



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:24 pm BST

PDB ID : 4GD3
Title : Structure of E. coli hydrogenase-1 in complex with cytochrome b
Authors : Volbeda, A.; Fontecilla-Camps, J.C.; Darnault, C.
Deposited on : 2012-07-31
Resolution : 3.30 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

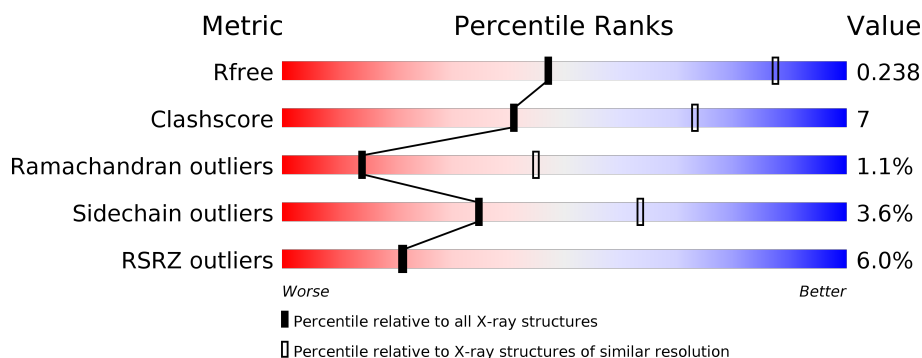
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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>3%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	R	335	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	S	335	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	T	335	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>
2	J	582	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>•</div> </div> </div>
2	K	582	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	L	582	
2	M	582	
3	A	235	
3	B	235	

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	SF4	Q	401	-	-	X	-
6	CL	K	601	-	-	X	-
6	CL	K	605	-	-	X	-
6	CL	M	601	-	-	X	-
6	CL	M	605	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 31252 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	304	Total	C	N	O	S	0	7	0
			2329	1477	400	430	22			
1	T	300	Total	C	N	O	S	0	4	0
			2283	1445	393	423	22			
1	Q	304	Total	C	N	O	S	0	7	0
			2329	1477	400	430	22			
1	R	300	Total	C	N	O	S	0	4	0
			2283	1445	393	423	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	242	CYS	PRO	ENGINEERED MUTATION	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	242	CYS	PRO	ENGINEERED MUTATION	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	242	CYS	PRO	ENGINEERED MUTATION	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	242	CYS	PRO	ENGINEERED MUTATION	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

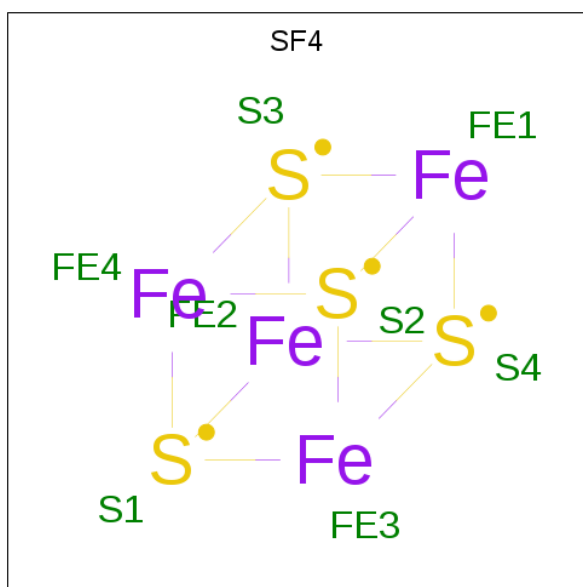
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	33	0
			4733	3011	822	871	29			
2	M	581	Total	C	N	O	S	0	35	0
			4743	3020	825	869	29			
2	J	581	Total	C	N	O	S	0	33	0
			4733	3011	822	871	29			
2	K	581	Total	C	N	O	S	0	35	0
			4743	3020	825	869	29			

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

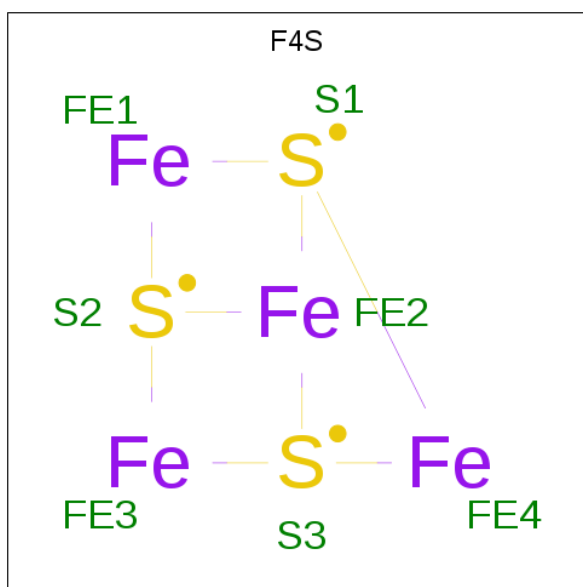
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			
3	B	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			

- 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	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	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	Q	1	Total	Fe	S	0	0
			8	4	4		
4	R	1	Total	Fe	S	0	0
			8	4	4		
4	R	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: F4S) (formula: Fe₄S₃).

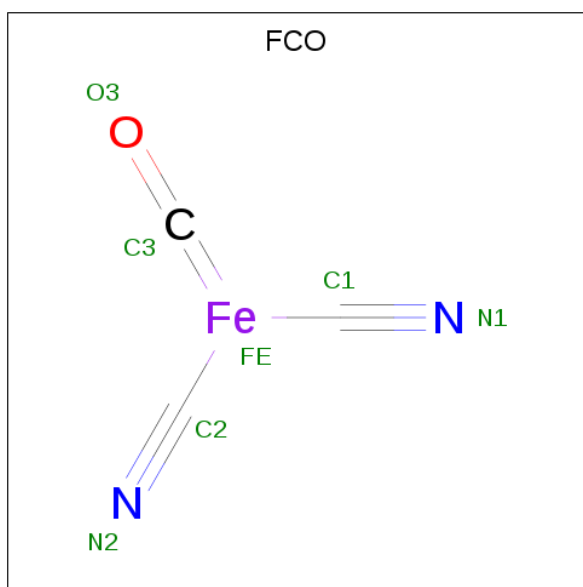


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			7	4	3		
5	T	1	Total	Fe	S	0	0
			7	4	3		
5	Q	1	Total	Fe	S	0	0
			7	4	3		
5	R	1	Total	Fe	S	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Cl	0	0
			1	1		
6	Q	2	Total	Cl	0	0
			2	2		
6	K	2	Total	Cl	0	0
			2	2		
6	L	1	Total	Cl	0	0
			1	1		
6	S	2	Total	Cl	0	0
			2	2		
6	M	2	Total	Cl	0	0
			2	2		

- 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).

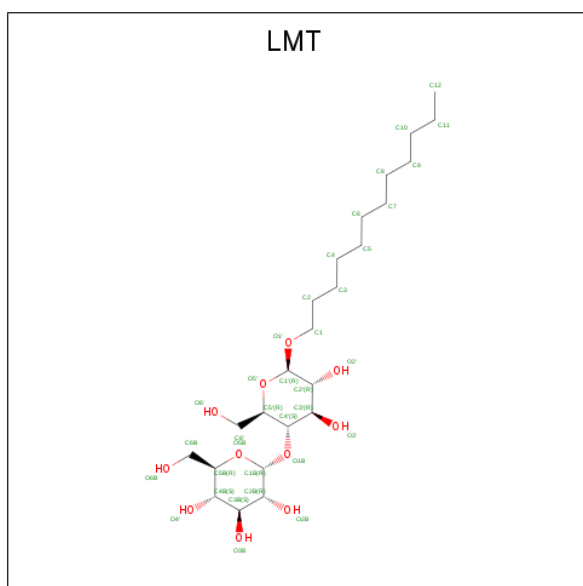
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		

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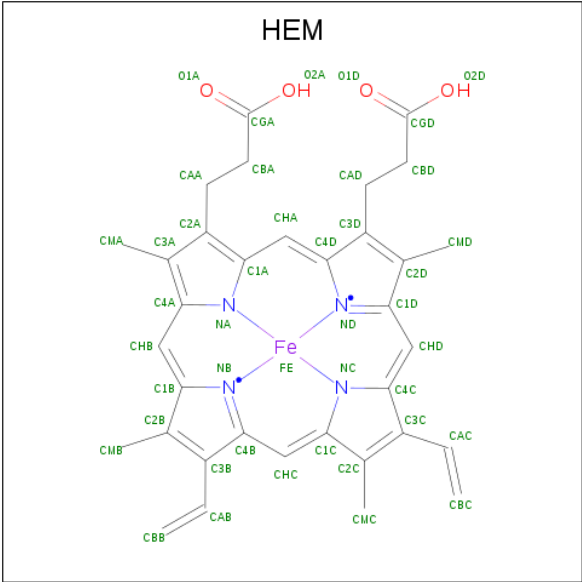
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total	Mg	0	0
			1	1		
9	K	1	Total	Mg	0	0
			1	1		
9	M	1	Total	Mg	0	0
			1	1		

- Molecule 10 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	T	1	Total	C	O	0	0
			23	12	11		
10	R	1	Total	C	O	0	0
			23	12	11		
10	A	1	Total	C	O	0	0
			23	12	11		
10	B	1	Total	C	O	0	0
			23	12	11		

