wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 02:09 PM EDT

PDB ID	:	4GD3 / pdb_00004gd3
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

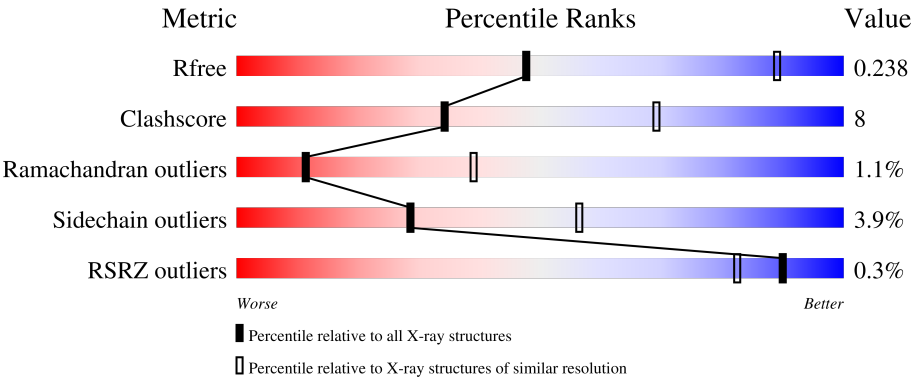
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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.



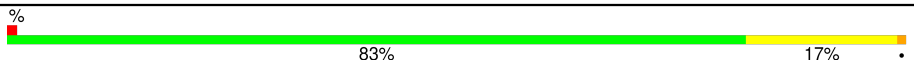
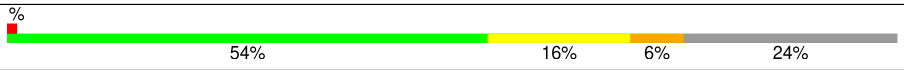
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	Q	335	69% 19% • 9%
1	R	335	69% 18% • 10%
1	S	335	69% 18% • 9%
1	T	335	67% 20% • 10%
2	J	582	84% 15% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	582	
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

Continued on next page...

Continued from previous page...

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

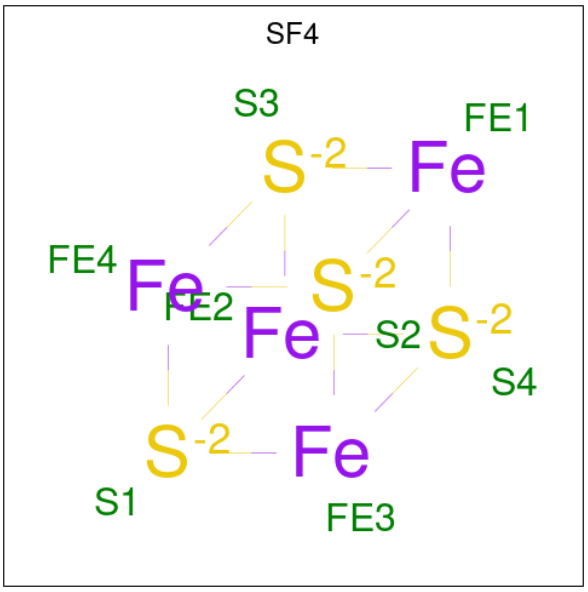
- Molecule 2 is a protein called Hydrogenase-1 large chain.

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.

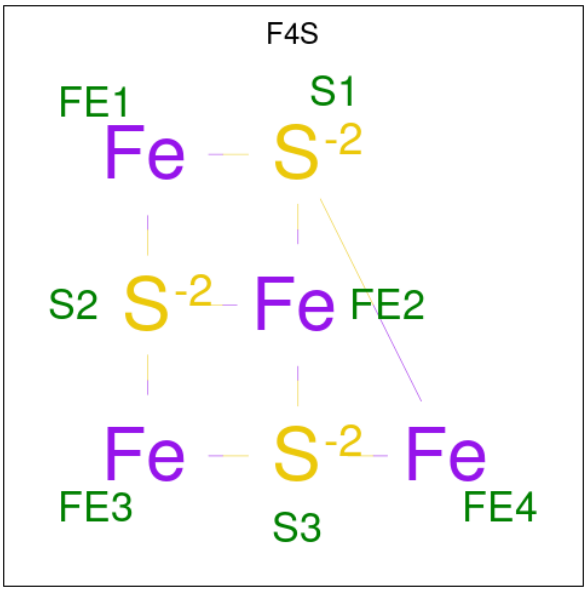
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			
3	B	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 5 is FE4-S3 CLUSTER (CCD ID: F4S) (formula: Fe_4S_3).

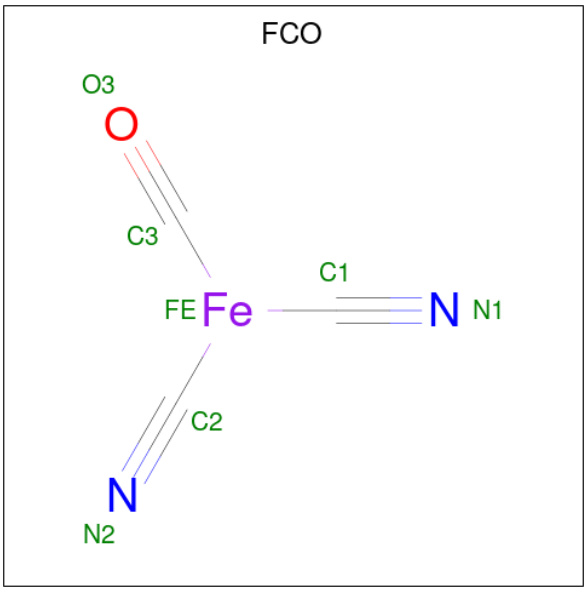


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total Fe S 7 4 3	0	0
5	T	1	Total Fe S 7 4 3	0	0
5	Q	1	Total Fe S 7 4 3	0	0
5	R	1	Total Fe S 7 4 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).



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

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

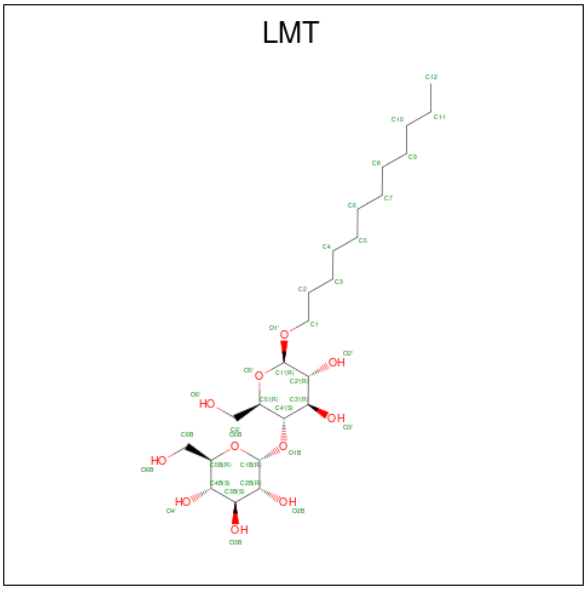
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

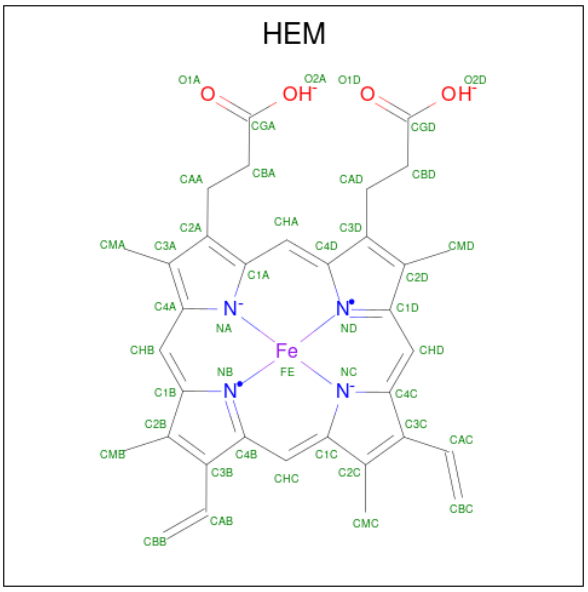
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Mg 1 1	0	0
9	J	1	Total Mg 1 1	0	0
9	K	1	Total Mg 1 1	0	0

