



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:50 pm BST

PDB ID : 1DY7
Title : Cytochrome cd1 Nitrite Reductase, CO complex
Authors : Sjogren, T.; Svensson-Ek, M.; Hajdu, J.; Brzezinski, P.
Deposited on : 2000-01-28
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

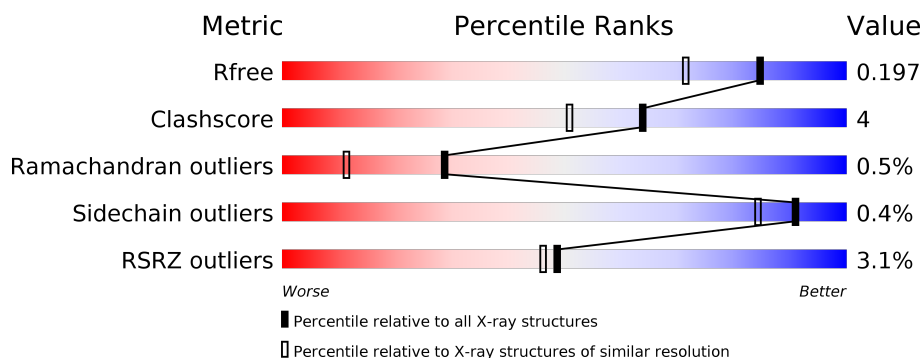
1 Overall quality at a glance

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))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	567	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 71% 5% 23% </div> </div>
1	B	567	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 5% 86% 8% • 5% </div> </div>

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	GOL	A	611	-	-	X	-
4	GOL	B	611	-	-	X	-
4	GOL	B	612	-	X	X	-

2 Entry composition [i](#)

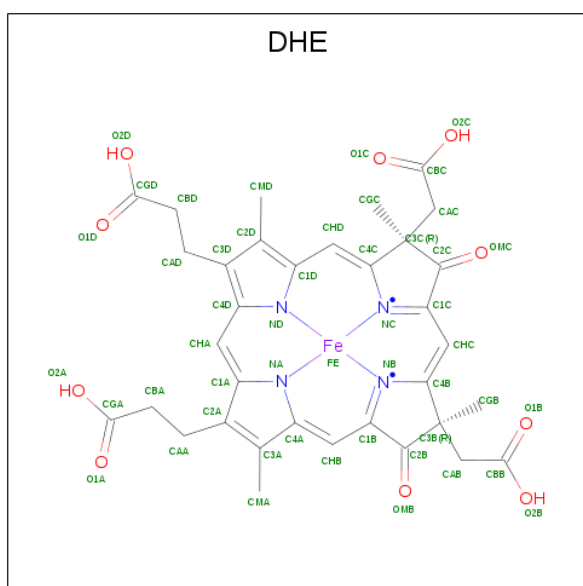
There are 7 unique types of molecules in this entry. The entry contains 8592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRITE REDUCTASE.

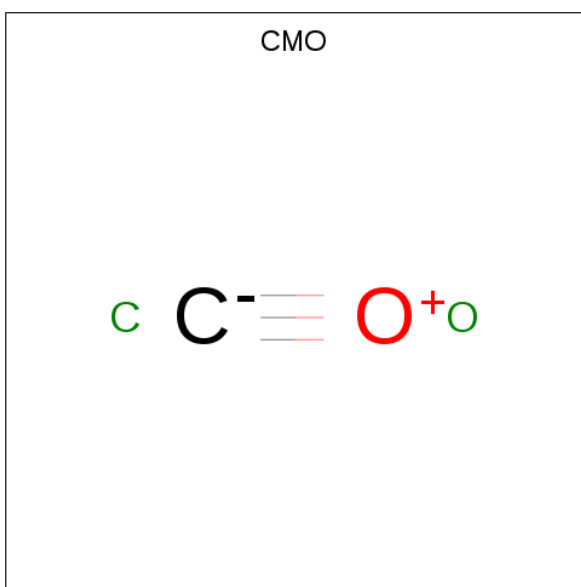
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3406	2160	568	668	10			
1	B	536	Total	C	N	O	S	0	0	0
			4161	2634	694	819	14			

- Molecule 2 is HEME D (three-letter code: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
2	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		
3	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



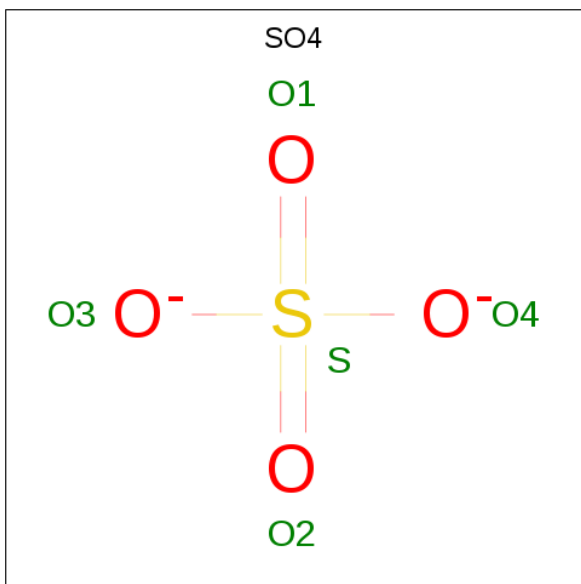
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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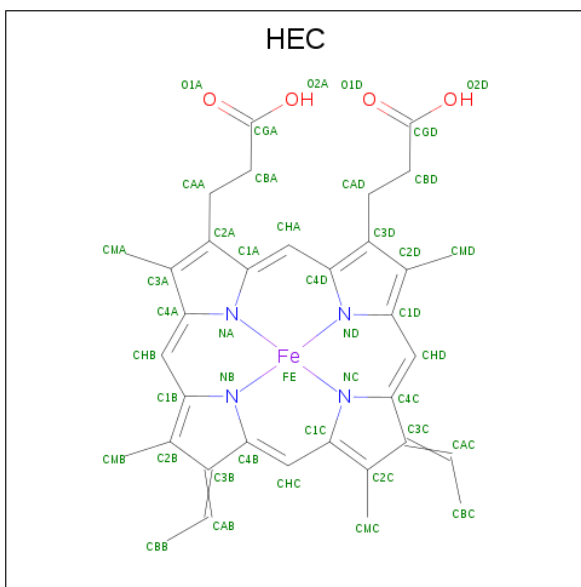
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