- 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

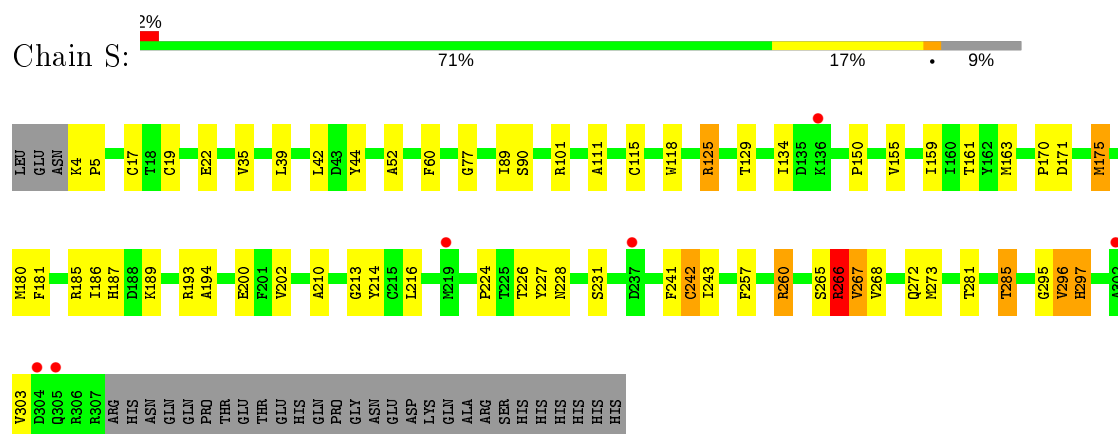
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	S	5	Total	O	0	0
			5	5		
12	L	4	Total	O	0	0
			4	4		
12	T	3	Total	O	0	0
			3	3		
12	M	8	Total	O	0	0
			8	8		
12	Q	5	Total	O	0	0
			5	5		
12	J	4	Total	O	0	0
			4	4		
12	R	2	Total	O	0	0
			2	2		
12	K	9	Total	O	0	0
			9	9		

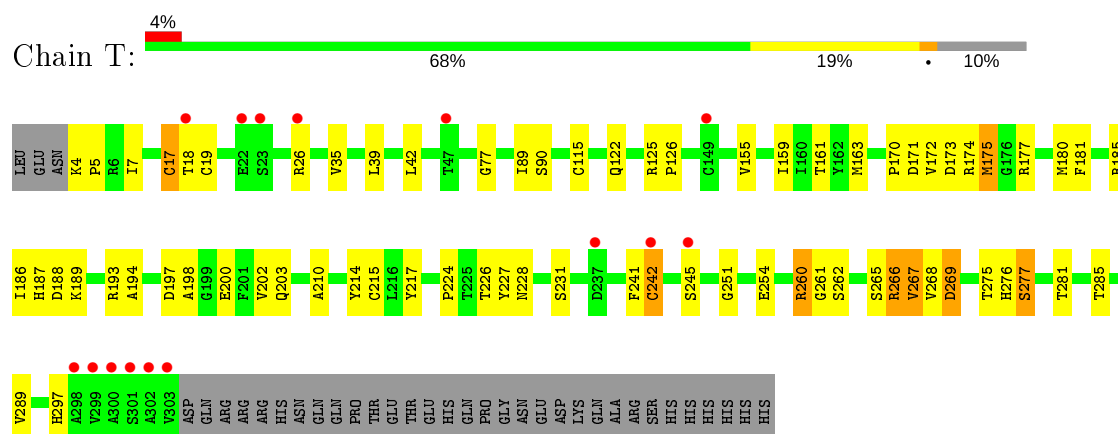
3 Residue-property plots [i](#)

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.

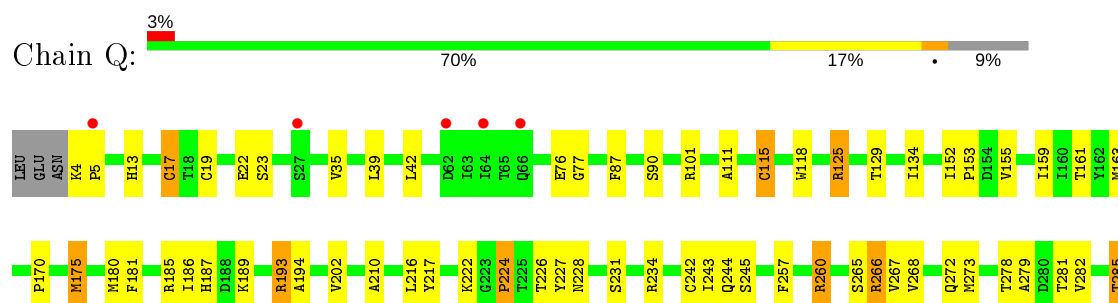
- Molecule 1: Hydrogenase-1 small chain

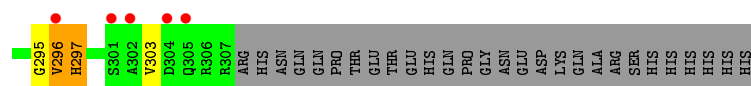


- Molecule 1: Hydrogenase-1 small chain

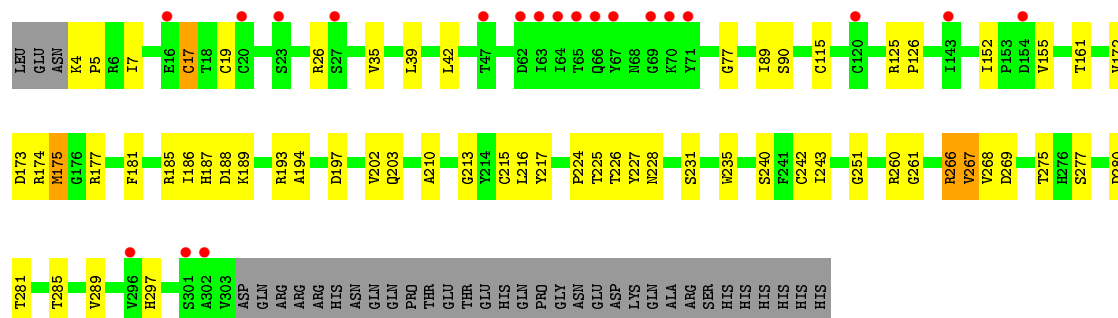
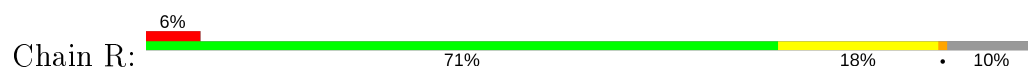


- Molecule 1: Hydrogenase-1 small chain

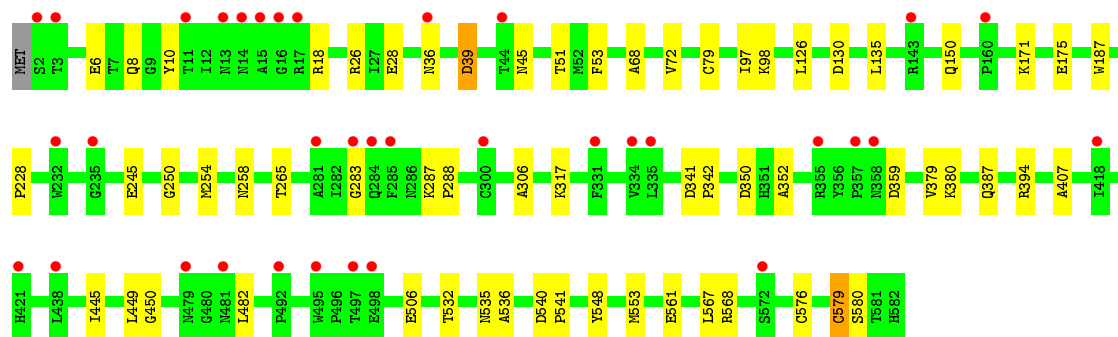
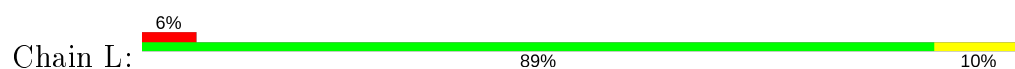




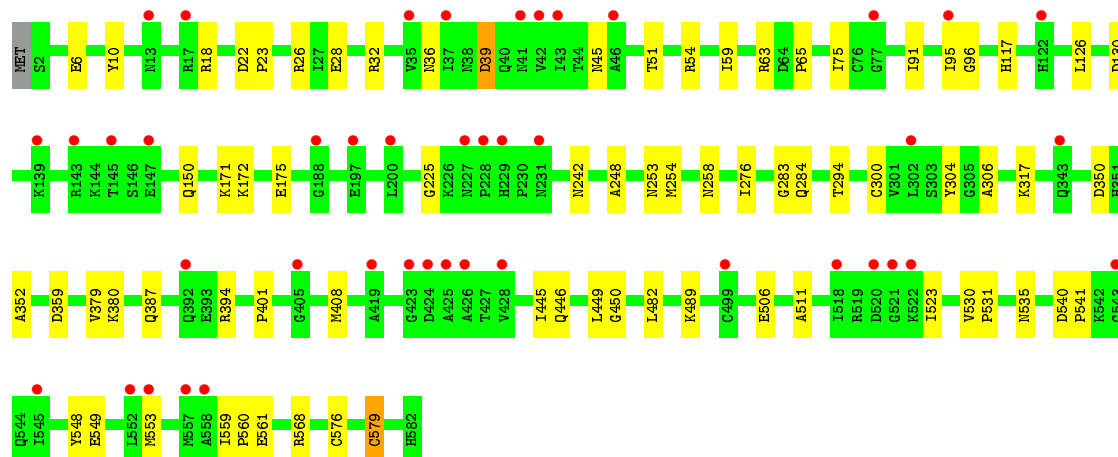
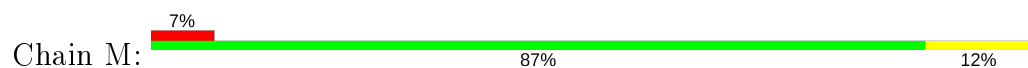
• Molecule 1: Hydrogenase-1 small chain



