



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 02:31 am BST

PDB ID : 6G94
Title : Structure of E. coli hydrogenase-1 C19G variant in complex with cytochrome b
Authors : Volbeda, A.; Fontecilla-Camps, J.C.
Deposited on : 2018-04-10
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

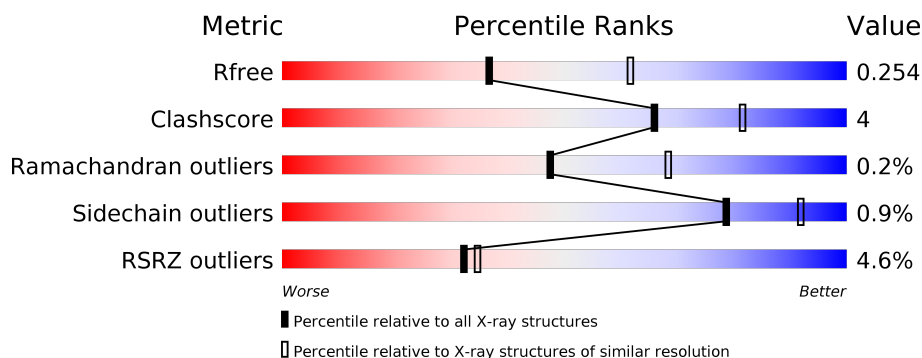
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	Q	335	<div> <div>10%</div> <div>81% 7% 12%</div> </div>
1	R	335	<div> <div>10%</div> <div>76% 10% 13%</div> </div>
1	S	335	<div> <div>10%</div> <div>80% 8% 12%</div> </div>
1	T	335	<div> <div>4%</div> <div>77% 10% 12%</div> </div>
2	J	582	<div> <div>10%</div> <div>90% 10%</div> </div>
2	K	582	<div> <div>3%</div> <div>91% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	582	<div><div>%</div><div><div></div><div>91%</div><div>9%</div></div></div>
2	M	582	<div><div>4%</div><div><div></div><div>89%</div><div>11%</div></div></div>
3	A	235	<div><div>14%</div><div><div></div><div>62%</div><div>11%</div><div>27%</div></div></div>
3	B	235	<div><div>15%</div><div><div></div><div>59%</div><div>9%</div><div>32%</div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 30463 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 Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	296	Total	C	N	O	S	0	0	0
			2242	1420	385	417	20			
1	T	296	Total	C	N	O	S	0	0	0
			2220	1408	379	413	20			
1	Q	295	Total	C	N	O	S	0	0	0
			2234	1416	383	415	20			
1	R	291	Total	C	N	O	S	0	0	0
			2203	1394	378	411	20			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	19	GLY	CYS	conflict	UNP P69739
S	328	ARG	-	expression tag	UNP P69739
S	329	SER	-	expression tag	UNP P69739
S	330	HIS	-	expression tag	UNP P69739
S	331	HIS	-	expression tag	UNP P69739
S	332	HIS	-	expression tag	UNP P69739
S	333	HIS	-	expression tag	UNP P69739
S	334	HIS	-	expression tag	UNP P69739
S	335	HIS	-	expression tag	UNP P69739
T	19	GLY	CYS	conflict	UNP P69739
T	328	ARG	-	expression tag	UNP P69739
T	329	SER	-	expression tag	UNP P69739
T	330	HIS	-	expression tag	UNP P69739
T	331	HIS	-	expression tag	UNP P69739
T	332	HIS	-	expression tag	UNP P69739
T	333	HIS	-	expression tag	UNP P69739
T	334	HIS	-	expression tag	UNP P69739
T	335	HIS	-	expression tag	UNP P69739
Q	19	GLY	CYS	conflict	UNP P69739
Q	328	ARG	-	expression tag	UNP P69739
Q	329	SER	-	expression tag	UNP P69739

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	330	HIS	-	expression tag	UNP P69739
Q	331	HIS	-	expression tag	UNP P69739
Q	332	HIS	-	expression tag	UNP P69739
Q	333	HIS	-	expression tag	UNP P69739
Q	334	HIS	-	expression tag	UNP P69739
Q	335	HIS	-	expression tag	UNP P69739
R	19	GLY	CYS	conflict	UNP P69739
R	328	ARG	-	expression tag	UNP P69739
R	329	SER	-	expression tag	UNP P69739
R	330	HIS	-	expression tag	UNP P69739
R	331	HIS	-	expression tag	UNP P69739
R	332	HIS	-	expression tag	UNP P69739
R	333	HIS	-	expression tag	UNP P69739
R	334	HIS	-	expression tag	UNP P69739
R	335	HIS	-	expression tag	UNP P69739

- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	1	0
			4526	2874	787	838	27			
2	M	581	Total	C	N	O	S	0	0	0
			4512	2869	787	829	27			
2	J	581	Total	C	N	O	S	0	0	0
			4528	2876	792	833	27			
2	K	581	Total	C	N	O	S	0	0	0
			4526	2873	791	835	27			

- Molecule 3 is a protein called Probable Ni/Fe-hydrogenase 1 B-type cytochrome subunit.