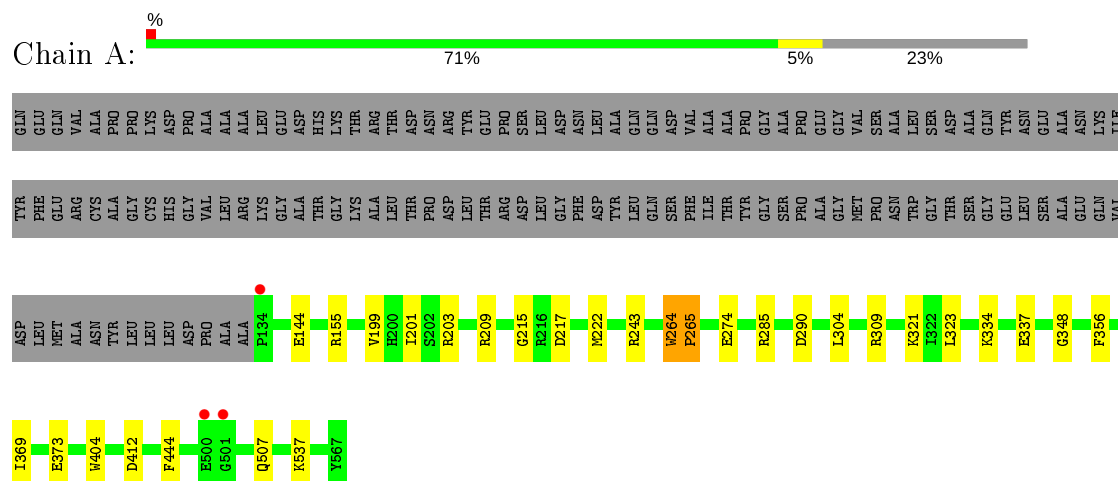
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	405	Total O 405 405	0	0
7	B	442	Total O 442 442	0	0

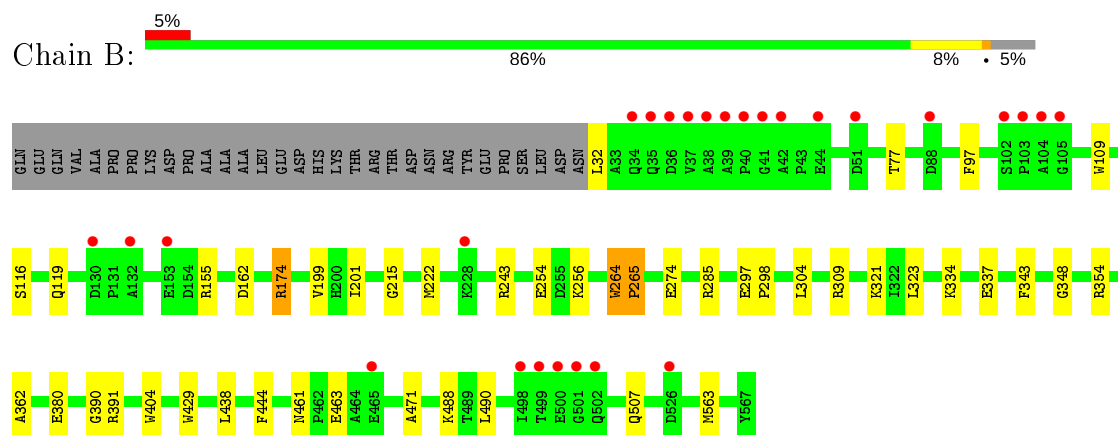
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



• Molecule 1: NITRITE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.94Å 61.04Å 100.39Å 90.00° 111.77° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 26.34 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (30.00-1.60) 88.7 (26.34-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.199 0.178 , 0.197	Depositor DCC
R_{free} test set	7127 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8592	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, GOL, DHE, SO4, 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	0.45	0/3491	1.04	13/4746 (0.3%)
1	B	0.43	0/4263	1.02	16/5799 (0.3%)
All	All	0.44	0/7754	1.03	29/10545 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	B	309	ARG	CD-NE-CZ	10.98	138.98	123.60
1	B	309	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	285	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	B	155	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	309	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	285	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	309	ARG	CD-NE-CZ	6.74	133.04	123.60
1	B	265	PRO	CA-N-CD	-6.61	102.25	111.50
1	A	373	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	264	TRP	CA-C-O	-6.22	107.03	120.10
1	B	264	TRP	CA-C-O	-6.04	107.41	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	243	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	391	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	243	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	162	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	265	PRO	CA-N-CD	-5.58	103.69	111.50
1	B	285	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	354	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	243	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	412	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	264	TRP	CA-CB-CG	-5.27	103.69	113.70
1	B	390	GLY	N-CA-C	-5.21	100.08	113.10
1	B	265	PRO	N-CA-CB	5.20	109.54	103.30
1	A	404	TRP	CA-CB-CG	5.20	123.57	113.70
1	B	404	TRP	CA-CB-CG	5.18	123.55	113.70
1	A	290	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	209	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	TRP	Mainchain,Peptide
1	B	264	TRP	Mainchain,Peptide

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	3406	0	3294	16	0
1	B	4161	0	4013	30	0
2	A	49	0	28	3	0
2	B	49	0	28	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	6	0	8	4	0
4	B	12	0	16	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	B	43	0	30	2	0
7	A	405	0	0	6	0
7	B	442	0	0	5	0
All	All	8592	0	7417	63	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 4.