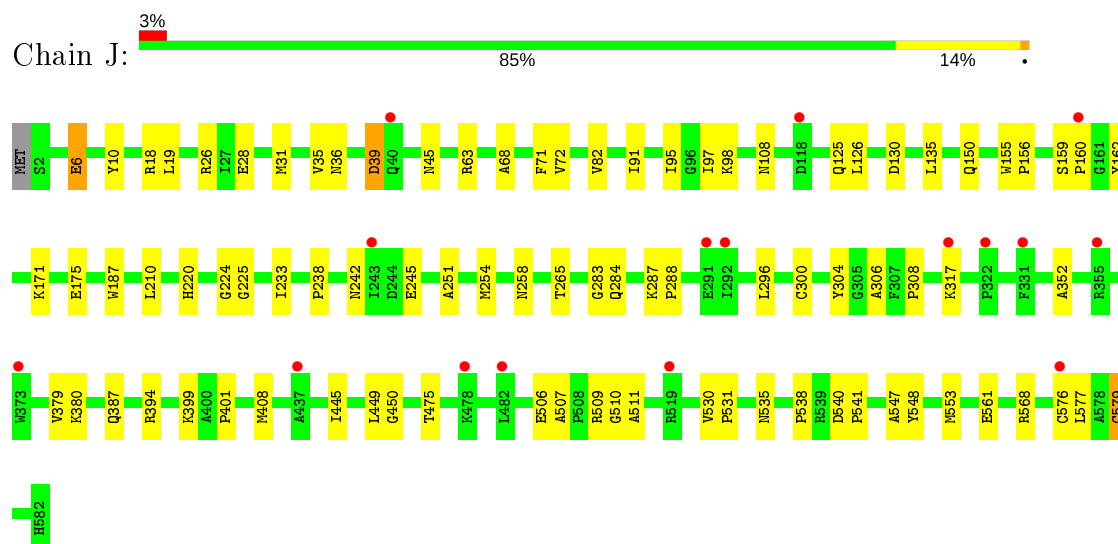
• Molecule 2: Hydrogenase-1 large chain



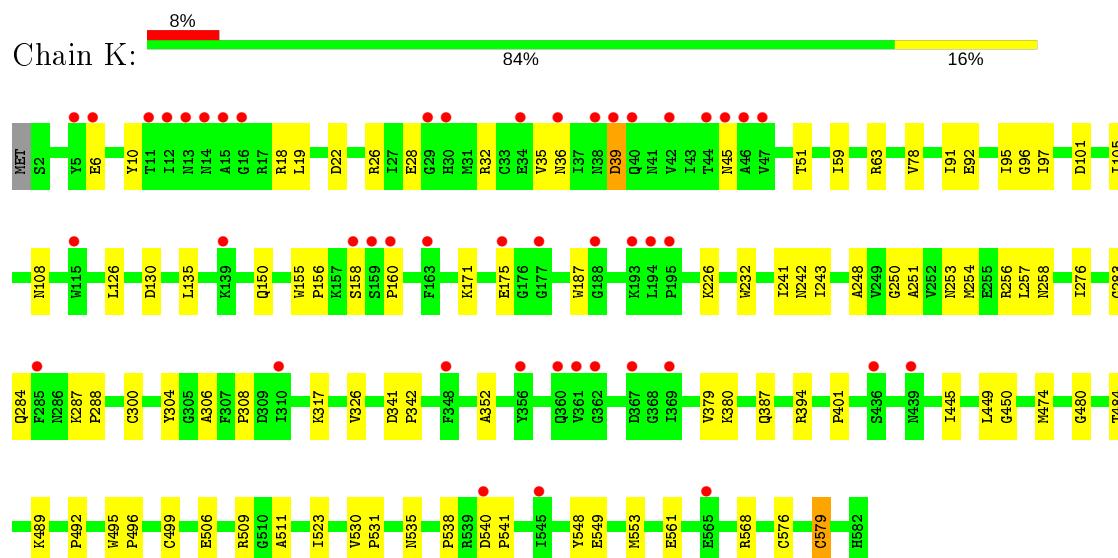
• Molecule 2: Hydrogenase-1 large chain



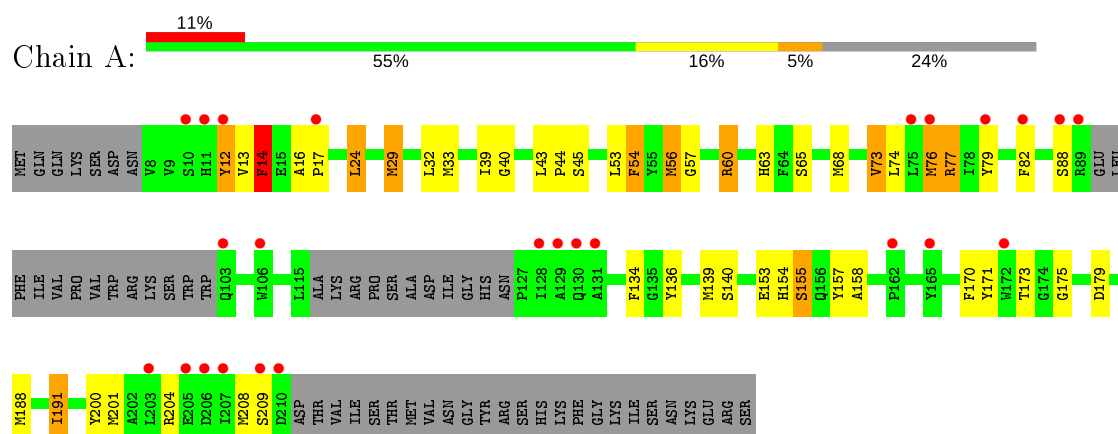
- Molecule 2: Hydrogenase-1 large chain



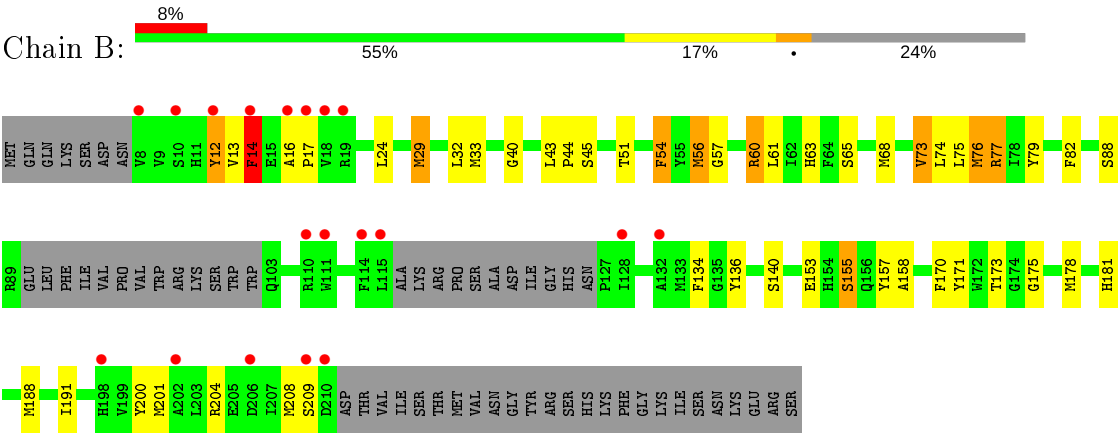
- Molecule 2: Hydrogenase-1 large chain



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



● Molecule 3: 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	126.00 Å 165.30 Å 212.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 49.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-3.30) 99.2 (49.12-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.236 0.205 , 0.238	Depositor DCC
R_{free} test set	3633 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31252	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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, CL, SF4, LMT, F4S, 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	0.55	1/2407 (0.0%)	0.65	0/3275
1	R	0.51	0/2352	0.59	0/3200
1	S	0.50	0/2407	0.62	0/3275
1	T	0.51	0/2352	0.60	0/3200
2	J	0.46	0/4940	0.56	0/6715
2	K	0.45	0/4956	0.55	0/6736
2	L	0.43	0/4940	0.55	0/6715
2	M	0.45	0/4956	0.56	0/6736
3	A	0.55	2/1406 (0.1%)	0.63	1/1916 (0.1%)
3	B	0.56	1/1406 (0.1%)	0.63	1/1916 (0.1%)
All	All	0.48	4/32122 (0.0%)	0.58	2/43684 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	TYR	CA-C	-5.87	1.37	1.52
3	A	201	MET	C-N	-5.61	1.21	1.34
3	A	200	TYR	CA-C	-5.42	1.38	1.52
1	Q	115	CYS	CB-SG	-5.26	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	MET	C-N-CA	5.47	135.36	121.70
3	B	201	MET	C-N-CA	5.29	134.93	121.70

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	Q	2329	0	2277	49	0
1	R	2283	0	2218	45	0
1	S	2329	0	2277	47	0
1	T	2283	0	2218	50	0
2	J	4733	0	4675	57	0
2	K	4743	0	4697	73	0
2	L	4733	0	4675	41	0
2	M	4743	0	4697	54	0
3	A	1360	0	1246	30	0
3	B	1360	0	1246	33	0
4	Q	16	0	0	3	0
4	R	16	0	0	1	0
4	S	16	0	0	2	0
4	T	16	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	J	1	0	0	0	0
6	K	2	0	0	4	0
6	L	1	0	0	0	0
6	M	2	0	0	4	0
6	Q	2	0	0	0	0
6	S	2	0	0	0	0
7	J	7	0	0	0	0
7	K	7	0	0	1	0
7	L	7	0	0	1	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	A	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	23	0	21	0	0
10	R	23	0	21	1	0
10	T	23	0	21	1	0
11	A	43	0	30	4	0
11	B	43	0	30	3	0
12	J	4	0	0	0	0
12	K	9	0	0	0	0
12	L	4	0	0	0	0
12	M	8	0	0	0	0
12	Q	5	0	0	0	0
12	R	2	0	0	0	0
12	S	5	0	0	0	0
12	T	3	0	0	0	0
All	All	31252	0	30370	436	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 7.