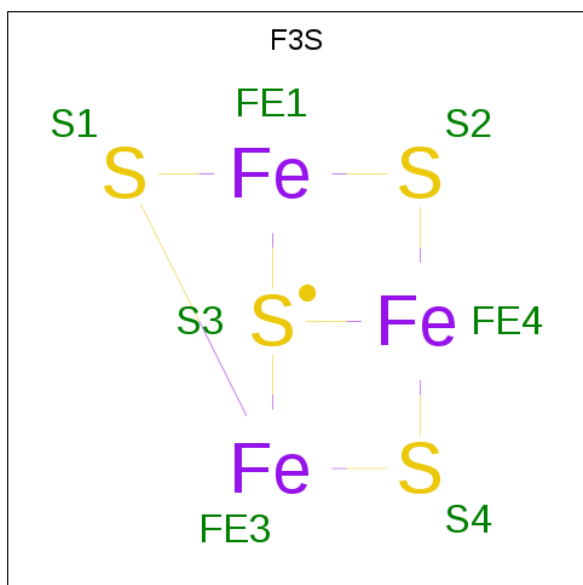
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	172	Total	C	N	O	S	0	0	0
			1310	888	204	207	11			
3	B	160	Total	C	N	O	S	0	0	0
			1242	842	196	194	10			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



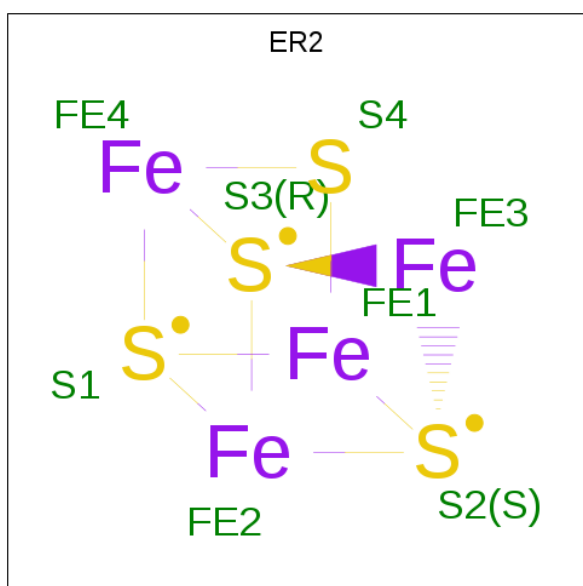
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	R	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



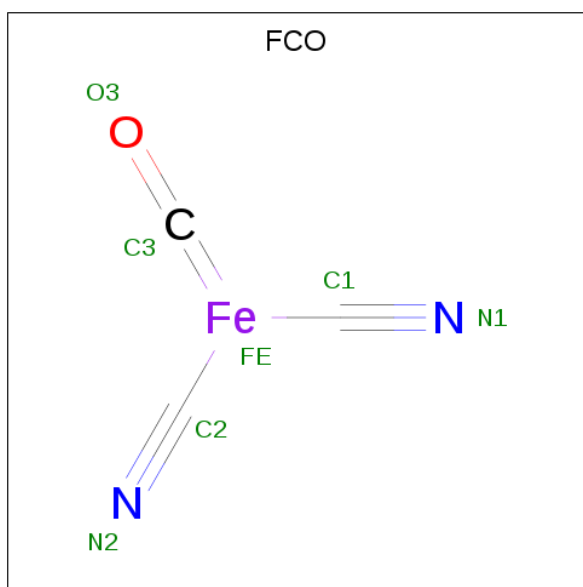
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			7	3	4		
5	T	1	Total	Fe	S	0	0
			7	3	4		
5	Q	1	Total	Fe	S	0	0
			7	3	4		
5	R	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is Fe₄S₄ (three-letter code: ER2) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	S	1	Total	Fe	S	0	0
			8	4	4		
6	T	1	Total	Fe	S	0	0
			8	4	4		
6	Q	1	Total	Fe	S	0	0
			8	4	4		
6	R	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C₃FeN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	1	Total	Ni	0	0
			1	1		
8	L	1	Total	Ni	0	0
			1	1		
8	K	1	Total	Ni	0	0
			1	1		
8	M	1	Total	Ni	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		

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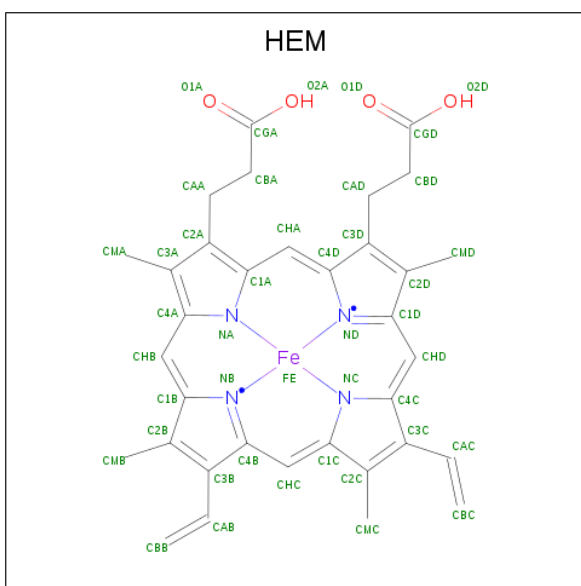
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total	Mg	0	0
			1	1		
9	K	1	Total	Mg	0	0
			1	1		
9	M	1	Total	Mg	0	0
			1	1		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	1	Total	Cl	0	0
			1	1		
10	L	1	Total	Cl	0	0
			1	1		
10	K	1	Total	Cl	0	0
			1	1		
10	M	1	Total	Cl	0	0
			1	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