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

- 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		

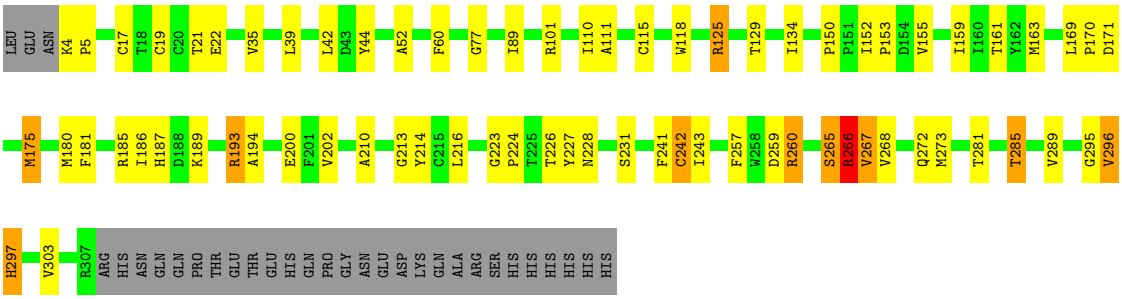
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hydrogenase-1 small chain

Chain S:

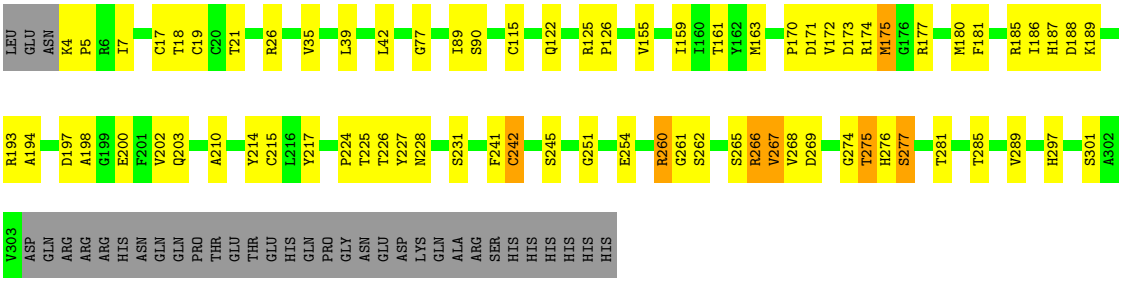




• Molecule 1: Hydrogenase-1 small chain

Chain T:

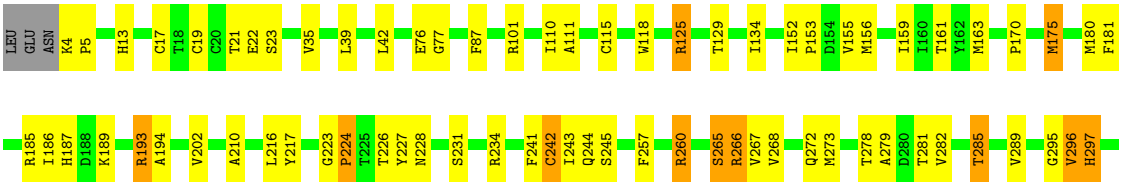


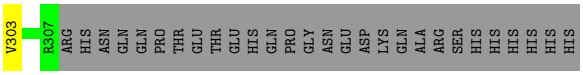


• Molecule 1: Hydrogenase-1 small chain

Chain Q:



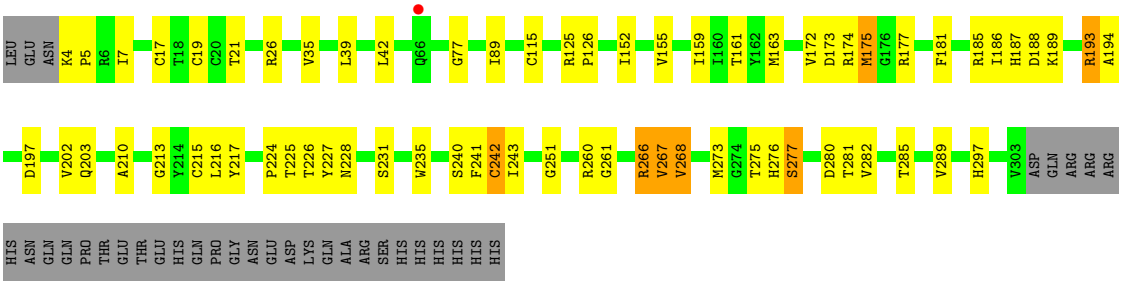




• Molecule 1: Hydrogenase-1 small chain

Chain R:

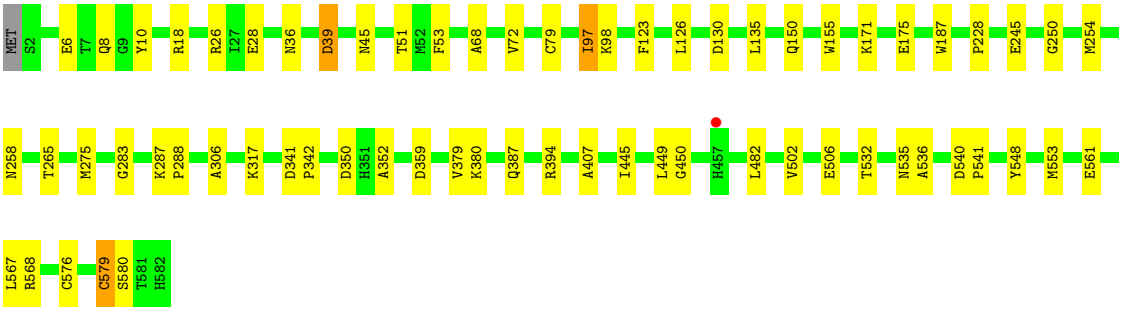




• Molecule 2: Hydrogenase-1 large chain

Chain L:





• Molecule 2: Hydrogenase-1 large chain

Chain M:

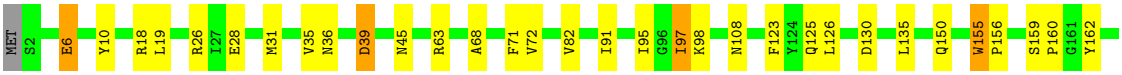


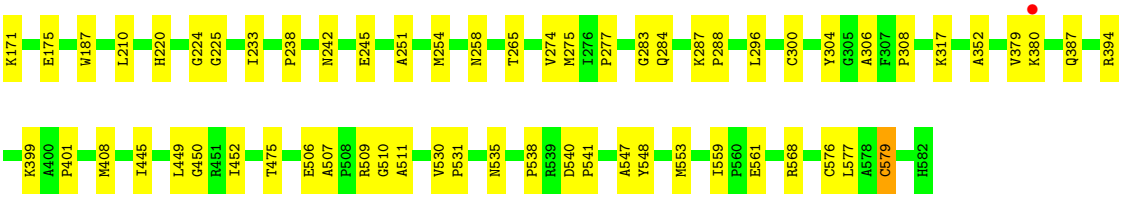


• Molecule 2: Hydrogenase-1 large chain

Chain J:



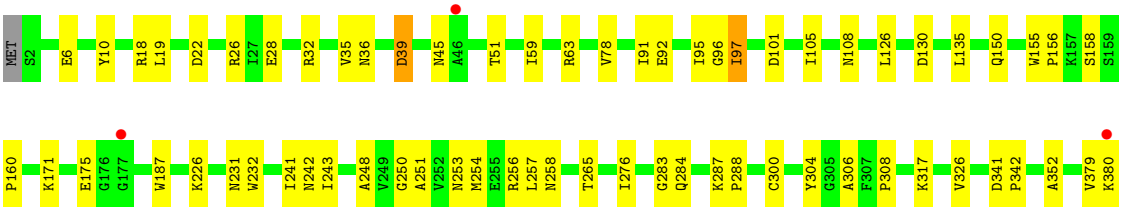




• Molecule 2: Hydrogenase-1 large chain

Chain K:

