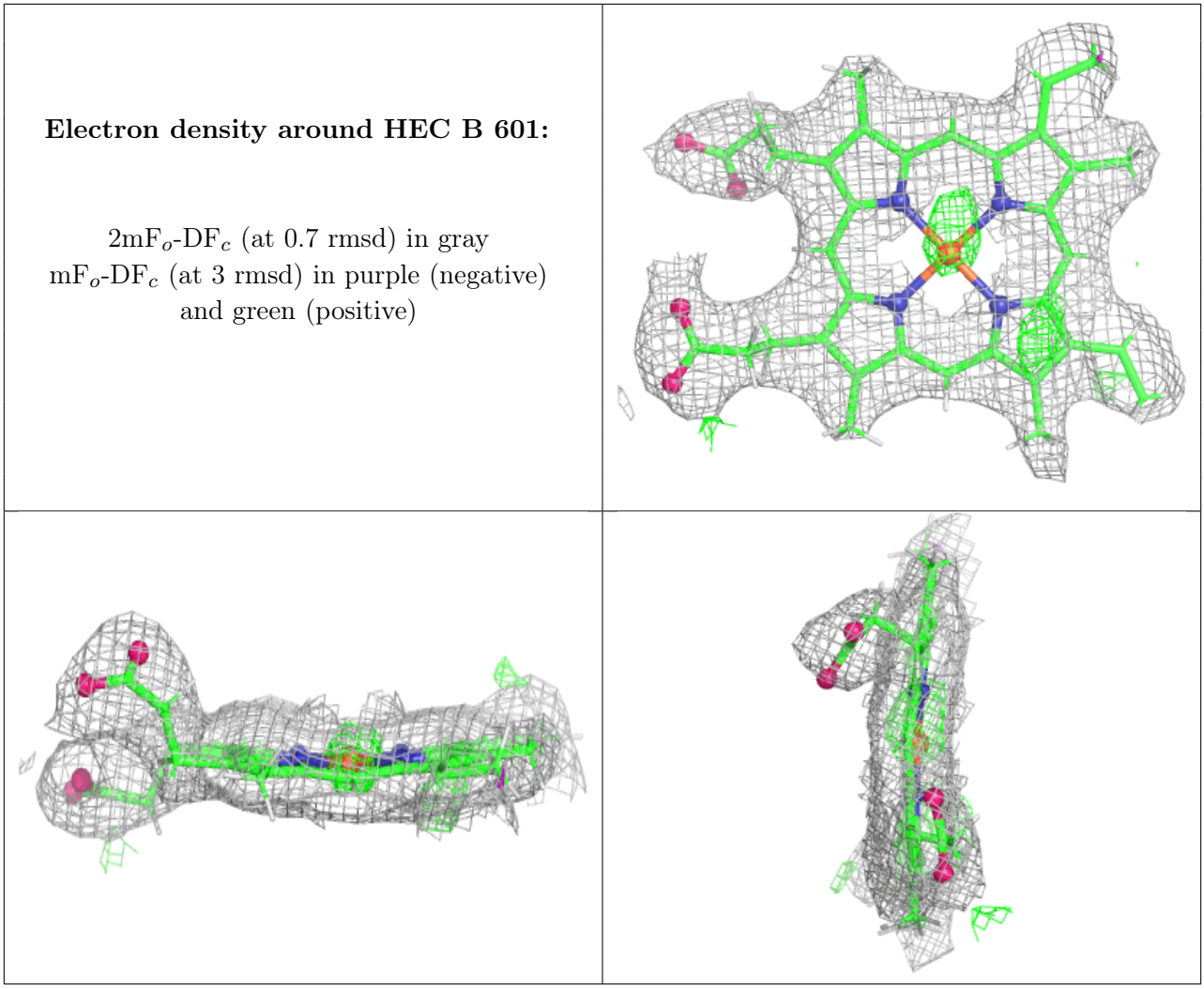
Electron density around HEC A 601:

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



Electron density around HEC B 601:

$2mF_o$-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

There are no such residues in this entry.