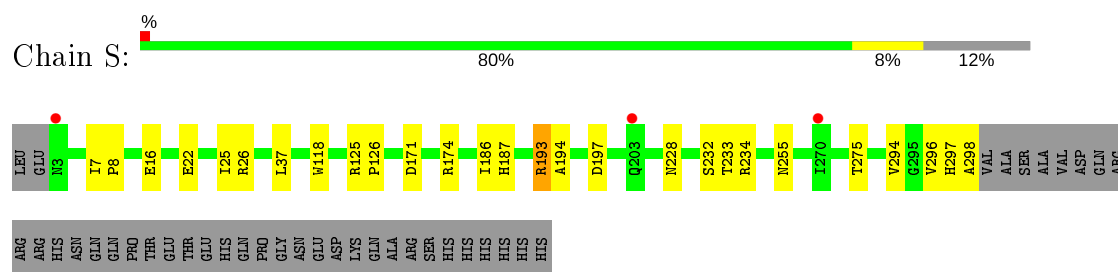
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	S	62	Total O 62 62	0	0
12	L	111	Total O 111 111	0	0
12	T	59	Total O 59 59	0	0
12	M	113	Total O 113 113	0	0
12	Q	62	Total O 62 62	0	0
12	J	112	Total O 112 112	0	0
12	R	63	Total O 63 63	0	0
12	K	108	Total O 108 108	0	0
12	A	6	Total O 6 6	0	0
12	B	6	Total O 6 6	0	0

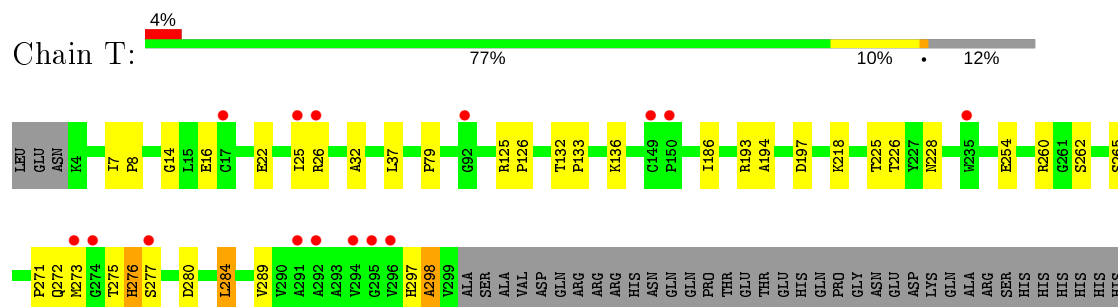
3 Residue-property plots [i](#)

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.

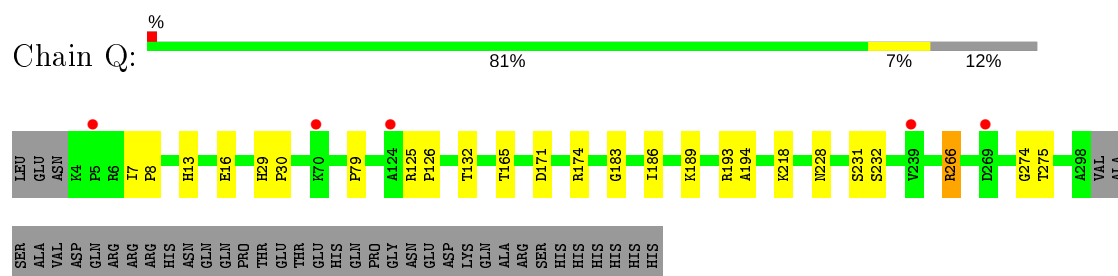
- Molecule 1: Hydrogenase-1 small chain



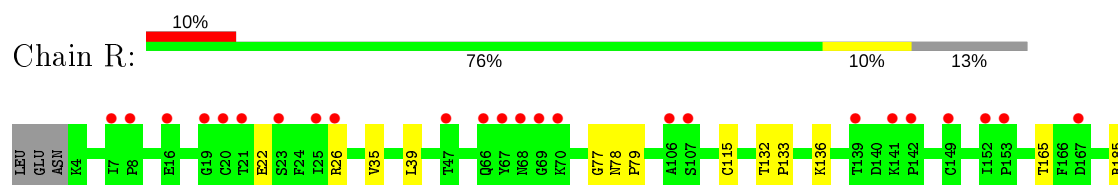
- Molecule 1: Hydrogenase-1 small chain

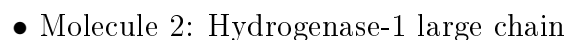
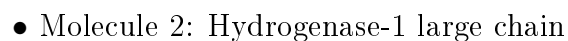
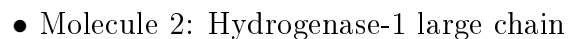