All (63) 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:A:611:GOL:C2	4:A:611:GOL:C1	1.86	1.50
4:B:611:GOL:C1	4:B:611:GOL:C2	1.87	1.49
4:B:612:GOL:C1	4:B:612:GOL:C2	1.86	1.49
1:B:174:ARG:HH12	4:B:612:GOL:H12	1.17	1.08
1:B:174:ARG:HH22	4:B:612:GOL:H31	1.30	0.97
4:B:611:GOL:C1	4:B:611:GOL:C3	2.51	0.88
4:B:612:GOL:C1	4:B:612:GOL:C3	2.56	0.84
4:A:611:GOL:C1	4:A:611:GOL:C3	2.61	0.78
1:B:174:ARG:HH12	4:B:612:GOL:C1	1.96	0.76
1:A:201:ILE:HD12	1:A:203:ARG:HG2	1.68	0.74
1:B:174:ARG:HH22	4:B:612:GOL:C3	2.04	0.69
4:B:612:GOL:C1	4:B:612:GOL:O2	2.41	0.69
1:B:116:SER:H	1:B:119:GLN:HE21	1.38	0.68
1:B:174:ARG:NH1	4:B:612:GOL:H12	2.00	0.66
4:B:612:GOL:C2	4:B:612:GOL:O1	2.46	0.63
4:B:611:GOL:C1	4:B:611:GOL:H31	2.29	0.61
4:B:612:GOL:C1	4:B:612:GOL:H31	2.28	0.61
1:B:174:ARG:NH2	4:B:612:GOL:H31	2.10	0.59
1:A:537:LYS:HG2	7:A:2368:HOH:O	2.02	0.58
1:B:490:LEU:HD23	4:B:611:GOL:H2	1.86	0.58
4:B:611:GOL:C1	4:B:611:GOL:O2	2.50	0.57
1:A:356:PHE:HB3	1:A:369:ILE:HG13	1.88	0.56
1:A:323:LEU:HD22	1:A:337:GLU:HG2	1.87	0.56
1:A:334:LYS:NZ	7:A:2210:HOH:O	2.37	0.55
2:B:602:DHE:HMD1	2:B:602:DHE:HBD2	1.90	0.54
1:A:155:ARG:HG2	7:A:2100:HOH:O	2.07	0.54
1:A:334:LYS:HB3	1:A:334:LYS:NZ	2.23	0.53
1:B:116:SER:H	1:B:119:GLN:NE2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HG22	2:A:602:DHE:HAD1	1.92	0.52
1:B:323:LEU:HD22	1:B:337:GLU:HG2	1.91	0.52
4:A:611:GOL:C2	4:A:611:GOL:O1	2.52	0.52
1:B:488:LYS:CG	4:B:611:GOL:H32	2.40	0.52
1:A:356:PHE:HB3	1:A:369:ILE:CG1	2.42	0.49
2:A:602:DHE:HBD2	2:A:602:DHE:HMD1	1.95	0.49
1:B:109:TRP:CE2	6:B:601:HEC:HBB2	2.48	0.49
1:B:321:LYS:NZ	7:B:2231:HOH:O	2.46	0.48
1:A:144:GLU:HG3	7:A:2007:HOH:O	2.14	0.47
4:B:611:GOL:O1	4:B:611:GOL:C2	2.53	0.47
1:A:222:MET:HE1	1:A:274:GLU:HA	1.97	0.47
1:B:488:LYS:HZ3	4:B:611:GOL:C3	2.27	0.46
1:B:488:LYS:HZ3	4:B:611:GOL:H31	1.81	0.46
4:A:611:GOL:C1	4:A:611:GOL:O2	2.57	0.46
1:A:304:LEU:HD21	1:A:348:GLY:HA2	1.98	0.46
1:B:256:LYS:NZ	7:B:2163:HOH:O	2.48	0.46
1:B:32:LEU:N	7:B:2001:HOH:O	2.48	0.45
1:A:321:LYS:NZ	7:A:2193:HOH:O	2.49	0.45
1:B:380:GLU:HG3	1:B:429:TRP:O	2.17	0.45
1:A:444:PHE:CE1	2:A:602:DHE:HBD1	2.51	0.44
1:A:199:VAL:HA	1:A:215:GLY:HA2	2.00	0.44
1:B:222:MET:HE1	1:B:274:GLU:HA	1.99	0.44
1:B:444:PHE:CE1	2:B:602:DHE:HBD1	2.53	0.44
1:B:438:LEU:HG	1:B:471:ALA:HB2	1.99	0.43
1:B:297:GLU:N	1:B:298:PRO:HD3	2.34	0.42
7:A:2214:HOH:O	1:B:334:LYS:HE2	2.20	0.42
1:B:488:LYS:HG3	4:B:611:GOL:H32	2.02	0.42
6:B:601:HEC:HBD2	6:B:601:HEC:HHA	2.02	0.42
1:B:254:GLU:HG3	7:B:2154:HOH:O	2.19	0.41
1:B:77:THR:HG23	7:B:2020:HOH:O	2.19	0.41
1:B:304:LEU:HD21	1:B:348:GLY:HA2	2.02	0.41
1:A:201:ILE:HD12	1:A:203:ARG:CG	2.46	0.40
1:B:461:ASN:OD1	1:B:463:GLU:HB2	2.21	0.40
1:B:343:PHE:CG	1:B:362:ALA:HB3	2.56	0.40
1:B:199:VAL:HA	1:B:215:GLY:HA2	2.03	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	432/567 (76%)	413 (96%)	17 (4%)	2 (0%)	29	11
1	B	534/567 (94%)	513 (96%)	18 (3%)	3 (1%)	25	8
All	All	966/1134 (85%)	926 (96%)	35 (4%)	5 (0%)	29	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	B	265	PRO
1	B	507	GLN
1	A	265	PRO
1	B	174	ARG

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	366/469 (78%)	366 (100%)	0	100	100
1	B	442/469 (94%)	439 (99%)	3 (1%)	84	73
All	All	808/938 (86%)	805 (100%)	3 (0%)	91	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	PHE

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Mol	Chain	Res	Type
1	B	201	ILE
1	B	563	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	282	GLN
1	A	452	GLN
1	B	58	ASN
1	B	119	GLN
1	B	221	ASN
1	B	282	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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
3	CMO	A	603	-	0,1,1	0.00	-	-		
4	GOL	B	612	-	5,5,5	3.75	1 (20%)	5,5,5	2.62	3 (60%)
2	DHE	B	602	1	38,56,56	7.60	26 (68%)	37,94,94	4.20	23 (62%)
5	SO4	B	621	-	4,4,4	0.68	0	6,6,6	0.25	0
4	GOL	B	611	-	5,5,5	3.95	1 (20%)	5,5,5	2.53	3 (60%)
4	GOL	A	611	-	5,5,5	3.85	1 (20%)	5,5,5	2.01	2 (40%)
5	SO4	A	621	-	4,4,4	0.60	0	6,6,6	0.28	0
2	DHE	A	602	1	38,56,56	7.68	26 (68%)	37,94,94	4.37	23 (62%)
6	HEC	B	601	1	26,50,50	2.17	4 (15%)	18,82,82	2.32	11 (61%)
5	SO4	B	622	-	4,4,4	0.61	0	6,6,6	0.22	0
3	CMO	B	603	-	0,1,1	0.00	-	-		