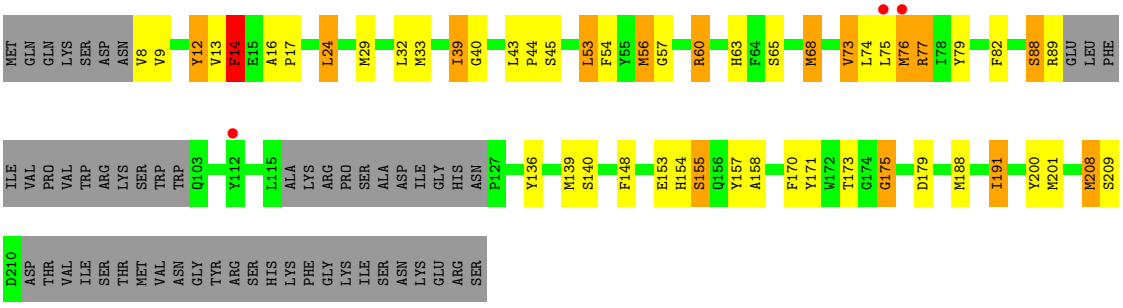




• Molecule 3: Ni/Fe-hydrogenase 1 B-type cytochrome subunit

Chain A:

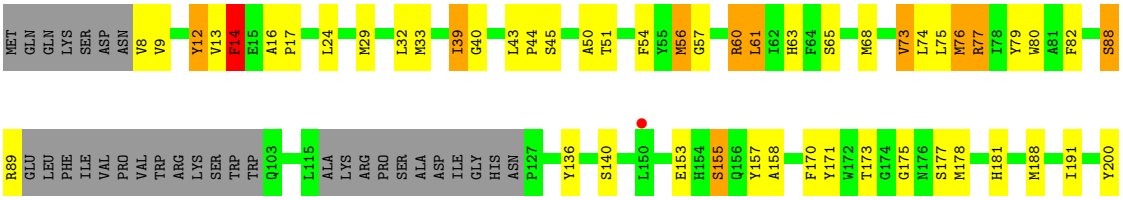




• Molecule 3: Ni/Fe-hydrogenase 1 B-type cytochrome subunit

Chain B:






M201
M208
S209
D210
ASP
THR
VAL
ILE
SER
THR
MET
VAL
ASN
GLY
TYR
ARG
SER
HIS
LYS
PHE
GLY
LYS
ILE
SER
ASN
LYS
GLU
ARG
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.00Å 165.30Å 212.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 25.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-3.30) 99.0 (25.00-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.236 0.205 , 0.238	Depositor DCC
R_{free} test set	3633 reflections (4.92%)	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 , 77.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, HEM, SF4, F4S, CL, MG, NI, 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	0.71	0/2407	0.94	1/3275 (0.0%)
1	R	0.65	0/2352	0.89	1/3200 (0.0%)
1	S	0.67	0/2407	0.92	2/3275 (0.1%)
1	T	0.65	0/2352	0.89	0/3200
2	J	0.56	0/4940	0.87	5/6715 (0.1%)
2	K	0.57	0/4956	0.86	0/6736
2	L	0.53	0/4940	0.84	3/6715 (0.0%)
2	M	0.57	0/4956	0.85	3/6736 (0.0%)
3	A	0.74	2/1406 (0.1%)	1.01	4/1916 (0.2%)
3	B	0.74	2/1406 (0.1%)	1.00	2/1916 (0.1%)
All	All	0.61	4/32122 (0.0%)	0.88	21/43684 (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	-12.03	1.37	1.52
3	A	200	TYR	CA-C	-11.10	1.38	1.52
3	A	201	MET	C-N	-8.96	1.21	1.33
3	B	201	MET	C-N	-7.87	1.22	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	97	ILE	N-CA-C	7.80	118.70	111.45
3	A	201	MET	CA-C-N	7.24	135.36	121.54
3	A	201	MET	C-N-CA	7.24	135.36	121.54
3	B	201	MET	CA-C-N	7.01	134.93	121.54
3	B	201	MET	C-N-CA	7.01	134.93	121.54

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	2329	0	2277	54	0
1	R	2283	0	2218	50	0
1	S	2329	0	2277	51	0
1	T	2283	0	2218	52	0
2	J	4733	0	4675	59	0
2	K	4743	0	4697	75	0
2	L	4733	0	4675	42	0
2	M	4743	0	4697	56	0
3	A	1360	0	1246	35	0
3	B	1360	0	1247	37	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1	0	0	0	0
9	M	1	0	0	0	0
10	A	23	0	21	0	0
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	30371	466	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 8.

The worst 5 of 466 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:HH11	1:S:101[B]:ARG:CG	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:HH11	1:S:101[B]:ARG:HG2	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%)	5 25
1	R	302/335 (90%)	282 (93%)	14 (5%)	6 (2%)	6 27
1	S	309/335 (92%)	283 (92%)	19 (6%)	7 (2%)	5 25
1	T	302/335 (90%)	279 (92%)	17 (6%)	6 (2%)	6 27
2	J	612/582 (105%)	571 (93%)	39 (6%)	2 (0%)	36 65
2	K	614/582 (106%)	578 (94%)	35 (6%)	1 (0%)	43 71
2	L	612/582 (105%)	567 (93%)	44 (7%)	1 (0%)	43 71
2	M	614/582 (106%)	572 (93%)	42 (7%)	0	100 100
3	A	173/235 (74%)	147 (85%)	19 (11%)	7 (4%)	2 15
3	B	173/235 (74%)	147 (85%)	20 (12%)	6 (4%)	3 18
All	All	4020/4138 (97%)	3708 (92%)	269 (7%)	43 (1%)	11 39

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 (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	Q	247/274 (90%)	233 (94%)	14 (6%)	18 47
1	R	241/274 (88%)	235 (98%)	6 (2%)	42 64
1	S	247/274 (90%)	234 (95%)	13 (5%)	20 49
1	T	241/274 (88%)	233 (97%)	8 (3%)	33 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	512/481 (106%)	500 (98%)	12 (2%)	44 66
2	K	513/481 (107%)	503 (98%)	10 (2%)	50 68
2	L	512/481 (106%)	500 (98%)	12 (2%)	44 66
2	M	513/481 (107%)	503 (98%)	10 (2%)	50 68
3	A	123/203 (61%)	101 (82%)	22 (18%)	2 8
3	B	123/203 (61%)	101 (82%)	22 (18%)	2 8
All	All	3272/3426 (96%)	3143 (96%)	129 (4%)	28 56

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	61	LEU
3	B	75	LEU
1	Q	260	ARG
1	Q	224	PRO
3	B	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	286	ASN
2	K	125	GLN
2	J	332	ASN
2	K	36	ASN
2	K	258	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
10	LMT	A	302	-	24,24,36	0.56	0	35,35,47	0.93	1 (2%)
5	F4S	R	403	1	0,9,9	-	-	-		
5	F4S	T	403	1	0,9,9	-	-	-		
7	FCO	K	602	2	3,6,6	0.92	0	-		
4	SF4	T	402	1	0,12,12	-	-	-		
7	FCO	L	601	2	3,6,6	1.51	1 (33%)	-		
11	HEM	A	301	3	50,50,50	1.88	8 (16%)	67,82,82	1.19	4 (5%)
7	FCO	M	602	2	3,6,6	1.39	1 (33%)	-		
4	SF4	S	401	1	0,12,12	-	-	-		
4	SF4	T	401	1	0,12,12	-	-	-		
5	F4S	Q	403	1	0,9,9	-	-	-		
5	F4S	S	403	1	0,9,9	-	-	-		
4	SF4	R	401	1	0,12,12	-	-	-		
4	SF4	Q	401	1	0,12,12	-	-	-		
10	LMT	B	302	-	24,24,36	0.43	0	35,35,47	0.89	2 (5%)
7	FCO	J	601	2	3,6,6	1.42	1 (33%)	-		
10	LMT	T	404	-	24,24,36	0.53	0	35,35,47	1.24	3 (8%)
4	SF4	S	402	1	0,12,12	-	-	-		
4	SF4	R	402	1	0,12,12	-	-	-		
10	LMT	R	404	-	24,24,36	0.59	0	35,35,47	1.15	3 (8%)
4	SF4	Q	402	1	0,12,12	-	-	-		
11	HEM	B	301	3	50,50,50	1.80	9 (18%)	67,82,82	1.22	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	Q	401	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	A	302	-	-	2/8/48/61	0/2/2/2
5	F4S	R	403	1	-	-	0/4/3/3
10	LMT	B	302	-	-	2/8/48/61	0/2/2/2
5	F4S	T	403	1	-	-	0/4/3/3
10	LMT	T	404	-	-	2/8/48/61	0/2/2/2
4	SF4	S	402	1	-	-	0/6/5/5
4	SF4	T	401	1	-	-	0/6/5/5
4	SF4	T	402	1	-	-	0/6/5/5
11	HEM	A	301	3	-	4/14/54/54	-
4	SF4	R	402	1	-	-	0/6/5/5
10	LMT	R	404	-	-	2/8/48/61	0/2/2/2
5	F4S	Q	403	1	-	-	0/4/3/3
4	SF4	Q	402	1	-	-	0/6/5/5
5	F4S	S	403	1	-	-	0/4/3/3
4	SF4	R	401	1	-	-	0/6/5/5
4	SF4	S	401	1	-	-	0/6/5/5
11	HEM	B	301	3	-	2/14/54/54	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	301	HEM	C3D-C2D	8.12	1.54	1.36
11	B	301	HEM	C3D-C2D	7.49	1.52	1.36
11	A	301	HEM	FE-ND	4.77	2.09	1.94
11	A	301	HEM	FE-NA	3.93	2.08	1.95
11	B	301	HEM	FE-ND	3.68	2.06	1.94