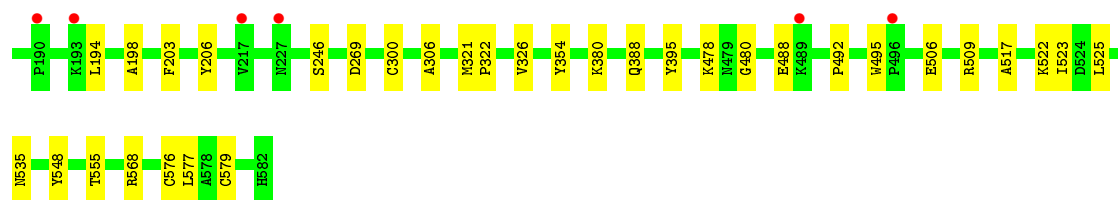
- Molecule 1: Hydrogenase-1 small chain



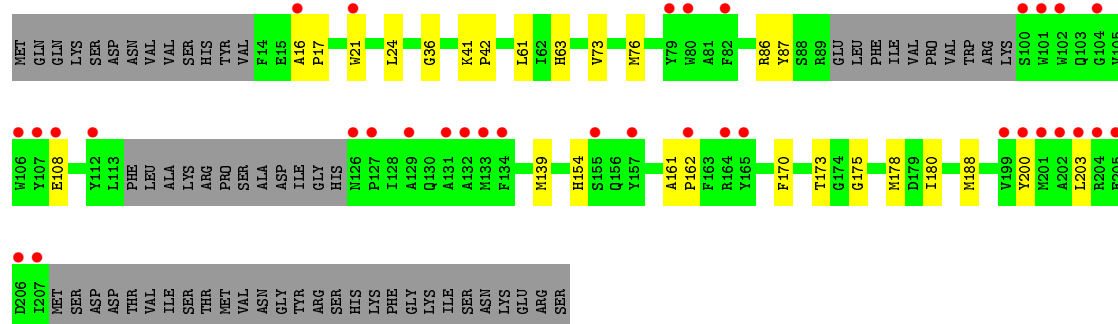
- Molecule 1: Hydrogenase-1 small chain



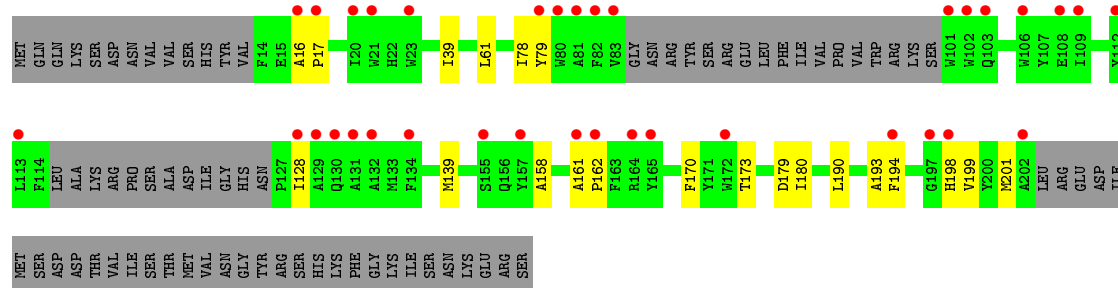




• Molecule 3: Probable Ni/Fe-hydrogenase 1 B-type cytochrome subunit



• Molecule 3: Probable Ni/Fe-hydrogenase 1 B-type cytochrome subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.41Å 165.03Å 206.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (25.00-2.50) 97.7 (49.67-2.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.222 , 0.253 0.223 , 0.254	Depositor DCC
R_{free} test set	7076 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30463	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, ER2, CL, SF4, F3S, HEM, FCO

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	Q	0.50	0/2292	0.57	0/3120
1	R	0.50	0/2260	0.59	0/3077
1	S	0.50	0/2300	0.61	0/3131
1	T	0.49	0/2278	0.60	0/3104
2	J	0.49	0/4647	0.58	1/6328 (0.0%)
2	K	0.48	0/4645	0.56	0/6327
2	L	0.51	0/4648	0.57	0/6332
2	M	0.48	0/4631	0.59	0/6308
3	A	0.59	0/1356	0.65	0/1848
3	B	0.55	0/1288	0.64	0/1753
All	All	0.50	0/30345	0.59	1/41328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	256	ARG	NE-CZ-NH2	-5.95	117.33	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2234	0	2164	20	0
1	R	2203	0	2121	22	0
1	S	2242	0	2170	18	0
1	T	2220	0	2129	28	0
2	J	4528	0	4390	34	0
2	K	4526	0	4379	31	0
2	L	4526	0	4376	33	0
2	M	4512	0	4371	38	0
3	A	1310	0	1188	21	0
3	B	1242	0	1141	14	0
4	Q	8	0	0	0	0
4	R	8	0	0	0	0
4	S	8	0	0	0	0
4	T	8	0	0	0	0
5	Q	7	0	0	0	0
5	R	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
6	Q	8	0	0	0	0
6	R	8	0	0	0	0
6	S	8	0	0	0	0
6	T	8	0	0	0	0
7	J	7	0	0	0	0
7	K	7	0	0	0	0
7	L	7	0	0	0	0
7	M	7	0	0	0	0
8	J	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
10	J	1	0	0	0	0
10	K	1	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	A	43	0	30	5	0
11	B	43	0	30	0	0
12	A	6	0	0	1	0
12	B	6	0	0	0	0
12	J	112	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	108	0	0	3	0
12	L	111	0	0	1	0
12	M	113	0	0	7	0
12	Q	62	0	0	1	0
12	R	63	0	0	0	0
12	S	62	0	0	1	0
12	T	59	0	0	0	0
All	All	30463	0	28489	231	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.