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	GOL	B	612	-	-	2/4/4/4	-
2	DHE	B	602	1	-	3/12/108/108	-
6	HEC	B	601	1	-	2/6/54/54	-
4	GOL	B	611	-	-	1/4/4/4	-
4	GOL	A	611	-	-	1/4/4/4	-
2	DHE	A	602	1	-	3/12/108/108	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	DHE	OMC-C2C	17.89	1.52	1.21
2	B	602	DHE	OMC-C2C	17.67	1.51	1.21
2	B	602	DHE	OMB-C2B	17.24	1.51	1.21
2	A	602	DHE	OMB-C2B	17.21	1.51	1.21
2	A	602	DHE	C3B-C2B	-14.93	1.34	1.52
2	A	602	DHE	C3C-C2C	-14.66	1.35	1.52
2	B	602	DHE	C3C-C2C	-14.47	1.35	1.52
2	B	602	DHE	C3B-C2B	-13.86	1.35	1.52
2	B	602	DHE	C4B-NB	-12.48	1.37	1.49
2	A	602	DHE	CHA-C1A	-12.31	1.38	1.51
2	B	602	DHE	CHA-C1A	-12.21	1.38	1.51
2	A	602	DHE	C4B-NB	-12.17	1.37	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	DHE	CHA-C4D	-11.85	1.39	1.51
2	B	602	DHE	CHA-C4D	-11.83	1.39	1.51
2	B	602	DHE	C4C-NC	-11.68	1.37	1.49
2	A	602	DHE	C4C-NC	-11.18	1.38	1.49
2	A	602	DHE	C1C-NC	-8.99	1.37	1.49
2	A	602	DHE	C1B-NB	-8.89	1.37	1.49
4	B	611	GOL	C1-C2	8.80	1.87	1.51
4	A	611	GOL	C1-C2	8.54	1.86	1.51
2	B	602	DHE	C1C-NC	-8.47	1.38	1.49
2	B	602	DHE	CHB-C1B	-8.39	1.38	1.53
4	B	612	GOL	C1-C2	8.37	1.86	1.51
2	A	602	DHE	CHB-C1B	-8.28	1.39	1.53
2	B	602	DHE	C1B-NB	-8.28	1.38	1.49
2	A	602	DHE	C3B-C4B	-7.49	1.44	1.55
2	B	602	DHE	C3B-C4B	-6.76	1.45	1.55
2	B	602	DHE	C3C-C4C	-6.57	1.46	1.55
2	B	602	DHE	CHD-C4C	-6.47	1.36	1.54
6	B	601	HEC	C3C-C2C	-6.30	1.34	1.40
2	B	602	DHE	CHC-C4B	-6.12	1.37	1.52
2	A	602	DHE	CHD-C4C	-6.07	1.37	1.54
6	B	601	HEC	C3B-C2B	-6.05	1.34	1.40
2	A	602	DHE	CHC-C4B	-5.92	1.38	1.52
2	A	602	DHE	C3C-C4C	-5.86	1.47	1.55
2	A	602	DHE	C1D-C2D	5.82	1.46	1.38
2	A	602	DHE	CHB-C4A	-5.59	1.37	1.51
2	B	602	DHE	C1D-C2D	5.55	1.45	1.38
2	A	602	DHE	C4D-C3D	5.31	1.45	1.38
2	B	602	DHE	CHD-C1D	-5.26	1.38	1.51
2	A	602	DHE	C1A-C2A	5.24	1.45	1.38
2	B	602	DHE	CHB-C4A	-5.13	1.38	1.51
2	A	602	DHE	C4A-C3A	5.13	1.45	1.38
2	B	602	DHE	C4A-C3A	5.02	1.45	1.38
2	B	602	DHE	C1A-C2A	4.93	1.44	1.38
2	B	602	DHE	C4D-C3D	4.91	1.44	1.38
2	A	602	DHE	CHD-C1D	-4.62	1.39	1.51
2	B	602	DHE	C1B-C2B	-3.81	1.44	1.50
2	B	602	DHE	CHC-C1C	-3.81	1.38	1.53
2	A	602	DHE	CHC-C1C	-3.81	1.38	1.53
2	A	602	DHE	C1B-C2B	-3.71	1.44	1.50
6	B	601	HEC	CBC-CAC	-3.35	1.36	1.49
2	B	602	DHE	CAA-C2A	2.91	1.56	1.52
2	A	602	DHE	CAA-C2A	2.74	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	DHE	CAB-C3B	-2.74	1.51	1.56
2	B	602	DHE	C1C-C2C	-2.63	1.46	1.50
2	B	602	DHE	CAB-C3B	-2.45	1.52	1.56
6	B	601	HEC	CBB-CAB	-2.25	1.41	1.49
2	A	602	DHE	CAC-C3C	-2.01	1.53	1.56