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	301	HEM	C4D-ND-C1D	4.94	111.06	105.21
11	B	301	HEM	C4D-ND-C1D	4.61	110.67	105.21
10	A	302	LMT	O5'-C1'-C2'	-3.29	104.51	110.30
11	A	301	HEM	CAA-CBA-CGA	-3.10	105.45	113.67
11	B	301	HEM	CAA-CBA-CGA	-3.01	105.69	113.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

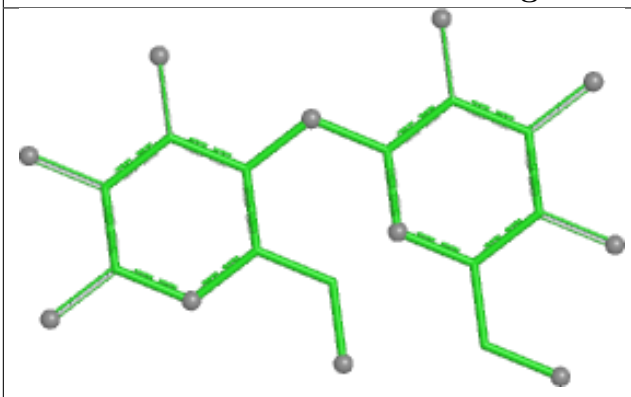
There are no ring outliers.

11 monomers are involved in 17 short contacts:

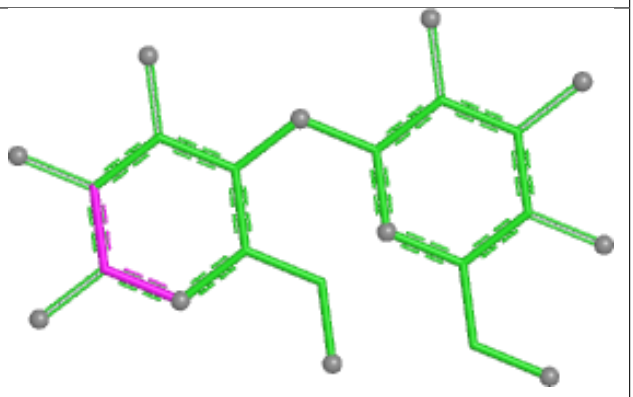
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	602	FCO	1	0
7	L	601	FCO	1	0
11	A	301	HEM	4	0
4	S	401	SF4	1	0
4	Q	401	SF4	2	0
10	T	404	LMT	1	0
4	S	402	SF4	1	0
4	R	402	SF4	1	0
10	R	404	LMT	1	0
4	Q	402	SF4	1	0
11	B	301	HEM	3	0