The worst 5 of 231 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)
3:B:78:ILE:HG13	3:B:79:TYR:H	1.21	1.02
3:B:78:ILE:HG13	3:B:79:TYR:N	1.77	0.95
2:J:3:THR:HB	12:J:717:HOH:O	1.70	0.91
3:A:16:ALA:HB1	3:A:17:PRO:HD2	1.65	0.79
1:T:260:ARG:HH21	3:A:175:GLY:HA2	1.54	0.72

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	Q	293/335 (88%)	280 (96%)	13 (4%)	0	100	100
1	R	289/335 (86%)	275 (95%)	13 (4%)	1 (0%)	41	61
1	S	294/335 (88%)	280 (95%)	14 (5%)	0	100	100
1	T	294/335 (88%)	279 (95%)	14 (5%)	1 (0%)	41	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	579/582 (100%)	558 (96%)	21 (4%)	0	100	100
2	K	579/582 (100%)	562 (97%)	17 (3%)	0	100	100
2	L	580/582 (100%)	564 (97%)	16 (3%)	0	100	100
2	M	579/582 (100%)	560 (97%)	18 (3%)	1 (0%)	47	68
3	A	166/235 (71%)	140 (84%)	24 (14%)	2 (1%)	13	24
3	B	154/235 (66%)	135 (88%)	15 (10%)	4 (3%)	5	8
All	All	3807/4138 (92%)	3633 (95%)	165 (4%)	9 (0%)	47	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	86	ARG
2	M	488	GLU
3	A	154	HIS
3	B	201	MET
1	R	272	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	235/273 (86%)	231 (98%)	4 (2%)	60	82
1	R	231/273 (85%)	228 (99%)	3 (1%)	69	87
1	S	236/273 (86%)	233 (99%)	3 (1%)	69	87
1	T	230/273 (84%)	227 (99%)	3 (1%)	69	87
2	J	474/481 (98%)	471 (99%)	3 (1%)	86	95
2	K	474/481 (98%)	472 (100%)	2 (0%)	91	97
2	L	475/481 (99%)	474 (100%)	1 (0%)	93	98
2	M	471/481 (98%)	467 (99%)	4 (1%)	81	93
3	A	114/203 (56%)	110 (96%)	4 (4%)	36	62
3	B	111/203 (55%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3051/3422 (89%)	3024 (99%)	27 (1%)	78 92

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	232	SER
2	J	269	ASP
3	A	108	GLU
1	Q	266	ARG
1	T	276	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	244	GLN
2	K	446	GLN
2	J	457	HIS
1	T	297	HIS
2	J	446	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 ⓘ

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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
11	HEM	A	301	3	27,50,50	1.17	3 (11%)	17,82,82	1.29	2 (11%)
5	F3S	R	402	1	0,9,9	0.00	-	-		
5	F3S	T	402	1	0,9,9	0.00	-	-		
6	ER2	R	403	1	0,11,11	0.00	-	-		
7	FCO	J	601	12,2	0,6,6	0.00	-	-		
7	FCO	L	601	12,2	0,6,6	0.00	-	-		
6	ER2	Q	403	1	0,11,11	0.00	-	-		
4	SF4	S	401	1	0,12,12	0.00	-	-		
11	HEM	B	301	3	27,50,50	1.09	2 (7%)	17,82,82	1.86	5 (29%)
5	F3S	Q	402	1	0,9,9	0.00	-	-		
6	ER2	T	403	1	0,11,11	0.00	-	-		
5	F3S	S	402	1	0,9,9	0.00	-	-		
7	FCO	K	601	12,2	0,6,6	0.00	-	-		
7	FCO	M	601	12,2	0,6,6	0.00	-	-		
4	SF4	T	401	1	0,12,12	0.00	-	-		
4	SF4	Q	401	1	0,12,12	0.00	-	-		
4	SF4	R	401	1	0,12,12	0.00	-	-		
6	ER2	S	403	1	0,11,11	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
11	HEM	A	301	3	-	2/6/54/54	-
5	F3S	R	402	1	-	-	0/3/3/3
5	F3S	T	402	1	-	-	0/3/3/3
6	ER2	R	403	1	-	-	0/4/4/4
6	ER2	Q	403	1	-	-	0/4/4/4
4	SF4	S	401	1	-	-	0/6/5/5
11	HEM	B	301	3	-	2/6/54/54	-
5	F3S	Q	402	1	-	-	0/3/3/3
6	ER2	T	403	1	-	-	0/4/4/4
5	F3S	S	402	1	-	-	0/3/3/3
4	SF4	T	401	1	-	-	0/6/5/5
4	SF4	Q	401	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	R	401	1	-	-	0/6/5/5
6	ER2	S	403	1	-	-	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	301	HEM	C3B-C2B	-3.29	1.35	1.40
11	B	301	HEM	C3C-C2C	-2.90	1.36	1.40
11	A	301	HEM	C3C-C2C	-2.57	1.36	1.40
11	B	301	HEM	C3B-C2B	-2.52	1.36	1.40
11	A	301	HEM	C4D-C3D	2.18	1.47	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	301	HEM	CMD-C2D-C1D	-3.22	123.52	128.46
11	B	301	HEM	CMD-C2D-C3D	3.00	130.59	124.94
11	B	301	HEM	CAD-CBD-CGD	2.95	117.61	112.67
11	A	301	HEM	CMD-C2D-C1D	-2.61	124.45	128.46
11	A	301	HEM	CMD-C2D-C3D	2.51	129.67	124.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	301	HEM	C2D-C3D-CAD-CBD
11	A	301	HEM	C4D-C3D-CAD-CBD
11	B	301	HEM	C2D-C3D-CAD-CBD
11	B	301	HEM	C4D-C3D-CAD-CBD