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	DHE	CHC-C1C-NC	13.73	128.01	110.94
2	B	602	DHE	CHC-C1C-NC	13.16	127.31	110.94
2	B	602	DHE	CAD-C3D-C4D	-10.57	119.87	127.30
2	A	602	DHE	CAD-C3D-C4D	-9.77	120.44	127.30
2	A	602	DHE	CHB-C1B-NB	7.95	125.75	110.75
2	B	602	DHE	CHB-C1B-NB	7.88	125.60	110.75
2	A	602	DHE	C4B-C3B-C2B	7.84	108.29	100.71
2	B	602	DHE	C4B-C3B-C2B	7.07	107.54	100.71
2	A	602	DHE	CAA-C2A-C1A	-6.20	122.94	127.30
2	B	602	DHE	CAA-C2A-C1A	-5.24	123.62	127.30
2	A	602	DHE	CGB-C3B-CAB	-5.17	102.27	110.77
2	B	602	DHE	C3C-C4C-NC	4.80	108.89	104.67
2	B	602	DHE	C4C-C3C-C2C	4.80	105.35	100.71
2	A	602	DHE	C3C-C4C-NC	4.70	108.80	104.67
2	B	602	DHE	C4D-CHA-C1A	4.68	124.29	112.87
2	B	602	DHE	CHC-C4B-C3B	4.51	127.19	118.34
4	B	611	GOL	C3-C2-C1	-4.48	94.30	111.70
6	B	601	HEC	CMD-C2D-C1D	-4.17	122.06	128.46
2	A	602	DHE	CHB-C1B-C2B	4.10	126.55	114.47
2	A	602	DHE	C4C-C3C-C2C	4.09	104.66	100.71
2	A	602	DHE	C4D-CHA-C1A	4.04	122.72	112.87
2	B	602	DHE	CHB-C1B-C2B	4.04	126.37	114.47
2	A	602	DHE	CHD-C1D-C2D	-3.99	122.54	129.45
2	A	602	DHE	CHC-C4B-C3B	3.97	126.12	118.34
2	A	602	DHE	CHA-C1A-C2A	-3.79	125.11	129.68
2	A	602	DHE	CBD-CAD-C3D	3.64	119.20	112.49
4	B	612	GOL	C3-C2-C1	-3.58	97.77	111.70
4	B	612	GOL	O2-C2-C1	-3.56	93.44	109.12
2	A	602	DHE	CAA-CBA-CGA	3.56	118.64	112.67
2	B	602	DHE	CHC-C1C-C2C	3.49	125.60	114.70
6	B	601	HEC	CBD-CAD-C3D	3.47	118.89	112.49
2	B	602	DHE	CAA-CBA-CGA	3.40	118.37	112.67
2	A	602	DHE	CHC-C1C-C2C	3.37	125.21	114.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	DHE	CHA-C4D-C3D	-3.17	125.85	129.68
6	B	601	HEC	CMC-C2C-C3C	3.17	129.54	125.82
2	B	602	DHE	CHD-C1D-C2D	-3.14	124.02	129.45
2	A	602	DHE	OMB-C2B-C3B	3.11	129.89	125.59
6	B	601	HEC	CMB-C2B-C1B	-3.09	123.72	128.46
2	B	602	DHE	CGB-C3B-CAB	-3.07	105.72	110.77
2	A	602	DHE	CAD-CBD-CGD	3.06	117.80	112.67
6	B	601	HEC	CMB-C2B-C3B	2.96	129.30	125.82
2	A	602	DHE	OMC-C2C-C3C	2.87	129.56	125.59
6	B	601	HEC	C4C-C3C-C2C	2.87	109.45	106.35
4	B	612	GOL	O1-C1-C2	-2.86	96.50	110.20
2	B	602	DHE	OMC-C2C-C3C	2.82	129.49	125.59
2	B	602	DHE	CBD-CAD-C3D	2.80	117.65	112.49
4	A	611	GOL	C3-C2-C1	-2.67	101.31	111.70
4	B	611	GOL	O2-C2-C1	-2.64	97.49	109.12
4	A	611	GOL	O3-C3-C2	2.62	122.75	110.20
2	B	602	DHE	C3B-C4B-NB	2.55	106.91	104.67
6	B	601	HEC	CMC-C2C-C1C	-2.52	124.59	128.46
2	B	602	DHE	CHA-C4D-C3D	-2.48	126.69	129.68
2	B	602	DHE	C1C-CHC-C4B	2.47	123.42	116.16
2	B	602	DHE	CHA-C1A-C2A	-2.47	126.70	129.68
6	B	601	HEC	CMD-C2D-C3D	2.42	129.50	124.94
2	A	602	DHE	CBA-CAA-C2A	-2.21	108.40	112.49
2	B	602	DHE	CMA-C3A-C2A	2.20	129.08	124.94
4	B	611	GOL	O1-C1-C2	-2.19	99.68	110.20
2	A	602	DHE	CMA-C3A-C2A	2.19	129.08	124.94
6	B	601	HEC	C4B-C3B-C2B	2.15	108.67	106.35
2	A	602	DHE	C3B-C4B-NB	2.12	106.54	104.67
2	B	602	DHE	CMD-C2D-C3D	2.10	128.90	124.94
2	B	602	DHE	OMB-C2B-C3B	2.09	128.48	125.59
6	B	601	HEC	CMA-C3A-C2A	2.07	128.85	124.94
6	B	601	HEC	C1D-C2D-C3D	2.07	108.44	107.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	DHE	C2D-C3D-CAD-CBD
2	B	602	DHE	C4D-C3D-CAD-CBD
4	B	612	GOL	C1-C2-C3-O3
4	B	611	GOL	C1-C2-C3-O3
2	A	602	DHE	C2D-C3D-CAD-CBD

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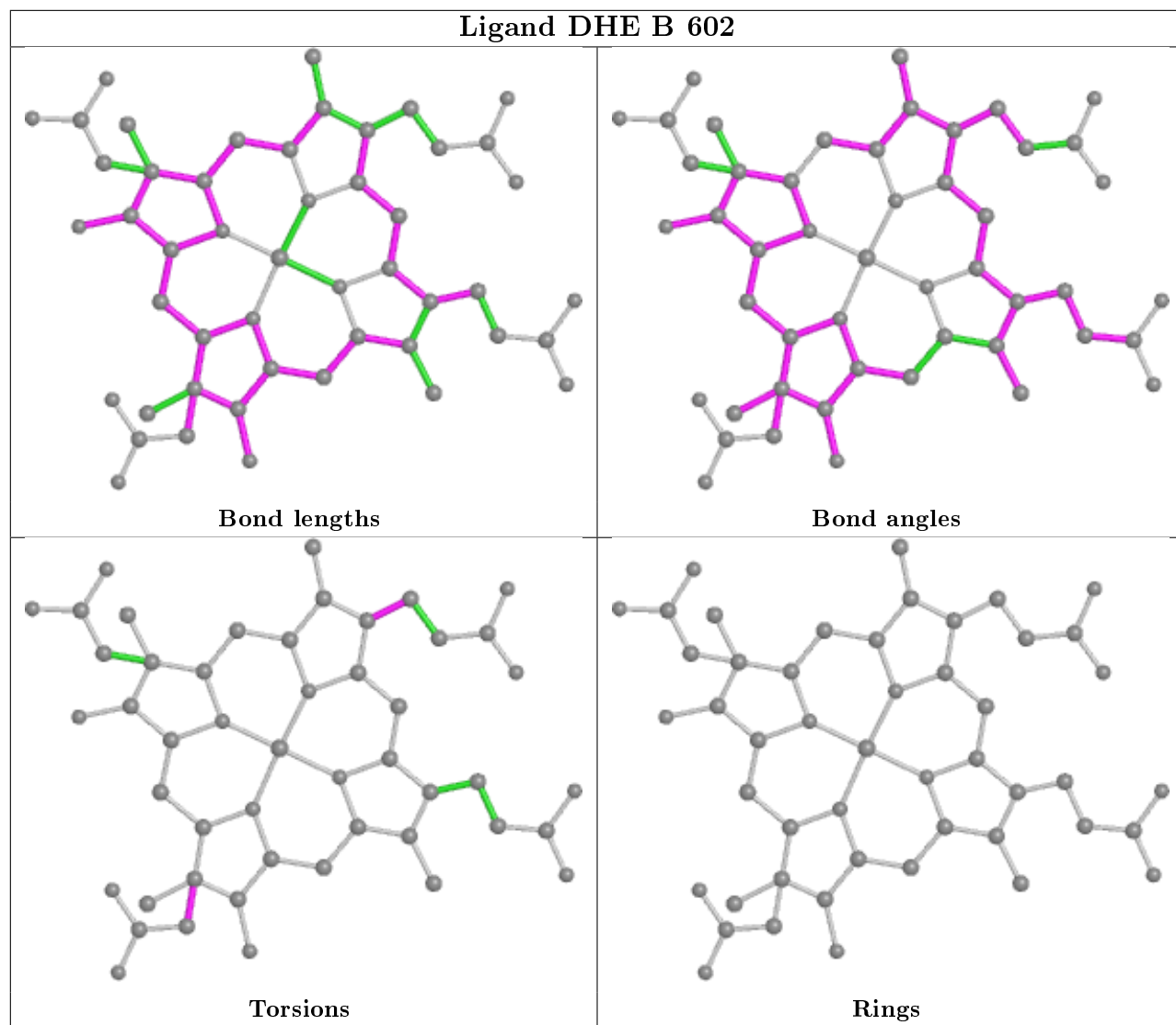
Mol	Chain	Res	Type	Atoms
2	A	602	DHE	C4D-C3D-CAD-CBD
4	B	612	GOL	O2-C2-C3-O3
4	A	611	GOL	O2-C2-C3-O3
6	B	601	HEC	C2D-C3D-CAD-CBD
6	B	601	HEC	C4D-C3D-CAD-CBD
2	B	602	DHE	CGB-C3B-CAB-CBB
2	A	602	DHE	CGB-C3B-CAB-CBB