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

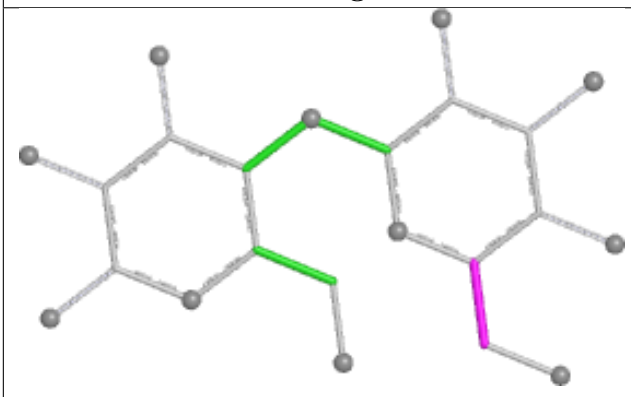
Ligand LMT A 302



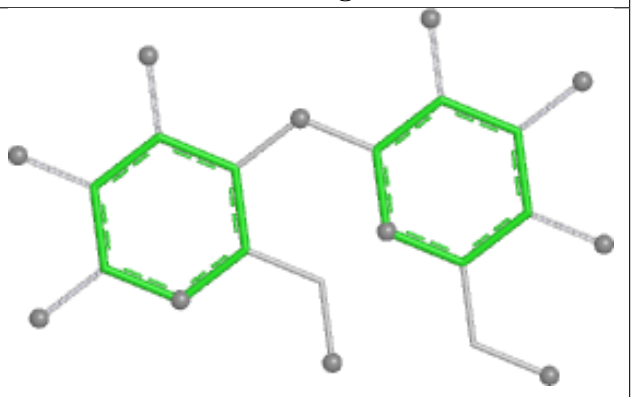
Bond lengths



Bond angles

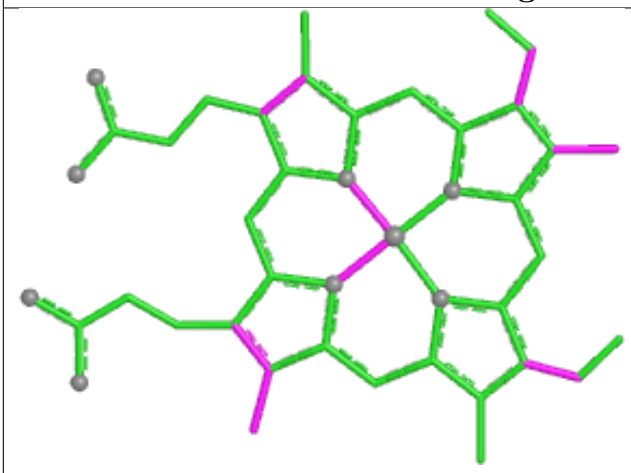


Torsions

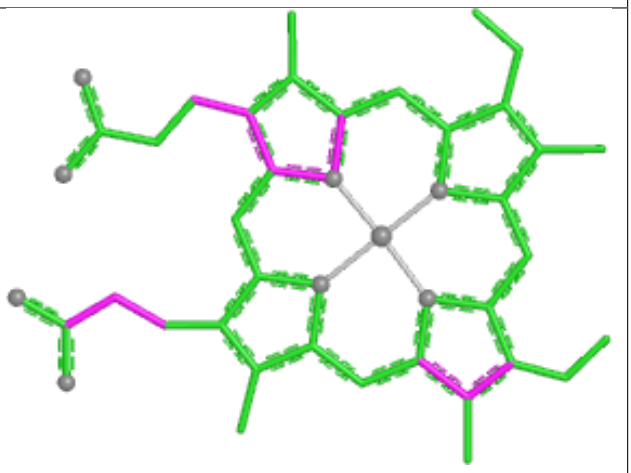


Rings

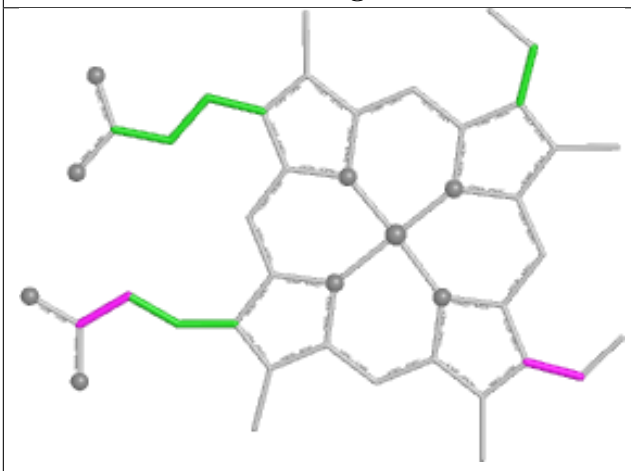
Ligand HEM A 301



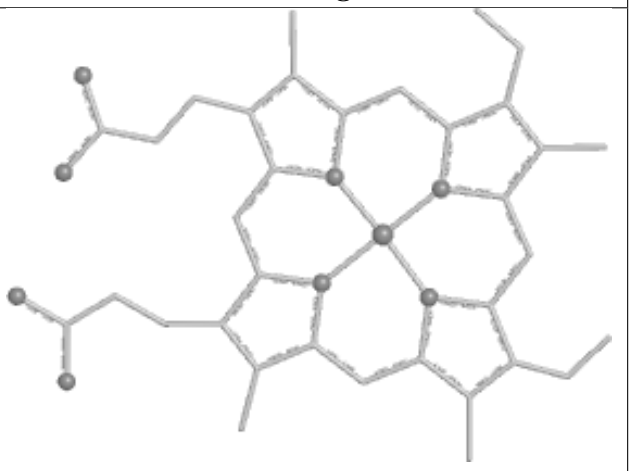
Bond lengths



Bond angles

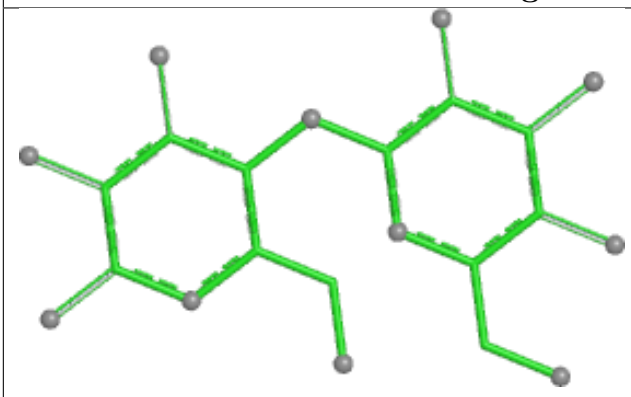


Torsions

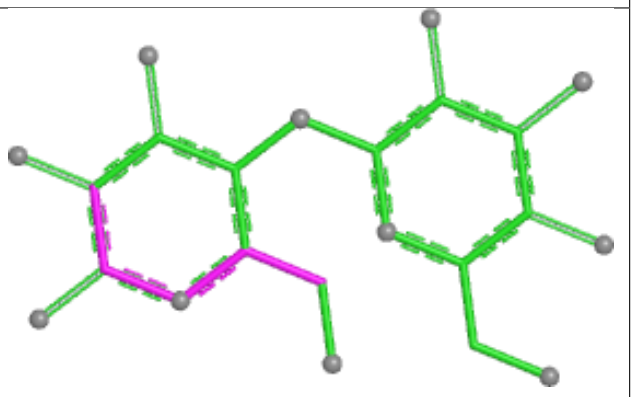


Rings

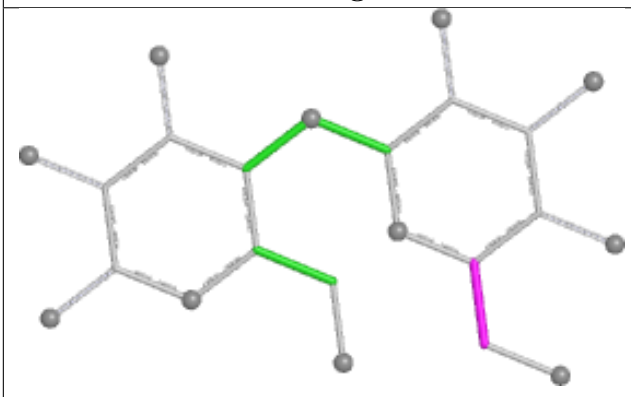
Ligand LMT B 302



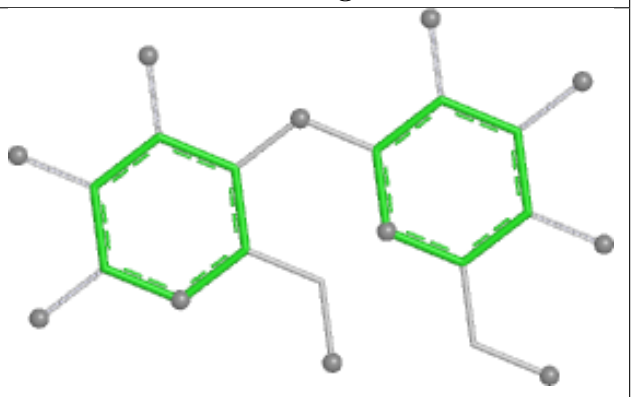
Bond lengths



Bond angles

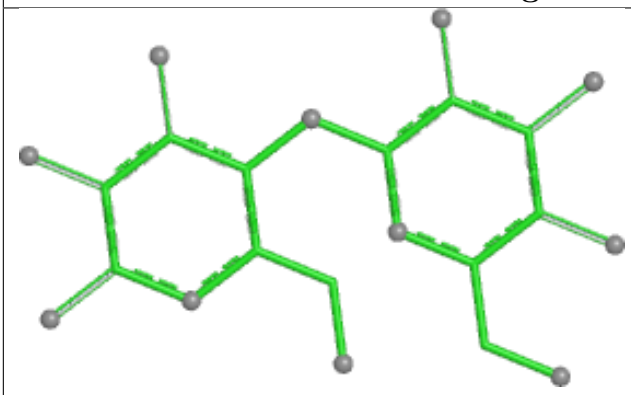


Torsions

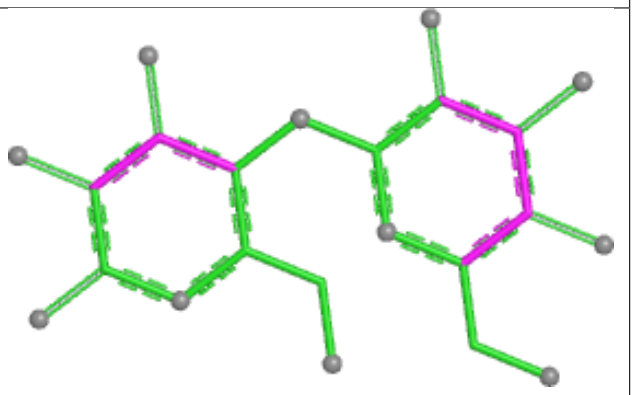


Rings

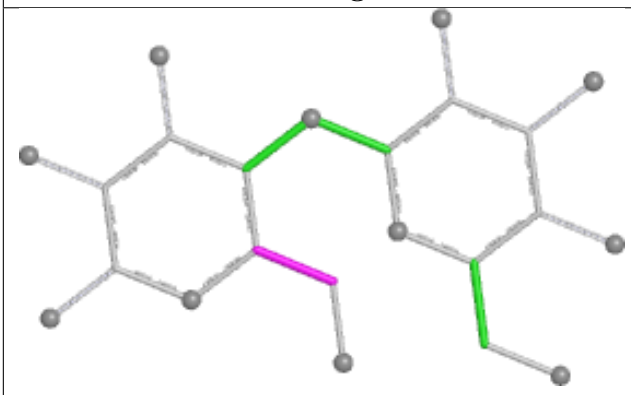
Ligand LMT T 404



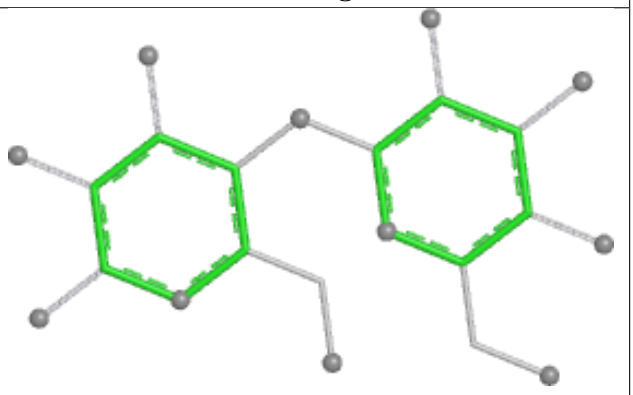
Bond lengths



Bond angles

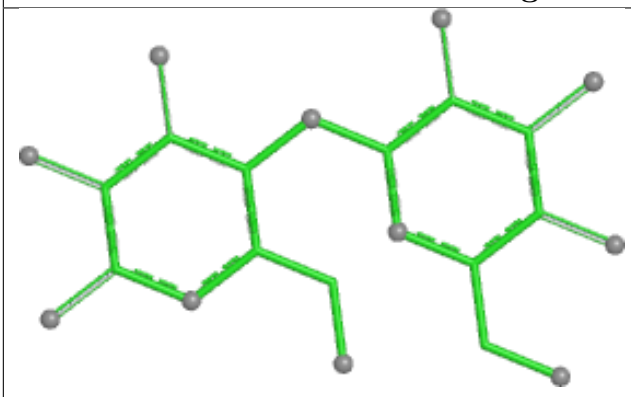


Torsions

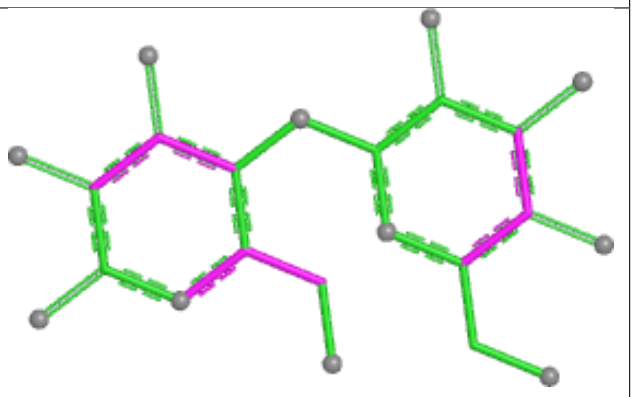


Rings

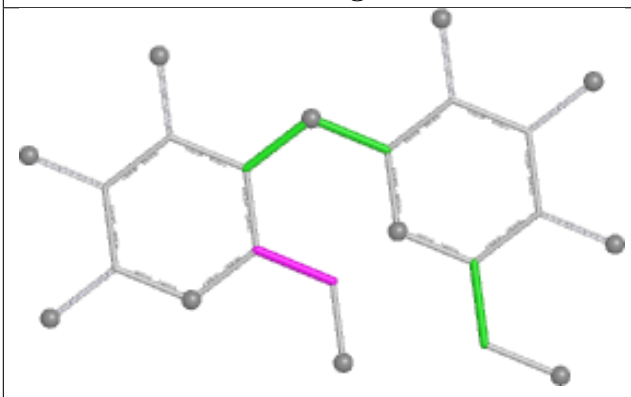
Ligand LMT R 404



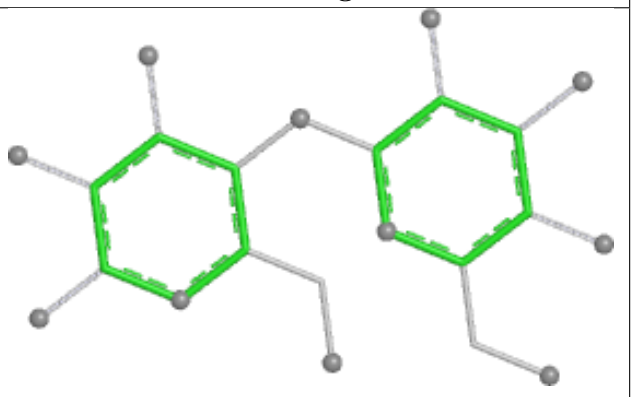