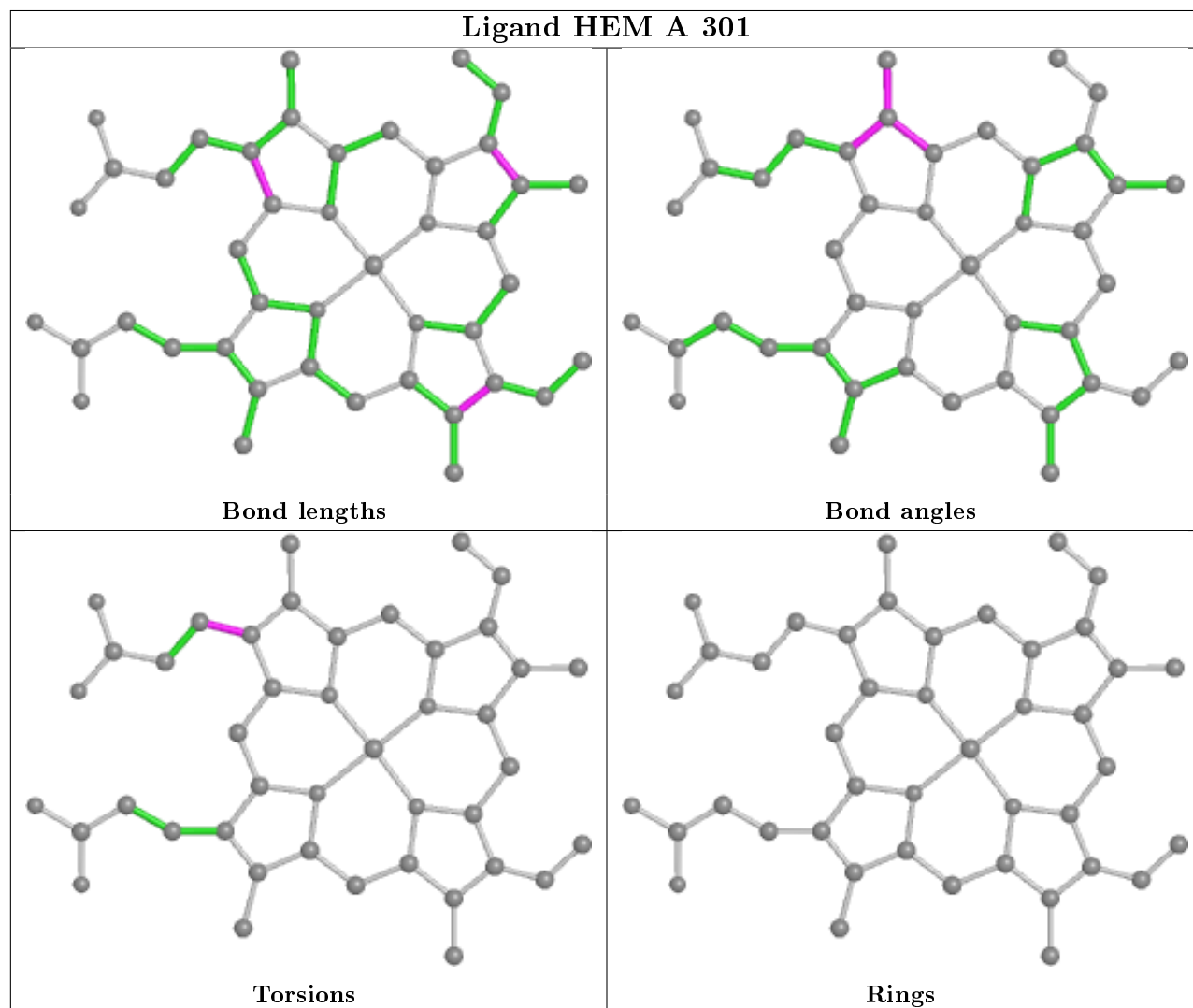
There are no ring outliers.