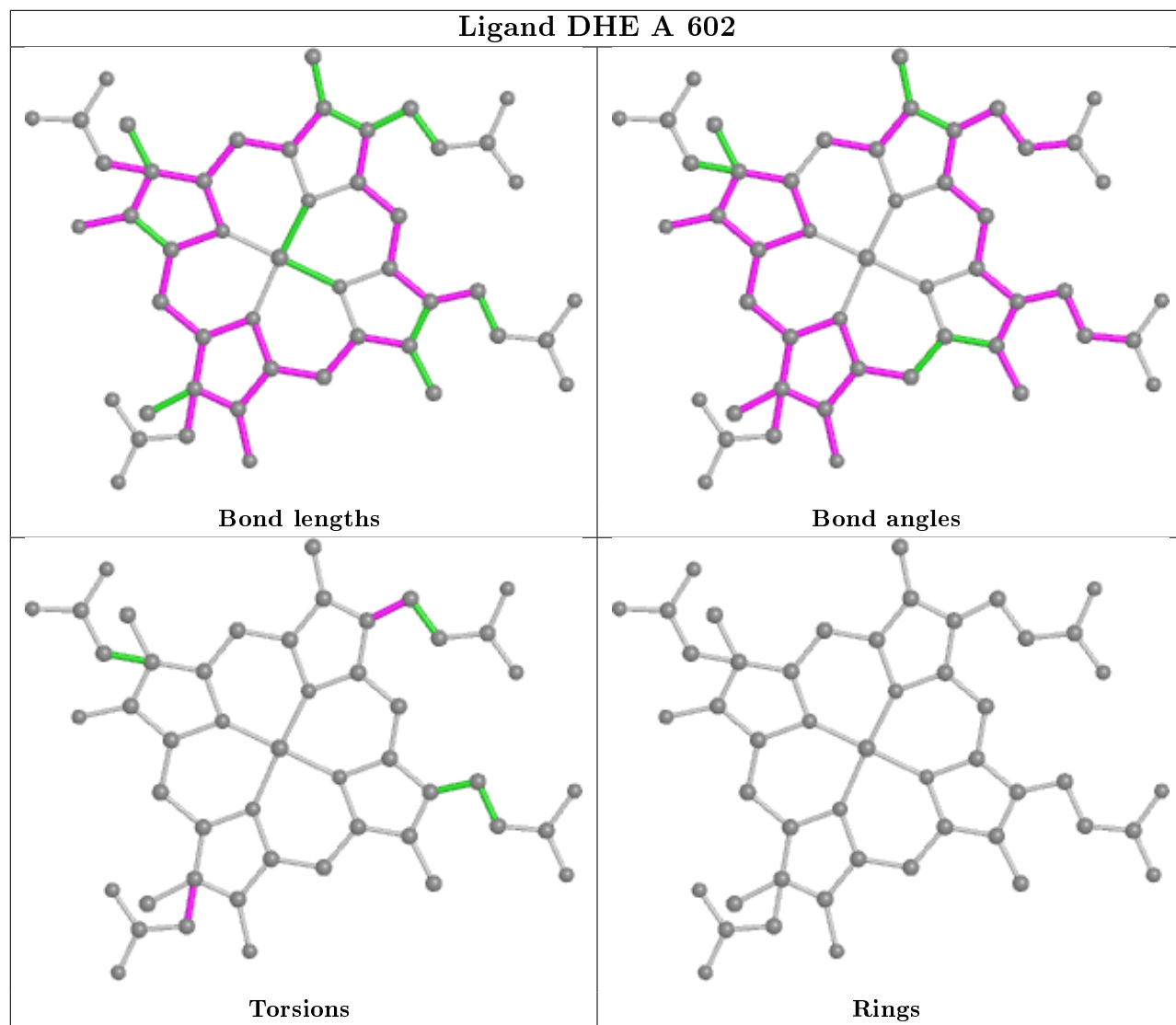
There are no ring outliers.