The worst 5 of 436 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:T:261:GLY:HA3	1:T:268:VAL:HB	1.33	1.11
1:S:101[B]:ARG:CG	1:S:101[B]:ARG:HH11	1.64	1.09
1:R:261:GLY:HA3	1:R:268:VAL:HB	1.38	1.05
1:Q:101[B]:ARG:HH11	1:Q:101[B]:ARG:CG	1.66	1.03
1:S:101[B]:ARG:HG2	1:S:101[B]:ARG:HH11	1.31	0.95

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	309/335 (92%)	282 (91%)	20 (6%)	7 (2%)	6	29
1	R	302/335 (90%)	282 (93%)	14 (5%)	6 (2%)	7	32
1	S	309/335 (92%)	283 (92%)	19 (6%)	7 (2%)	6	29
1	T	302/335 (90%)	279 (92%)	17 (6%)	6 (2%)	7	32
2	J	612/582 (105%)	571 (93%)	39 (6%)	2 (0%)	41	71
2	K	614/582 (106%)	578 (94%)	35 (6%)	1 (0%)	47	77
2	L	612/582 (105%)	567 (93%)	44 (7%)	1 (0%)	47	77
2	M	614/582 (106%)	572 (93%)	42 (7%)	0	100	100
3	A	173/235 (74%)	147 (85%)	19 (11%)	7 (4%)	3	18
3	B	173/235 (74%)	147 (85%)	20 (12%)	6 (4%)	3	21
All	All	4020/4138 (97%)	3708 (92%)	269 (7%)	43 (1%)	14	45

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	267	VAL
1	S	296	VAL
1	S	297	HIS
1	S	303	VAL
1	T	277	SER

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	247/274 (90%)	233 (94%)	14 (6%)	20	51
1	R	241/274 (88%)	234 (97%)	7 (3%)	42	69
1	S	247/274 (90%)	236 (96%)	11 (4%)	27	58
1	T	241/274 (88%)	233 (97%)	8 (3%)	38	66
2	J	512/481 (106%)	501 (98%)	11 (2%)	53	75
2	K	513/481 (107%)	507 (99%)	6 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	512/481 (106%)	501 (98%)	11 (2%)	53	75
2	M	513/481 (107%)	506 (99%)	7 (1%)	67	82
3	A	123/203 (61%)	102 (83%)	21 (17%)	2	9
3	B	123/203 (61%)	102 (83%)	21 (17%)	2	9
All	All	3272/3426 (96%)	3155 (96%)	117 (4%)	35	63

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	39	ASP
1	R	260	ARG
3	B	77	ARG
2	J	245[A]	GLU
2	J	561[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	406	ASN
2	J	61	GLN
2	K	406	ASN
1	Q	244	GLN
2	J	108	ASN

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 40 ligands modelled in this entry, 18 are monoatomic - leaving 22 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	$\# Z > 2$
5	F4S	Q	403	1	0,9,9	0.00	-	-		
7	FCO	J	601	2	0,6,6	0.00	-	-		
7	FCO	M	602	2	0,6,6	0.00	-	-		
5	F4S	R	403	1	0,9,9	0.00	-	-		
4	SF4	T	401	1	0,12,12	0.00	-	-		
4	SF4	T	402	1	0,12,12	0.00	-	-		
5	F4S	S	403	1	0,9,9	0.00	-	-		
7	FCO	L	601	2	0,6,6	0.00	-	-		
4	SF4	S	402	1	0,12,12	0.00	-	-		
4	SF4	Q	402	1	0,12,12	0.00	-	-		
10	LMT	A	302	-	24,24,36	0.56	0	35,35,47	0.92	1 (2%)
10	LMT	R	404	-	24,24,36	0.59	0	35,35,47	1.14	3 (8%)
4	SF4	Q	401	1	0,12,12	0.00	-	-		
5	F4S	T	403	1	0,9,9	0.00	-	-		
10	LMT	B	302	-	24,24,36	0.43	0	35,35,47	0.88	2 (5%)
10	LMT	T	404	-	24,24,36	0.53	0	35,35,47	1.23	3 (8%)
4	SF4	R	401	1	0,12,12	0.00	-	-		
11	HEM	A	301	3	27,50,50	2.18	5 (18%)	17,82,82	1.50	1 (5%)
7	FCO	K	602	2	0,6,6	0.00	-	-		
11	HEM	B	301	3	27,50,50	2.18	6 (22%)	17,82,82	1.43	1 (5%)
4	SF4	R	402	1	0,12,12	0.00	-	-		
4	SF4	S	401	1	0,12,12	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
5	F4S	Q	403	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F4S	R	403	1	-	-	0/3/3/3
10	LMT	R	404	-	-	2/8/48/61	0/2/2/2
5	F4S	S	403	1	-	-	0/3/3/3
4	SF4	S	402	1	-	-	0/6/5/5
4	SF4	R	401	1	-	-	0/6/5/5
4	SF4	Q	401	1	-	-	0/6/5/5
5	F4S	T	403	1	-	-	0/3/3/3
4	SF4	T	402	1	-	-	0/6/5/5
11	HEM	B	301	3	-	0/6/54/54	-
10	LMT	A	302	-	-	2/8/48/61	0/2/2/2
10	LMT	B	302	-	-	2/8/48/61	0/2/2/2
4	SF4	T	401	1	-	-	0/6/5/5
4	SF4	R	402	1	-	-	0/6/5/5
10	LMT	T	404	-	-	2/8/48/61	0/2/2/2
4	SF4	S	401	1	-	-	0/6/5/5
11	HEM	A	301	3	-	0/6/54/54	-
4	SF4	Q	402	1	-	-	0/6/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	301	HEM	C3D-C2D	5.60	1.54	1.37
11	B	301	HEM	C3D-C2D	5.15	1.52	1.37
11	B	301	HEM	C3B-C2B	-5.02	1.33	1.40
11	A	301	HEM	C3B-C2B	-4.35	1.34	1.40
11	B	301	HEM	C3C-C2C	-4.25	1.34	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	301	HEM	CAA-CBA-CGA	-4.31	105.45	112.67
11	B	301	HEM	CAA-CBA-CGA	-4.16	105.69	112.67
10	A	302	LMT	O5'-C1'-C2'	-3.24	104.51	110.28
10	B	302	LMT	O5'-C1'-C2'	-2.90	105.10	110.28
10	T	404	LMT	C3B-C4B-C5B	-2.82	105.21	110.24

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	302	LMT	O5B-C5B-C6B-O6B

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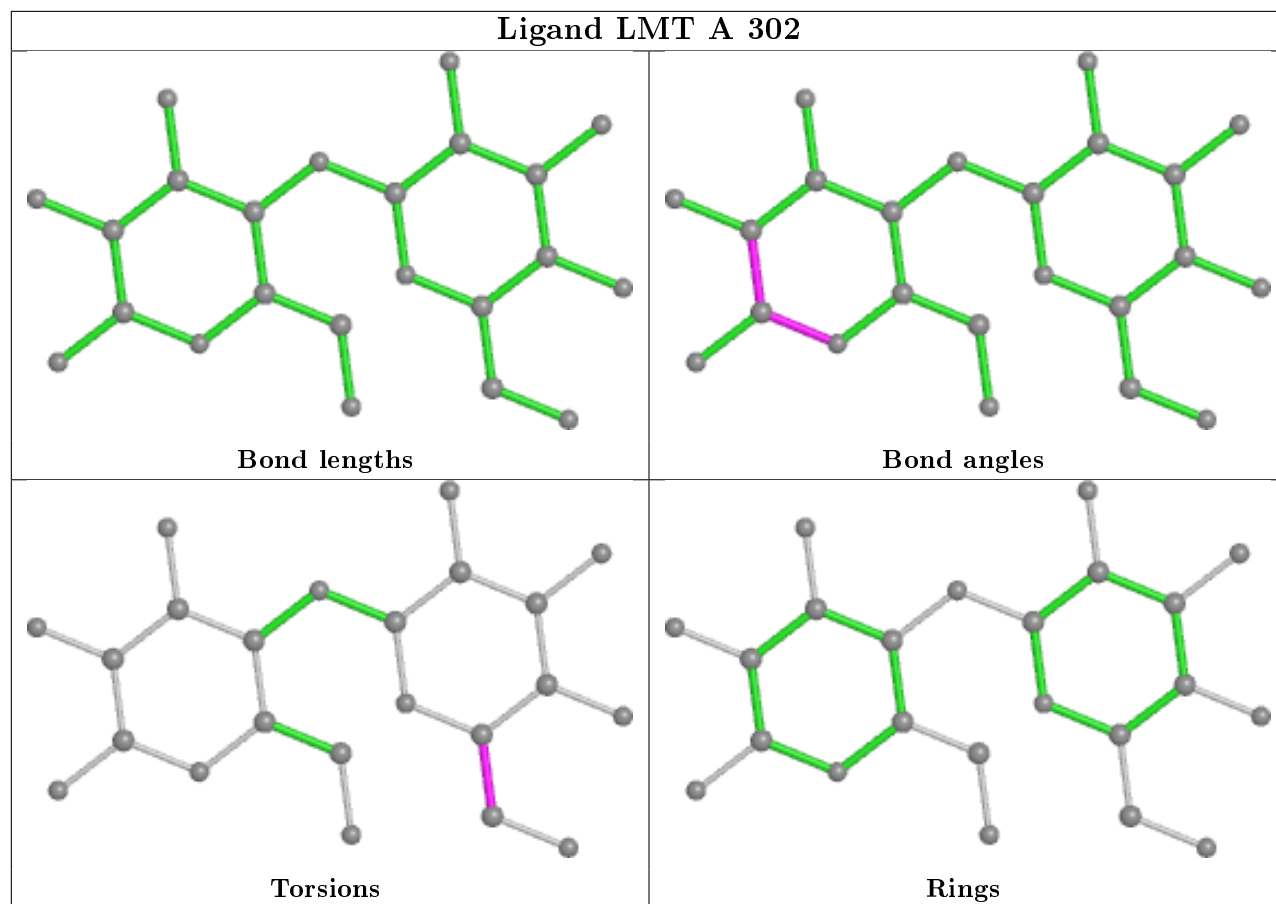
Mol	Chain	Res	Type	Atoms
10	B	302	LMT	O5B-C5B-C6B-O6B
10	A	302	LMT	C4B-C5B-C6B-O6B
10	B	302	LMT	C4B-C5B-C6B-O6B
10	T	404	LMT	C4'-C5'-C6'-O6'