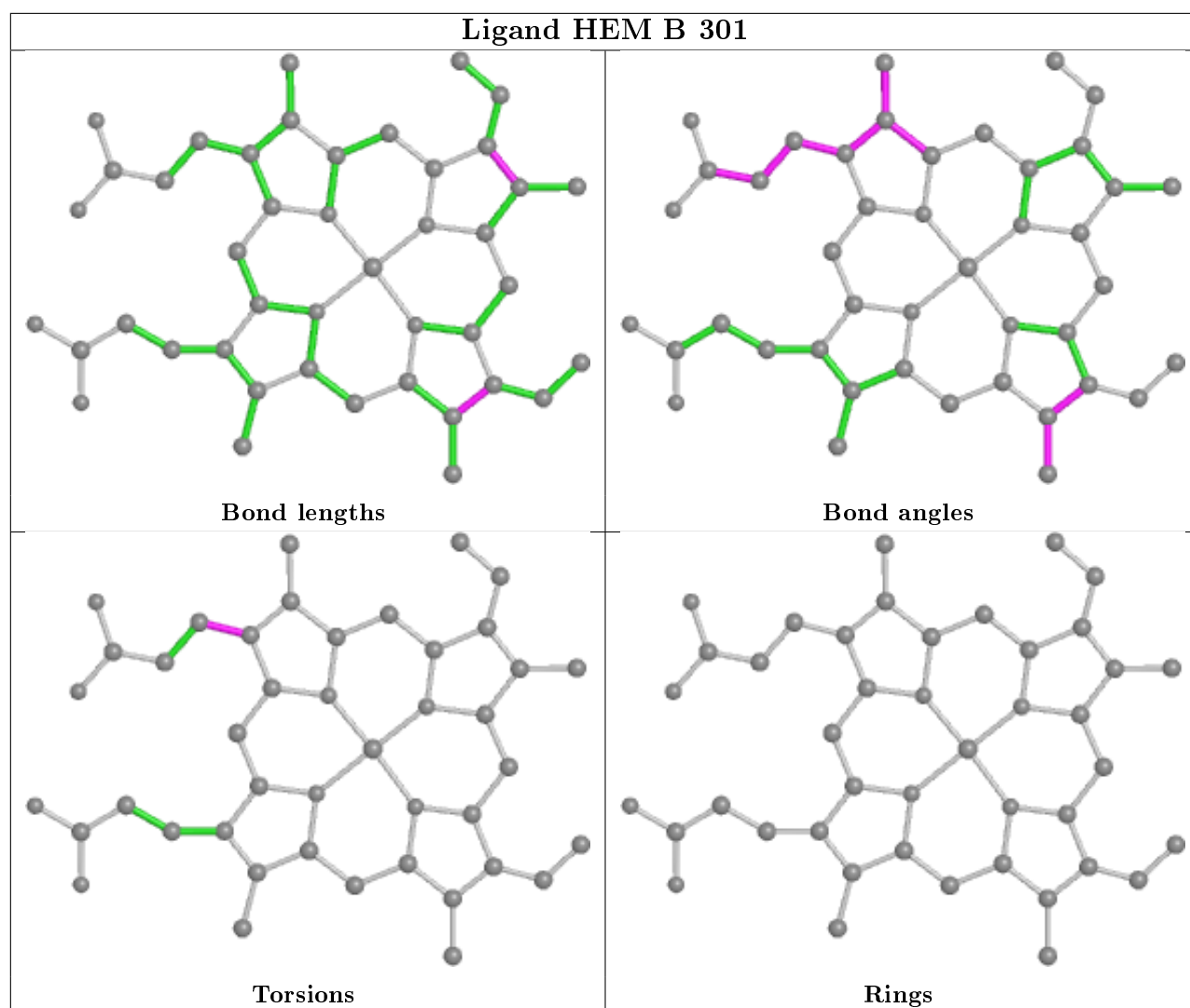
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	301	HEM	5	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	Q	295/335 (88%)	-0.08	5 (1%) 70 72	38, 48, 64, 87	0
1	R	291/335 (86%)	0.46	32 (10%) 5 5	38, 52, 73, 101	0
1	S	296/335 (88%)	-0.18	3 (1%) 82 84	33, 43, 62, 87	0
1	T	296/335 (88%)	0.26	15 (5%) 28 29	35, 51, 76, 117	0
2	J	581/582 (99%)	0.01	3 (0%) 91 91	40, 52, 66, 78	0
2	K	581/582 (99%)	0.04	19 (3%) 46 50	37, 49, 65, 85	0
2	L	581/582 (99%)	-0.09	6 (1%) 82 84	34, 46, 59, 76	0
2	M	581/582 (99%)	0.19	23 (3%) 38 41	36, 52, 70, 85	0
3	A	172/235 (73%)	0.69	34 (19%) 1 1	40, 61, 102, 112	0
3	B	160/235 (68%)	0.78	35 (21%) 0 0	45, 62, 106, 132	0
All	All	3834/4138 (92%)	0.12	175 (4%) 32 34	33, 50, 73, 132	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	155	SER	6.5
1	R	7	ILE	6.0
3	A	201	MET	5.9
3	B	109	ILE	5.6
3	B	102	TRP	5.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