Bond lengths



Bond angles

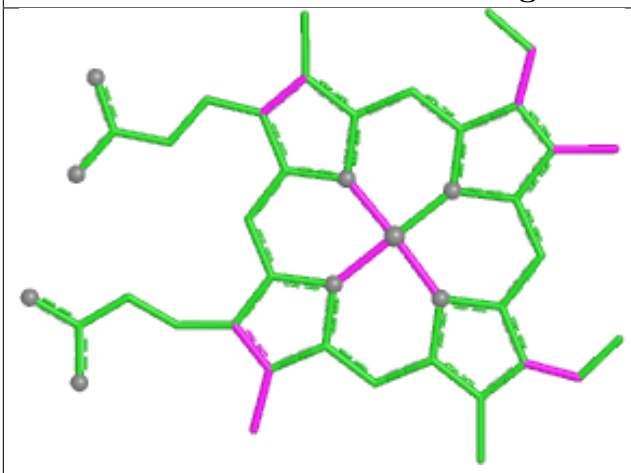


Torsions

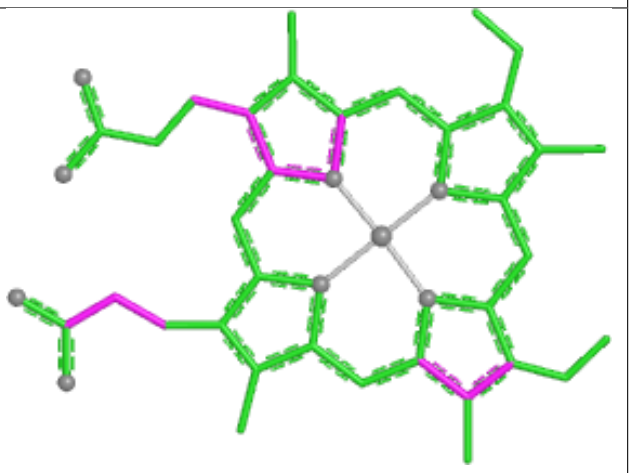


Rings

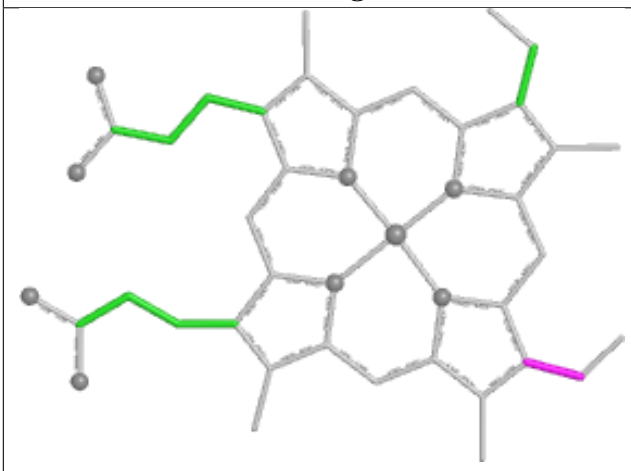
Ligand HEM B 301



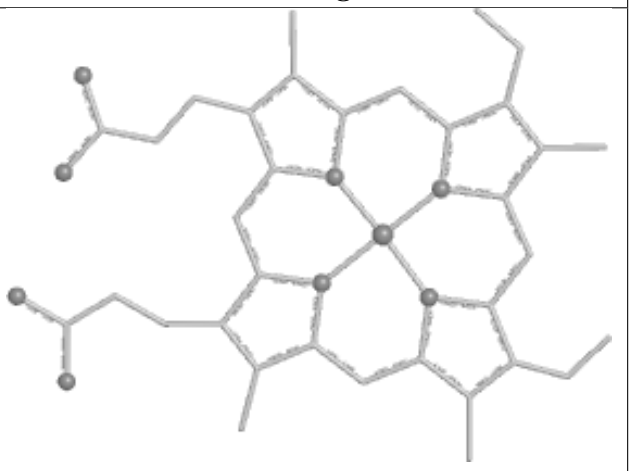
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Q	304/335 (90%)	-0.54	0 100 100	42, 82, 151, 200	8 (2%)
1	R	300/335 (89%)	-0.41	1 (0%) 90 82	53, 99, 138, 204	5 (1%)
1	S	304/335 (90%)	-0.55	0 100 100	44, 86, 134, 185	8 (2%)
1	T	300/335 (89%)	-0.48	0 100 100	52, 103, 161, 227	5 (1%)
2	J	581/582 (99%)	-0.46	1 (0%) 91 86	50, 99, 127, 142	37 (6%)
2	K	581/582 (99%)	-0.31	5 (0%) 81 65	39, 101, 133, 164	40 (6%)
2	L	581/582 (99%)	-0.43	1 (0%) 91 86	53, 107, 139, 164	37 (6%)
2	M	581/582 (99%)	-0.54	0 100 100	32, 99, 150, 188	40 (6%)
3	A	179/235 (76%)	-0.23	3 (1%) 69 50	74, 126, 212, 223	0
3	B	179/235 (76%)	-0.16	1 (0%) 85 73	78, 126, 227, 249	0
All	All	3890/4138 (94%)	-0.43	12 (0%) 90 82	32, 99, 159, 249	180 (4%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	380[A]	LYS	3.1
2	K	380[A]	LYS	3.1
2	K	46	ALA	2.9
2	K	457[A]	HIS	2.8
3	B	150	LEU	2.7