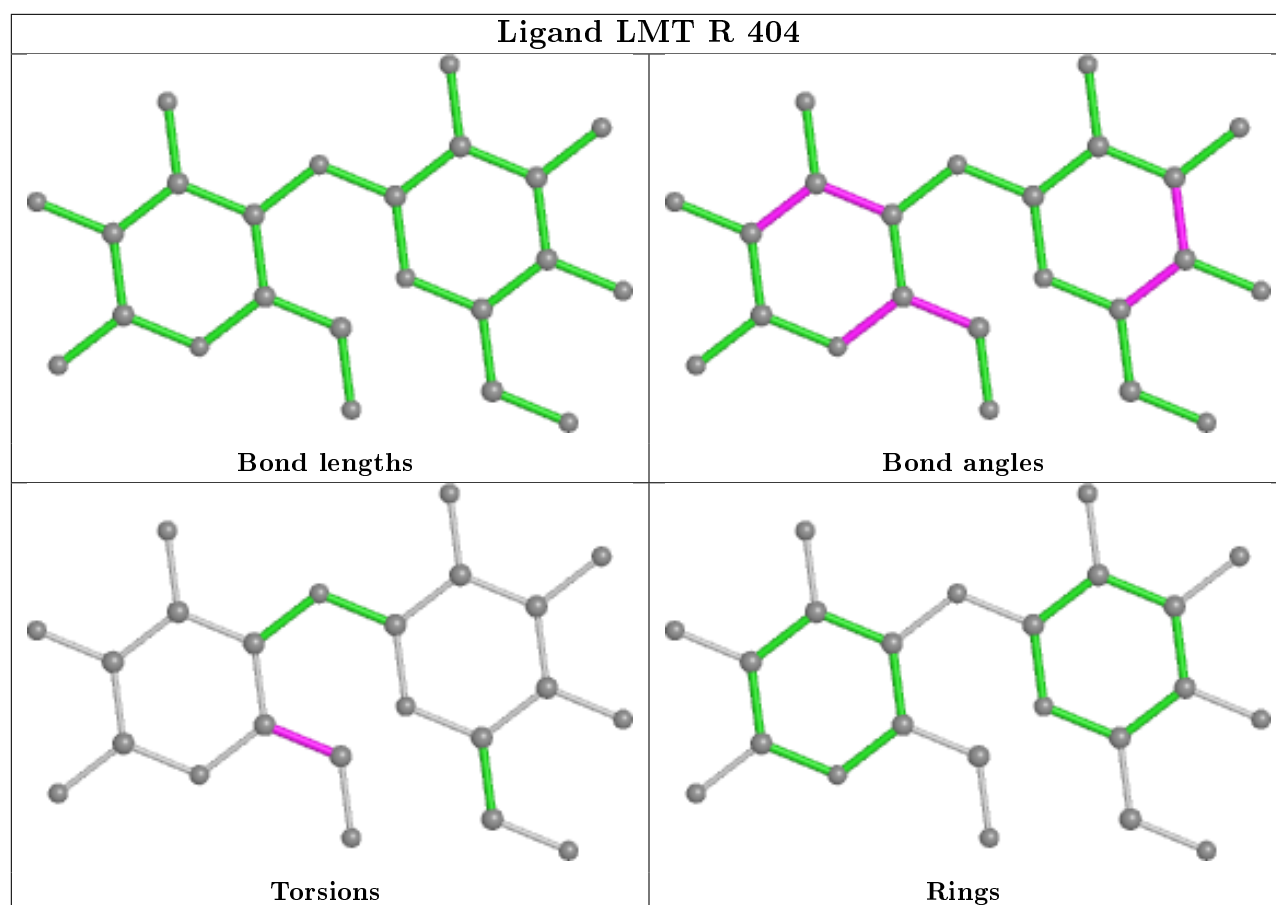
There are no ring outliers.

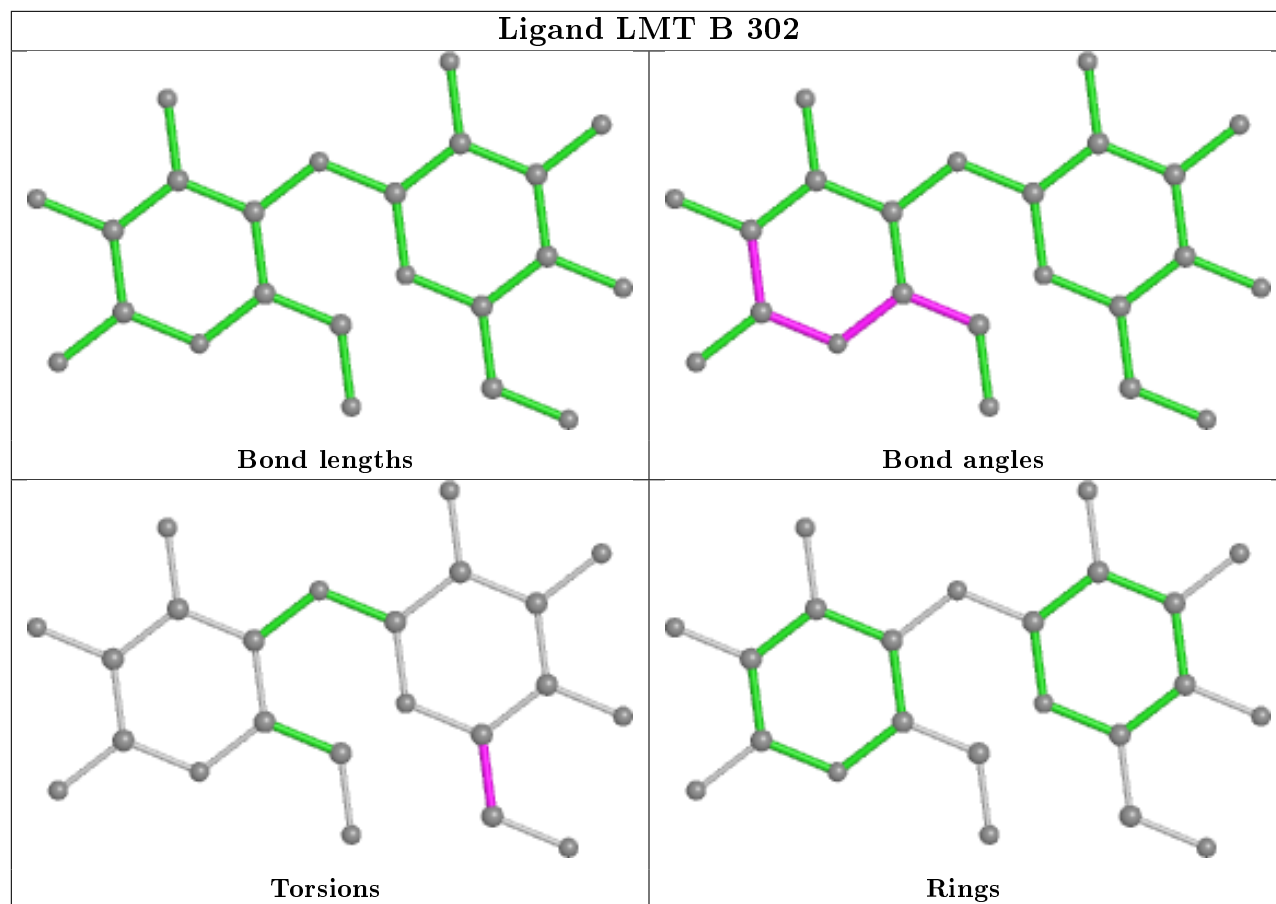
11 monomers are involved in 17 short contacts:

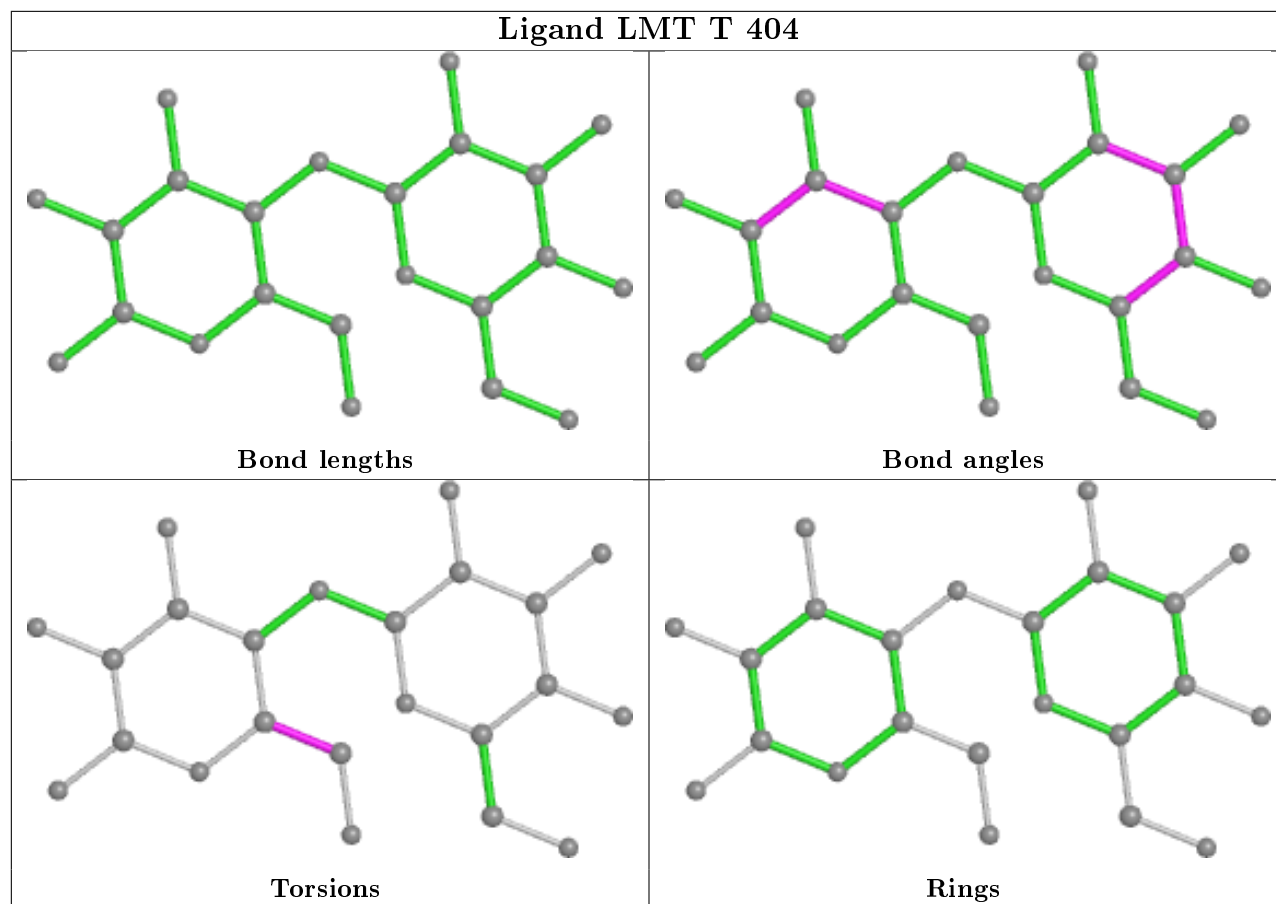
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	601	FCO	1	0
4	S	402	SF4	1	0
4	Q	402	SF4	1	0
10	R	404	LMT	1	0
4	Q	401	SF4	2	0
10	T	404	LMT	1	0
11	A	301	HEM	4	0
7	K	602	FCO	1	0
11	B	301	HEM	3	0
4	R	402	SF4	1	0
4	S	401	SF4	1	0

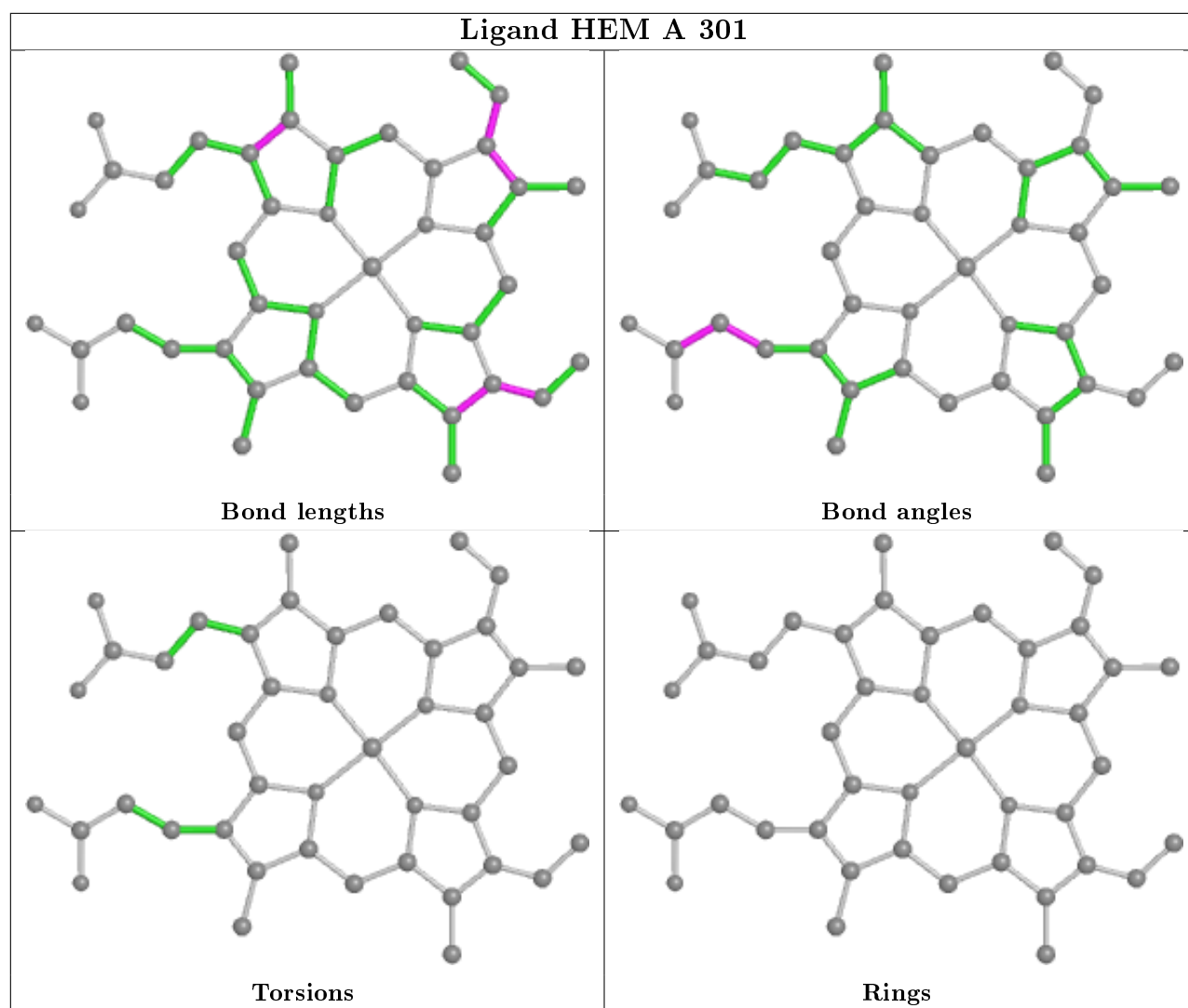
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