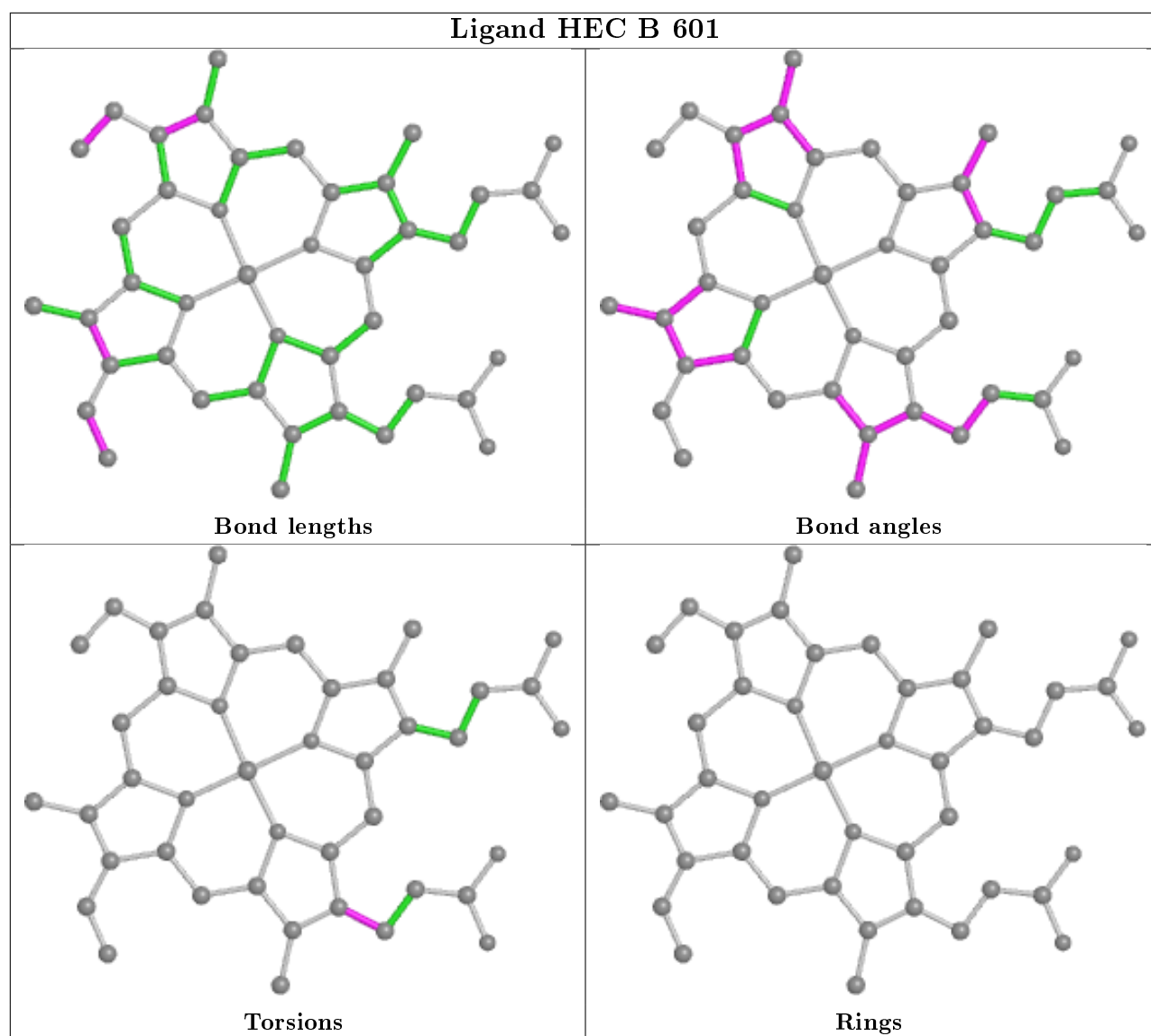
6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	612	GOL	11	0
2	B	602	DHE	2	0
4	B	611	GOL	10	0
4	A	611	GOL	4	0
2	A	602	DHE	3	0
6	B	601	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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	434/567 (76%)	-0.29	3 (0%) 87 87	9, 14, 23, 35	0
1	B	536/567 (94%)	-0.03	27 (5%) 28 26	10, 15, 32, 48	0
All	All	970/1134 (85%)	-0.15	30 (3%) 49 46	9, 15, 28, 48	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PRO	6.4
1	B	104	ALA	5.3
1	B	502	GLN	5.3
1	B	34	GLN	5.2
1	B	499	THR	4.3
1	B	36	ASP	4.1
1	B	35	GLN	4.0
1	B	37	VAL	3.6
1	B	38	ALA	3.4
1	B	500	GLU	3.3
1	B	501	GLY	3.0
1	A	134	PRO	3.0
1	A	501	GLY	2.8
1	B	39	ALA	2.7
1	B	42	ALA	2.6
1	B	105	GLY	2.5
1	A	500	GLU	2.4
1	B	51	ASP	2.4
1	B	102	SER	2.3
1	B	40	PRO	2.3
1	B	153	GLU	2.3
1	B	88	ASP	2.2
1	B	498	ILE	2.2
1	B	465	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLY	2.2
1	B	130	ASP	2.2
1	B	44	GLU	2.2
1	B	132	ALA	2.1
1	B	526	ASP	2.0
1	B	228	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 carbohydrates in this entry.

6.4 Ligands [i](#)

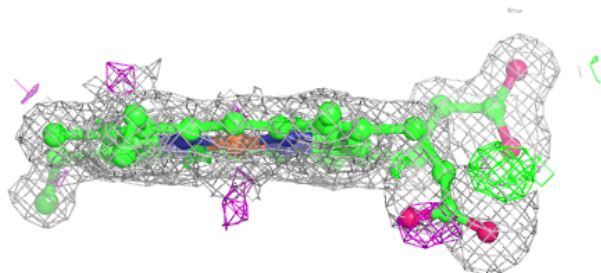
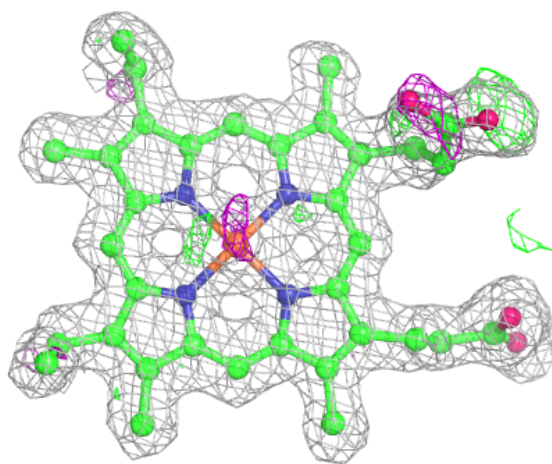
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	612	6/6	0.60	0.27	42,42,44,44	0
4	GOL	B	611	6/6	0.79	0.36	35,37,38,39	0
5	SO4	B	622	5/5	0.86	0.17	48,49,49,49	0
5	SO4	A	621	5/5	0.92	0.17	31,31,34,34	0
5	SO4	B	621	5/5	0.94	0.20	31,31,33,34	0
6	HEC	B	601	43/43	0.95	0.11	16,21,32,36	0
4	GOL	A	611	6/6	0.96	0.09	14,16,17,18	0
3	CMO	A	603	2/2	0.96	0.09	17,17,17,20	0
2	DHE	A	602	49/49	0.97	0.07	9,12,16,23	0
2	DHE	B	602	49/49	0.98	0.07	11,13,18,22	0
3	CMO	B	603	2/2	0.99	0.09	14,14,14,19	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.