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	LMT	R	404	23/35	0.73	0.08	145,151,157,158	0
10	LMT	B	302	23/35	0.79	0.07	119,140,162,163	0
10	LMT	A	302	23/35	0.80	0.07	114,132,152,153	0
10	LMT	T	404	23/35	0.80	0.08	135,143,147,149	0
6	CL	J	604	1/1	0.83	0.26	96,96,96,96	0
6	CL	Q	405	1/1	0.87	0.08	92,92,92,92	0
6	CL	M	605	1/1	0.88	0.26	91,91,91,91	0
6	CL	S	405	1/1	0.90	0.07	92,92,92,92	0
6	CL	K	601	1/1	0.92	0.11	103,103,103,103	0
6	CL	M	601	1/1	0.95	0.07	92,92,92,92	0
6	CL	Q	404	1/1	0.96	0.05	82,82,82,82	0
6	CL	S	404	1/1	0.97	0.05	90,90,90,90	0
6	CL	K	605	1/1	0.97	0.20	102,102,102,102	0
6	CL	L	604	1/1	0.98	0.06	100,100,100,100	0
9	MG	L	603	1/1	0.98	0.03	99,99,99,99	0
9	MG	J	603	1/1	0.98	0.03	87,87,87,87	0
9	MG	K	604	1/1	0.98	0.07	97,97,97,97	0
11	HEM	A	301	43/43	0.98	0.09	77,87,97,101	0
11	HEM	B	301	43/43	0.98	0.08	78,88,97,102	0
7	FCO	M	602	7/7	0.99	0.05	81,83,90,93	0
7	FCO	J	601	7/7	0.99	0.08	80,81,89,89	0
7	FCO	K	602	7/7	0.99	0.07	89,91,95,97	0
4	SF4	T	402	8/8	0.99	0.03	68,71,73,73	0
9	MG	M	604	1/1	0.99	0.04	95,95,95,95	0
4	SF4	Q	402	8/8	0.99	0.02	66,67,69,70	0
4	SF4	R	402	8/8	0.99	0.03	73,77,79,80	0
5	F4S	T	403	7/7	0.99	0.03	82,85,92,97	0
5	F4S	Q	403	7/7	0.99	0.02	64,68,73,77	0
5	F4S	R	403	7/7	0.99	0.03	83,86,92,97	0
4	SF4	S	401	8/8	0.99	0.03	63,64,67,70	0
4	SF4	S	402	8/8	0.99	0.03	70,72,73,73	0
7	FCO	L	601	7/7	0.99	0.07	88,90,98,99	0

Continued on next page...

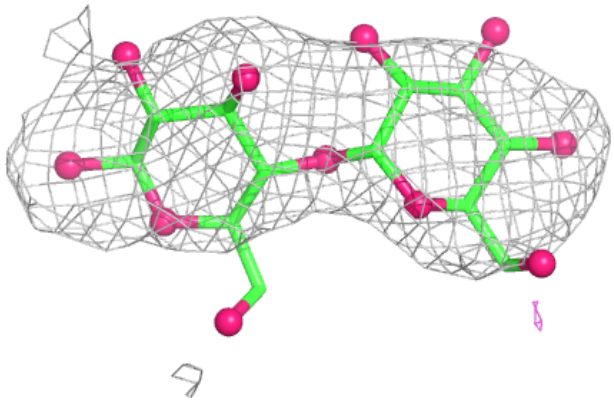
Continued from previous page...

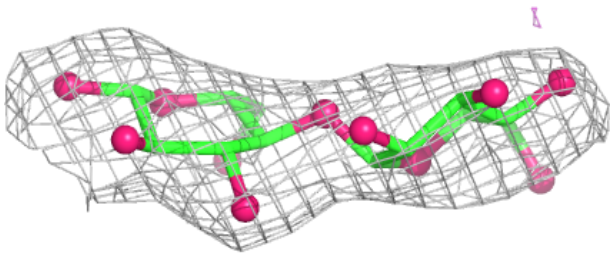
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	F4S	S	403	7/7	1.00	0.02	76,78,84,86	0
4	SF4	T	401	8/8	1.00	0.03	57,61,64,66	0
8	NI	L	602	1/1	1.00	0.02	91,91,91,91	0
8	NI	M	603	1/1	1.00	0.01	89,89,89,89	0
8	NI	J	602	1/1	1.00	0.02	81,81,81,81	0
8	NI	K	603	1/1	1.00	0.02	92,92,92,92	0
4	SF4	R	401	8/8	1.00	0.03	63,67,70,71	0
4	SF4	Q	401	8/8	1.00	0.02	61,62,67,68	0

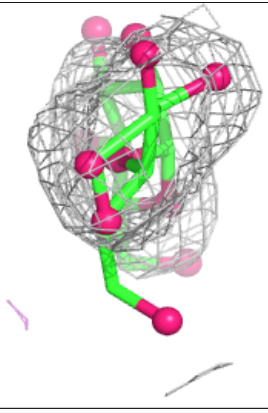
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

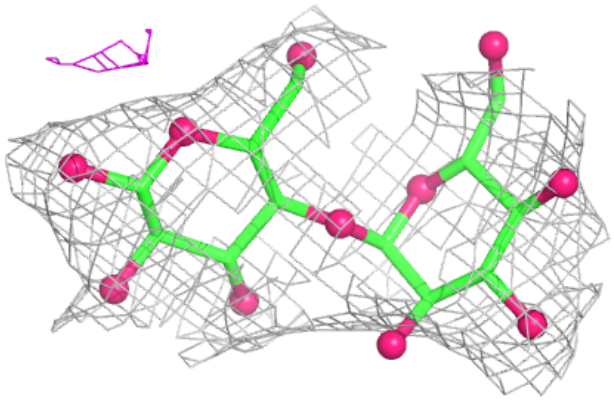


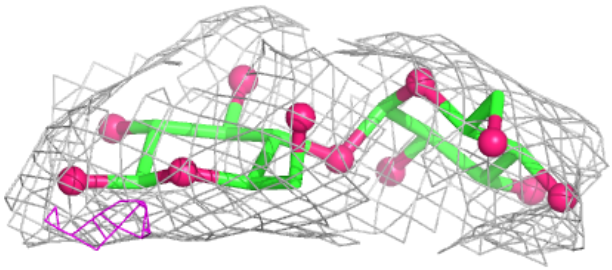


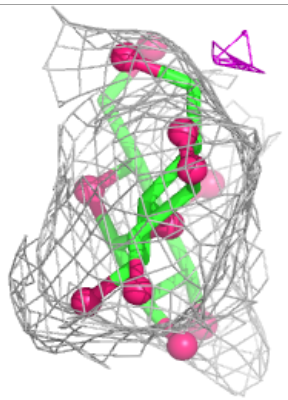


Electron density around LMT B 302:

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

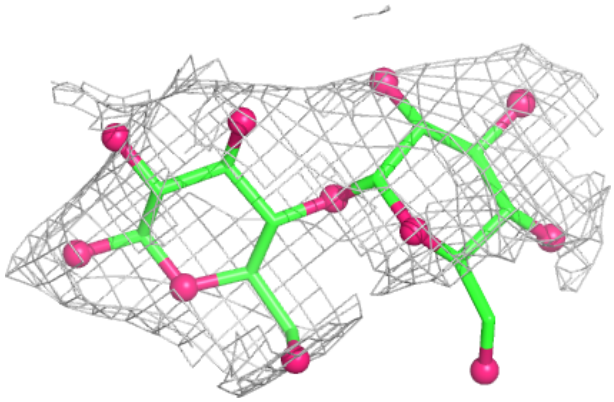


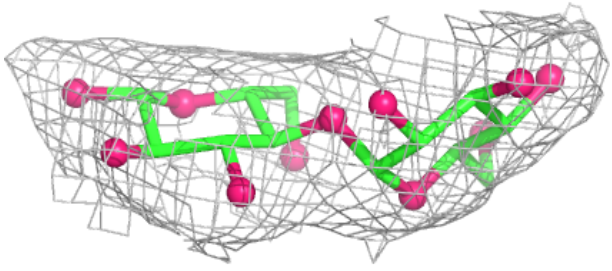


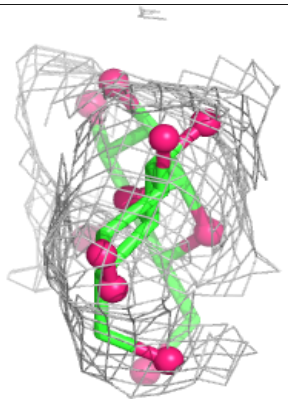


Electron density around LMT A 302:

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

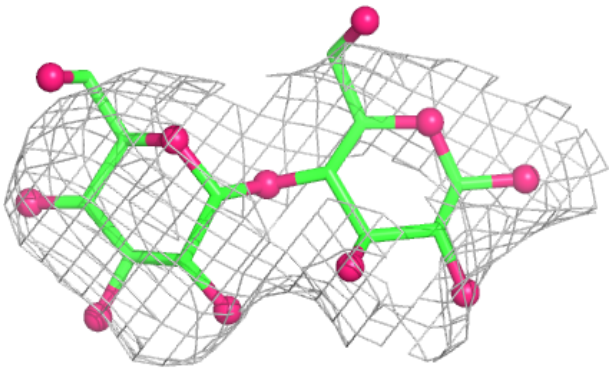


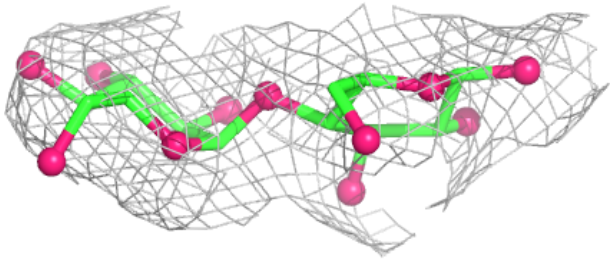


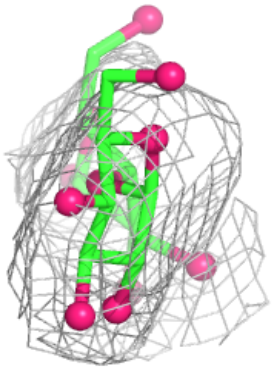


Electron density around LMT T 404:

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

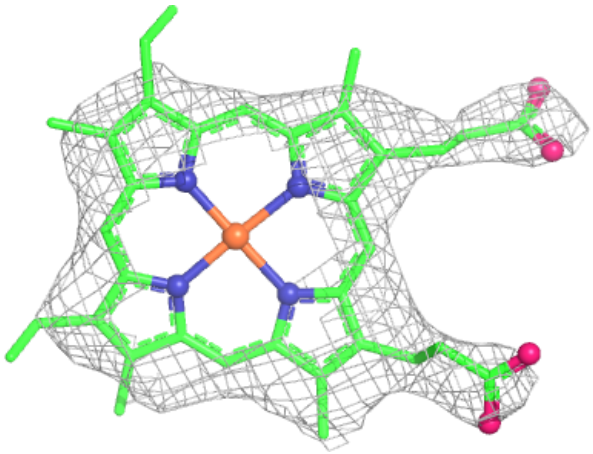


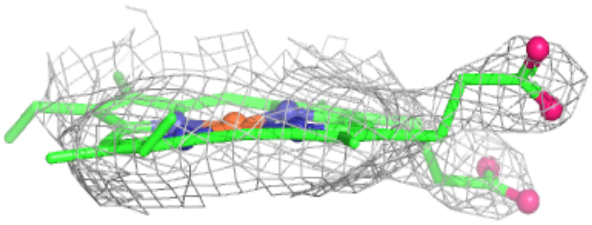


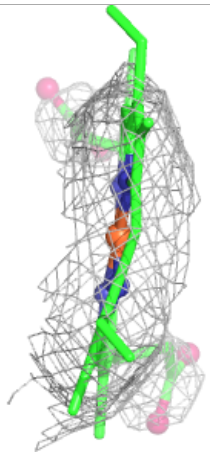


Electron density around HEM A 301:

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

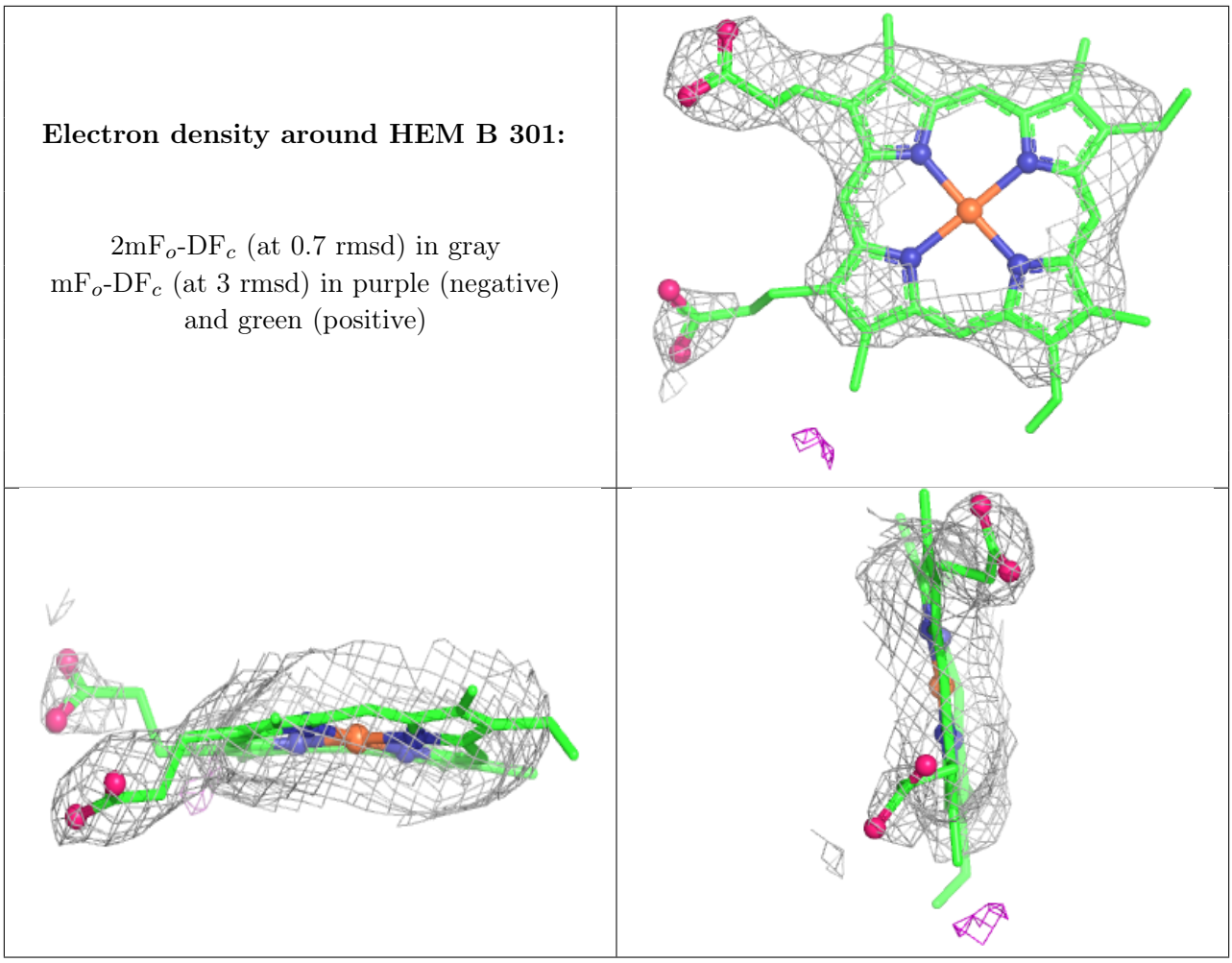






Electron density around HEM B 301:

$2mF_o$-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

There are no such residues in this entry.