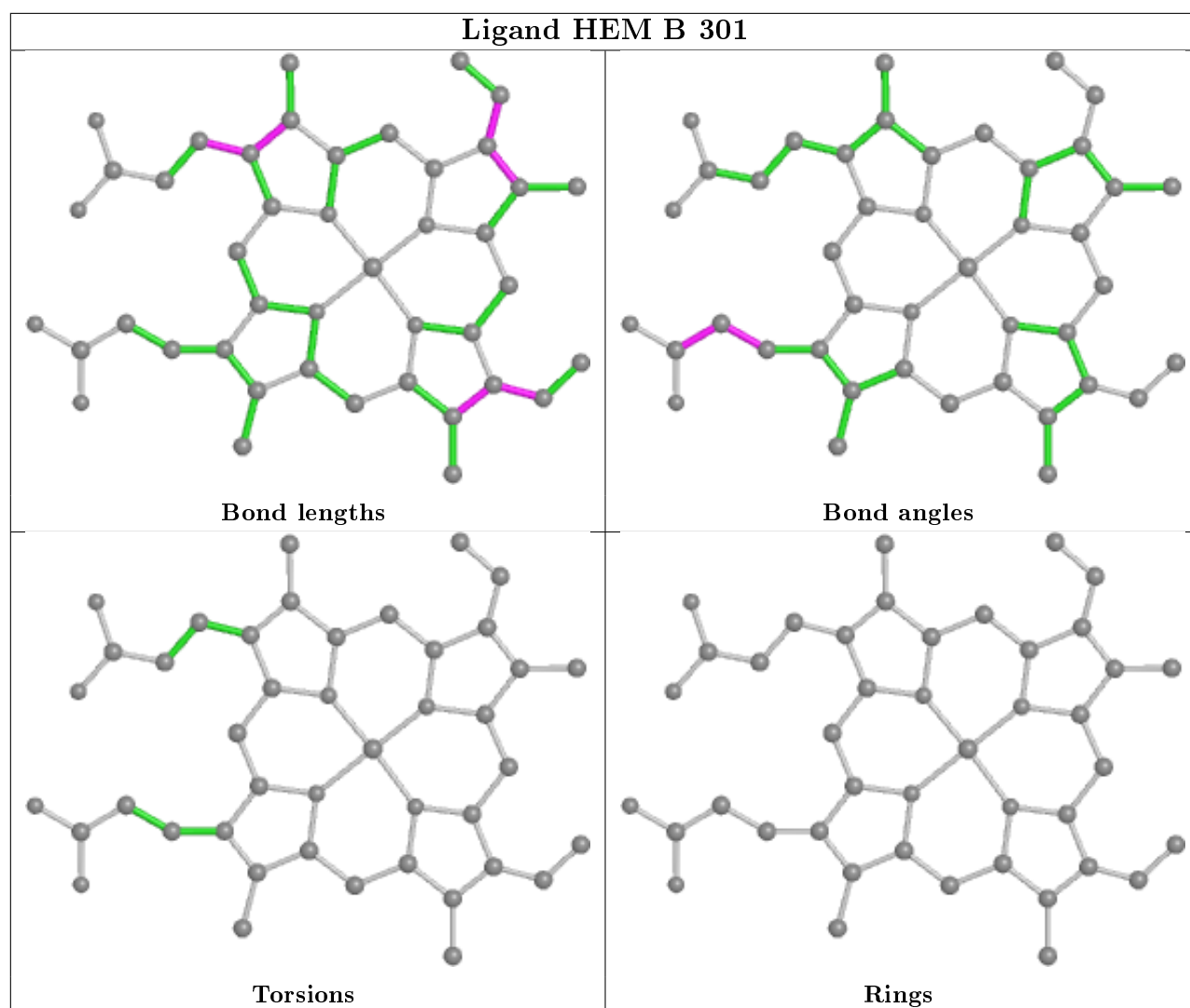












5.7 Other polymers [i](#)

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(Å²)	Q<0.9
1	Q	304/335 (90%)	-0.13	10 (3%)	46	44	59, 83, 151, 200	1 (0%)
1	R	300/335 (89%)	0.32	20 (6%)	17	17	69, 100, 138, 204	1 (0%)
1	S	304/335 (90%)	-0.09	6 (1%)	65	64	63, 87, 134, 185	1 (0%)
1	T	300/335 (89%)	0.00	15 (5%)	28	27	60, 103, 161, 227	1 (0%)
2	J	581/582 (99%)	0.12	16 (2%)	53	51	67, 101, 128, 142	4 (0%)
2	K	581/582 (99%)	0.28	46 (7%)	12	12	67, 103, 136, 164	5 (0%)
2	L	581/582 (99%)	0.24	35 (6%)	21	21	73, 109, 140, 164	4 (0%)
2	M	581/582 (99%)	0.23	43 (7%)	14	14	56, 103, 155, 188	5 (0%)
3	A	179/235 (76%)	0.40	25 (13%)	2	2	74, 126, 212, 223	0
3	B	179/235 (76%)	0.46	19 (10%)	6	6	78, 126, 227, 249	0
All	All	3890/4138 (94%)	0.18	235 (6%)	21	21	56, 101, 160, 249	22 (0%)

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	115	LEU	9.9
3	B	111	TRP	8.2
3	A	209	SER	6.5
2	K	46	ALA	6.4
3	B	210	ASP	6.3

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.

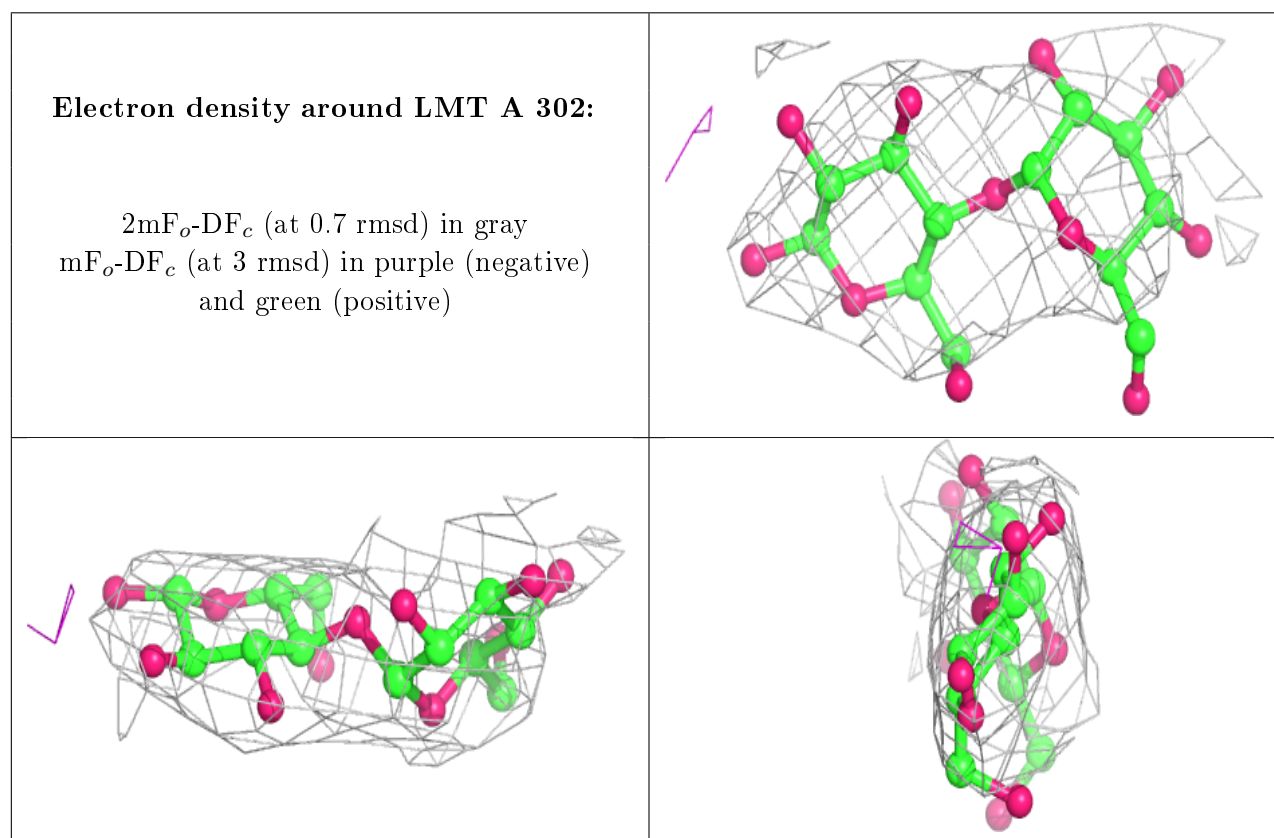
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LMT	A	302	23/35	0.77	0.29	114,132,152,153	0
10	LMT	R	404	23/35	0.80	0.38	145,151,157,158	0
10	LMT	T	404	23/35	0.80	0.28	135,143,147,149	0
6	CL	S	405	1/1	0.81	0.37	92,92,92,92	0
10	LMT	B	302	23/35	0.85	0.24	119,140,162,163	0
6	CL	K	601	1/1	0.86	0.35	103,103,103,103	0
6	CL	L	604	1/1	0.88	0.75	100,100,100,100	0
6	CL	M	605	1/1	0.89	0.86	91,91,91,91	0
6	CL	S	404	1/1	0.90	0.20	90,90,90,90	0
6	CL	Q	405	1/1	0.91	0.24	92,92,92,92	0
9	MG	K	604	1/1	0.93	0.18	97,97,97,97	0
6	CL	J	604	1/1	0.94	0.27	96,96,96,96	0
6	CL	K	605	1/1	0.94	0.60	102,102,102,102	0
6	CL	M	601	1/1	0.96	0.55	92,92,92,92	0
11	HEM	B	301	43/43	0.96	0.23	78,88,97,102	0
9	MG	J	603	1/1	0.96	0.08	87,87,87,87	0
9	MG	L	603	1/1	0.97	0.21	99,99,99,99	0
11	HEM	A	301	43/43	0.97	0.22	77,87,97,101	0
9	MG	M	604	1/1	0.97	0.11	95,95,95,95	0
8	NI	K	603	1/1	0.99	0.16	92,92,92,92	0
4	SF4	T	401	8/8	0.99	0.17	57,61,64,66	0
5	F4S	T	403	7/7	0.99	0.22	82,85,92,97	0
8	NI	L	602	1/1	0.99	0.17	91,91,91,91	0
4	SF4	T	402	8/8	0.99	0.20	68,71,73,73	0
5	F4S	S	403	7/7	0.99	0.12	76,78,84,86	0
7	FCO	L	601	7/7	0.99	0.20	88,90,98,99	0
7	FCO	J	601	7/7	0.99	0.32	80,81,89,89	0
8	NI	J	602	1/1	0.99	0.18	81,81,81,81	0
6	CL	Q	404	1/1	0.99	0.22	82,82,82,82	0
7	FCO	K	602	7/7	0.99	0.12	89,91,95,97	0
4	SF4	S	402	8/8	0.99	0.11	70,72,73,73	0
5	F4S	Q	403	7/7	0.99	0.18	64,68,73,77	0

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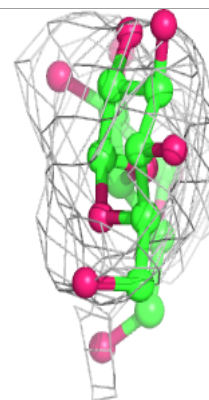
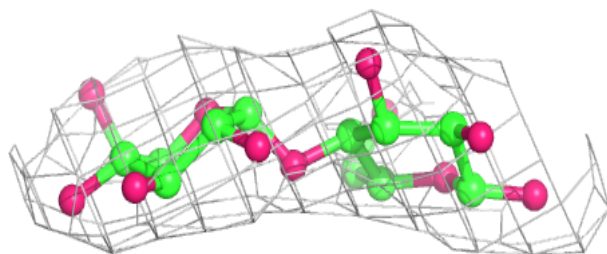
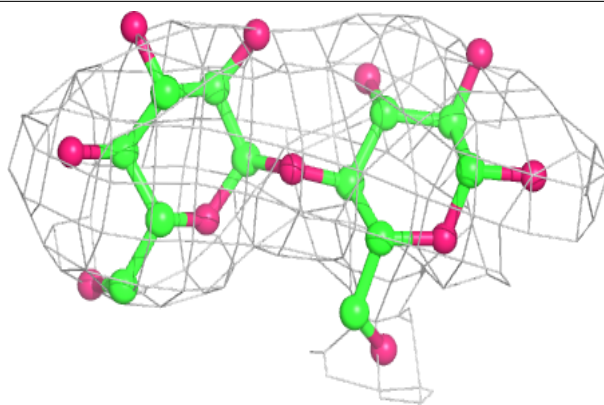
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SF4	R	402	8/8	0.99	0.20	73,77,79,80	0
4	SF4	Q	402	8/8	0.99	0.12	66,67,69,70	0
4	SF4	S	401	8/8	0.99	0.11	63,64,67,70	0
5	F4S	R	403	7/7	0.99	0.22	83,86,92,97	0
8	NI	M	603	1/1	1.00	0.17	89,89,89,89	0
4	SF4	Q	401	8/8	1.00	0.11	61,62,67,68	0
7	FCO	M	602	7/7	1.00	0.18	81,83,90,93	0
4	SF4	R	401	8/8	1.00	0.19	63,67,70,71	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.