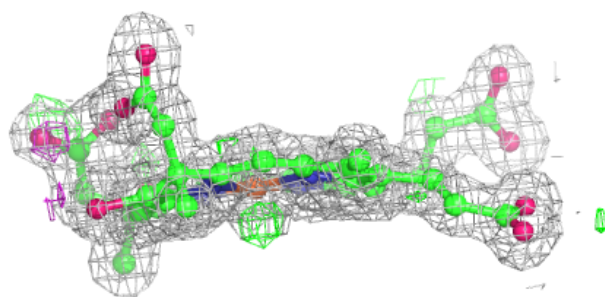
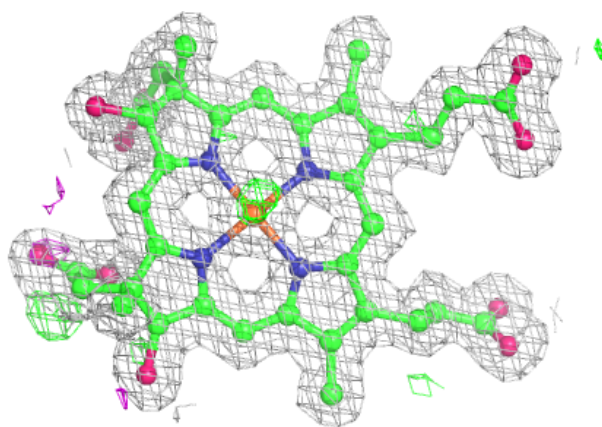
Electron density around HEC B 601:

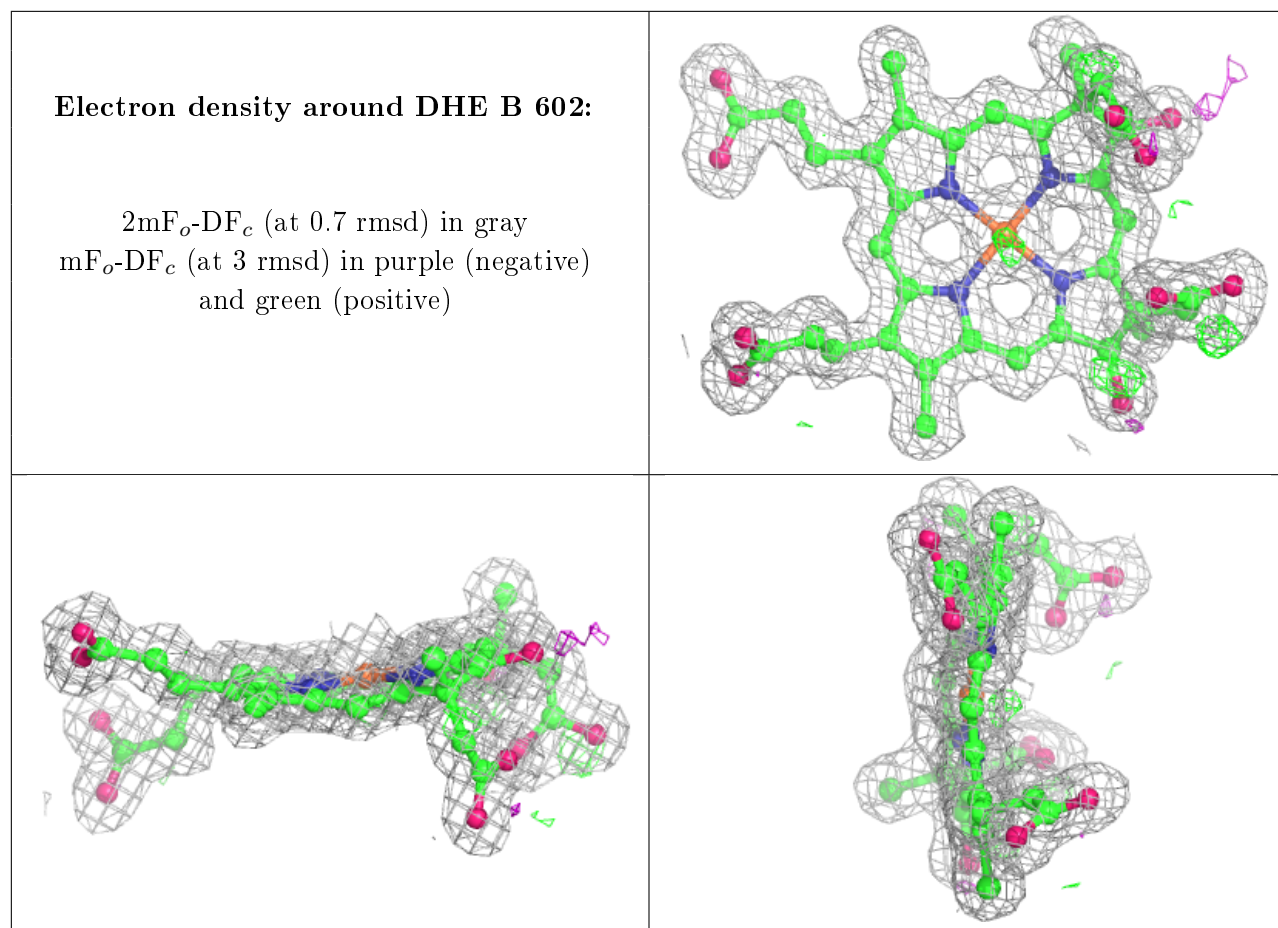
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.