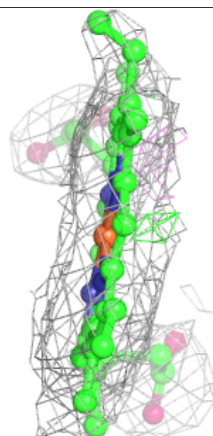
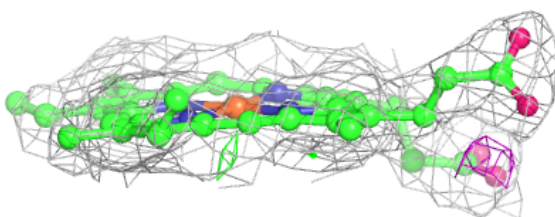
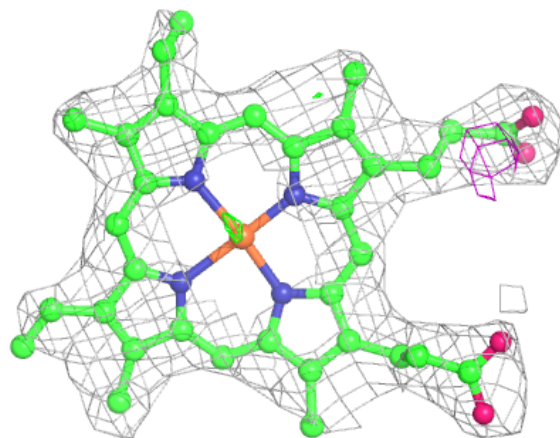
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	CL	J	604	1/1	0.64	0.27	43,43,43,43	1
10	CL	K	604	1/1	0.77	0.27	43,43,43,43	1
10	CL	M	604	1/1	0.90	0.30	35,35,35,35	1
10	CL	L	604	1/1	0.90	0.27	41,41,41,41	1
9	MG	L	603	1/1	0.93	0.06	42,42,42,42	0
9	MG	M	603	1/1	0.94	0.08	50,50,50,50	0
11	HEM	A	301	43/43	0.97	0.12	47,50,54,59	0
11	HEM	B	301	43/43	0.97	0.11	43,48,54,57	0
9	MG	K	603	1/1	0.97	0.10	45,45,45,45	0
9	MG	J	603	1/1	0.97	0.05	44,44,44,44	0
5	F3S	T	402	7/7	0.98	0.13	40,41,44,47	0
6	ER2	S	403	8/8	0.98	0.08	39,40,42,45	0
6	ER2	R	403	8/8	0.98	0.17	44,47,51,52	0
7	FCO	J	601	7/7	0.98	0.15	41,41,49,53	0
8	NI	K	602	1/1	0.98	0.08	43,43,43,43	0
5	F3S	S	402	7/7	0.98	0.08	38,40,40,45	0
8	NI	J	602	1/1	0.99	0.09	43,43,43,43	0
5	F3S	Q	402	7/7	0.99	0.07	39,40,41,42	0
6	ER2	T	403	8/8	0.99	0.17	42,43,47,49	0
4	SF4	T	401	8/8	0.99	0.12	39,40,41,45	0
5	F3S	R	402	7/7	0.99	0.14	39,41,42,42	0
6	ER2	Q	403	8/8	0.99	0.10	41,44,49,50	0
8	NI	M	602	1/1	0.99	0.09	44,44,44,44	0
7	FCO	K	601	7/7	0.99	0.09	39,41,45,46	0
7	FCO	M	601	7/7	0.99	0.13	42,45,49,49	0
4	SF4	Q	401	8/8	0.99	0.08	41,44,46,48	0
7	FCO	L	601	7/7	0.99	0.14	39,39,46,50	0
4	SF4	S	401	8/8	0.99	0.09	39,40,41,41	0
8	NI	L	602	1/1	0.99	0.12	39,39,39,39	0
4	SF4	R	401	8/8	0.99	0.10	40,42,44,45	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.

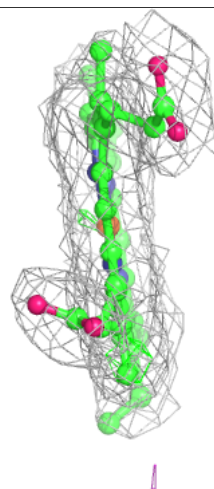
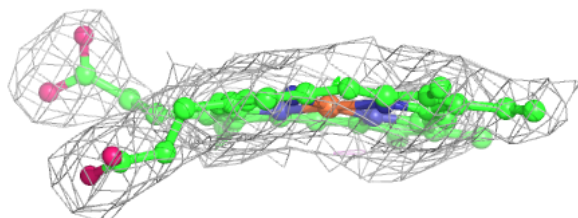
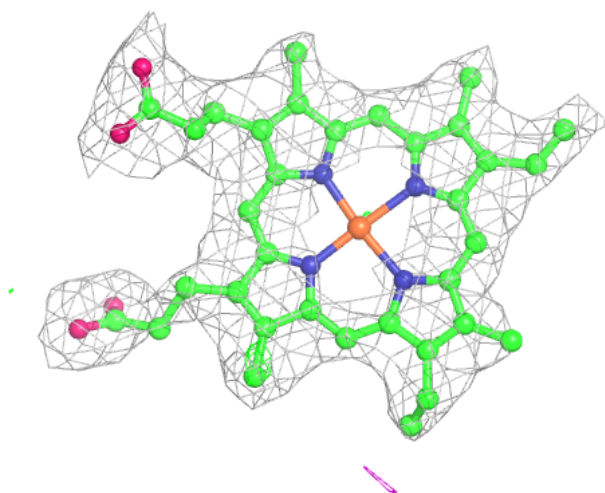
Electron density around HEM A 301:

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



Electron density around HEM B 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.