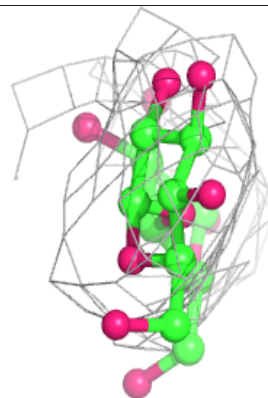
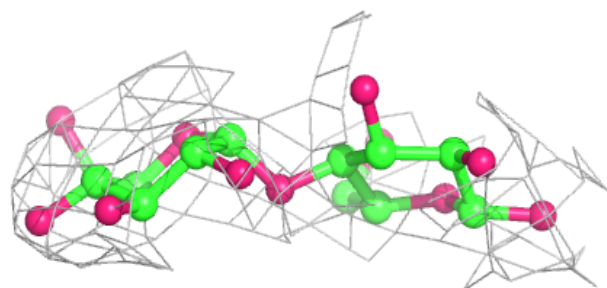
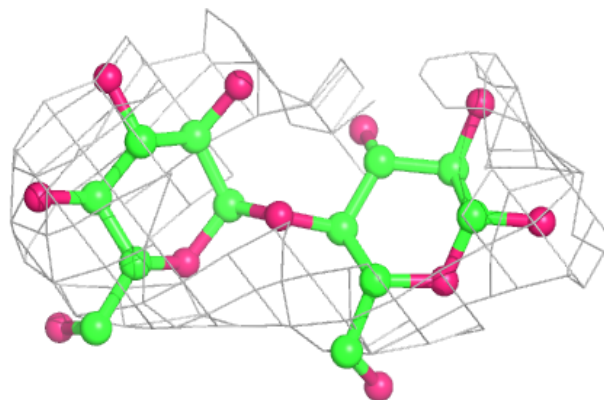


Electron density around LMT R 404:

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

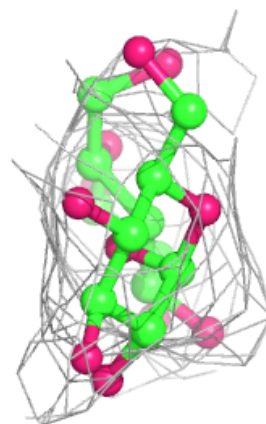
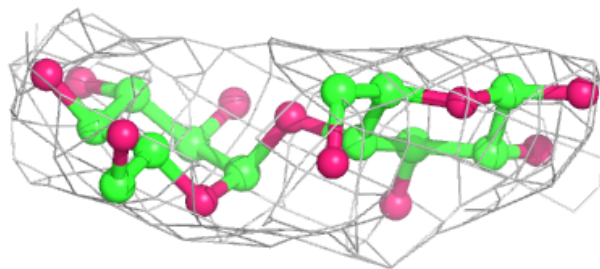
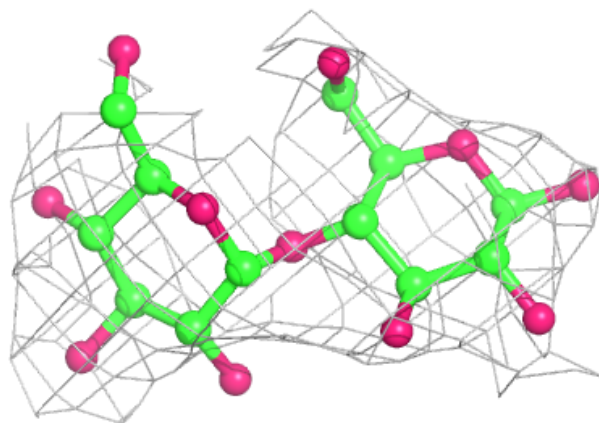
**Electron density around LMT T 404:**

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



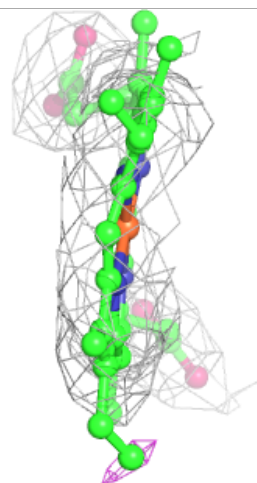
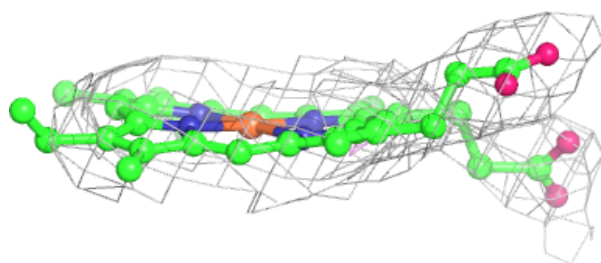
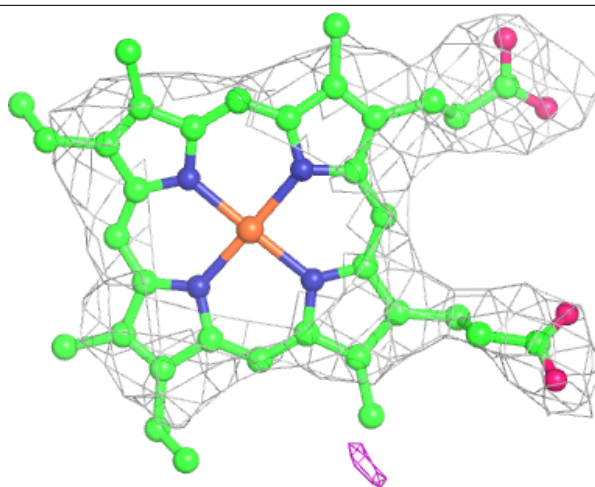
Electron density around LMT B 302:

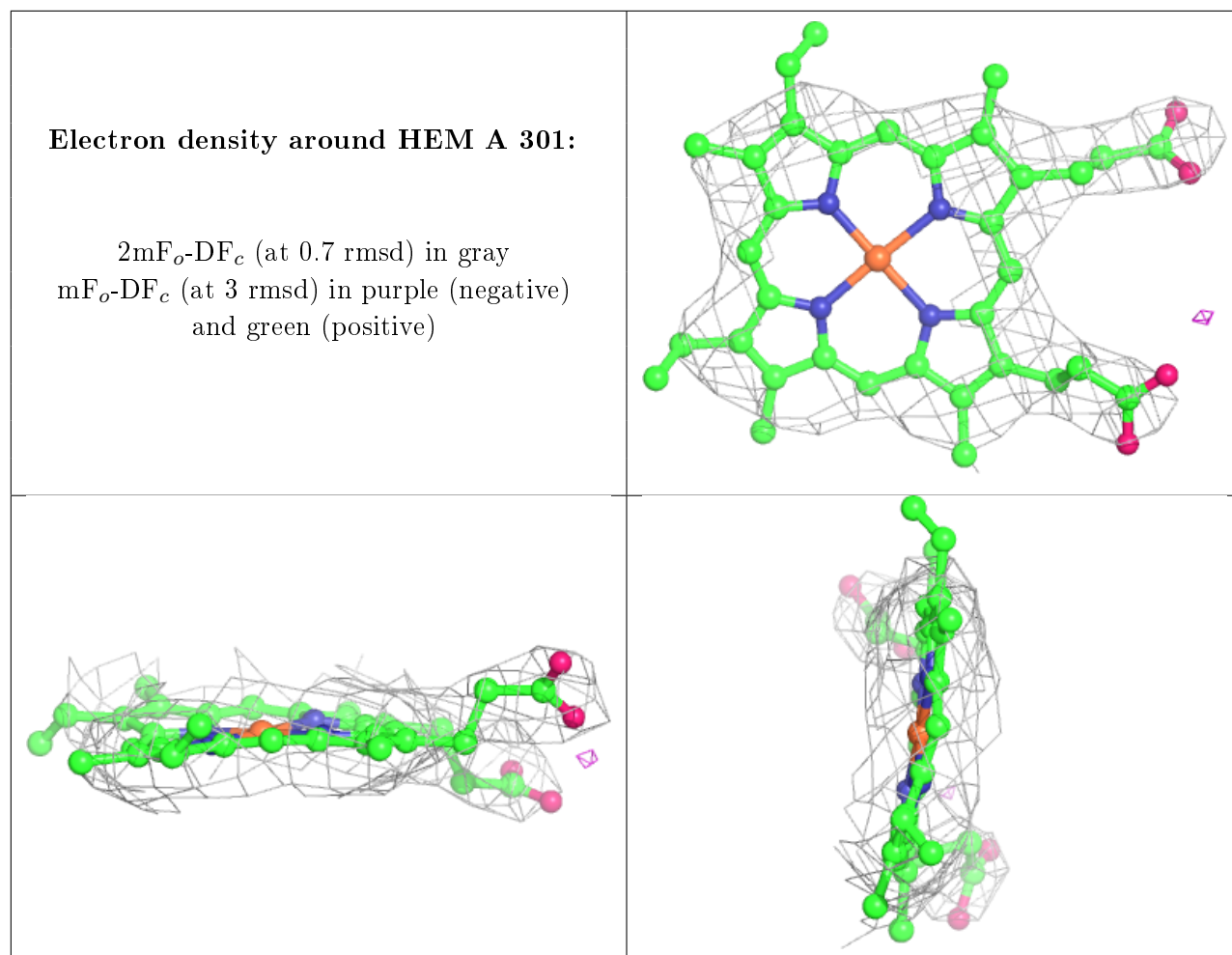
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.