wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2024 – 02:42 PM EST

PDB ID	:	1KQF
Title	:	FORMATE DEHYDROGENASE N FROM E. COLI
Authors	:	Jormakka, M.; Tornroth, S.; Byrne, B.; Iwata, S.
Deposited on	:	2002-01-05
Resolution	:	1.60 Å(reported)

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

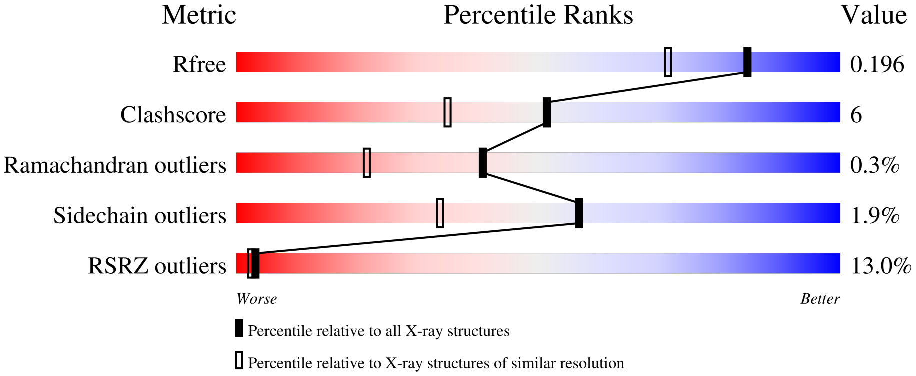
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

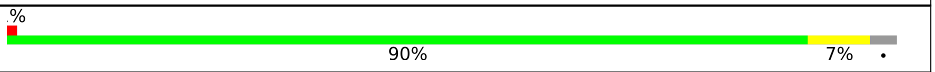
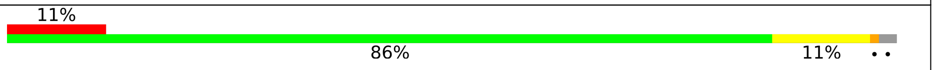
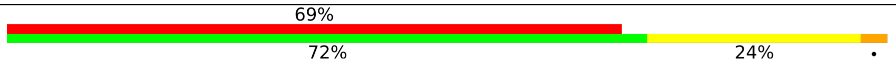
The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	**Whole archive (#Entries)**	**Similar resolution (#Entries, resolution range(Å))**
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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

Mol	**Chain**	**Length**	**Quality of chain**
1	A	1015	
2	B	294	
3	C	217	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13989 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	982	7719	4872	1352	1457	37	1	0	0	0

- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	289	2207	1383	381	421	22	0	0	0

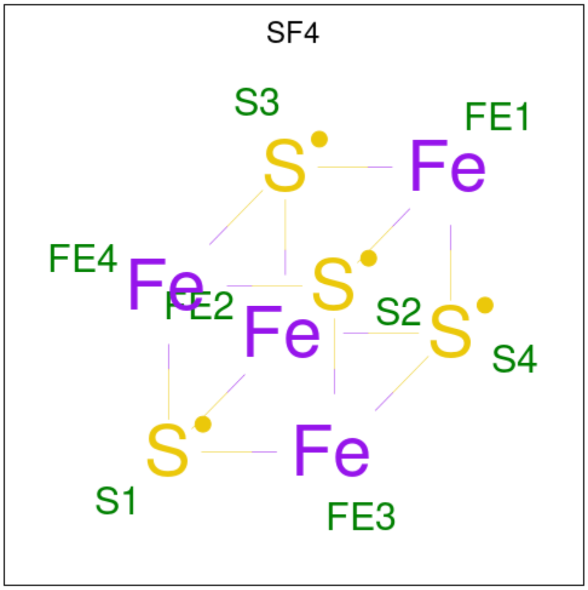
- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	216	1783	1192	301	276	14	0	0	0

- Molecule 4 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

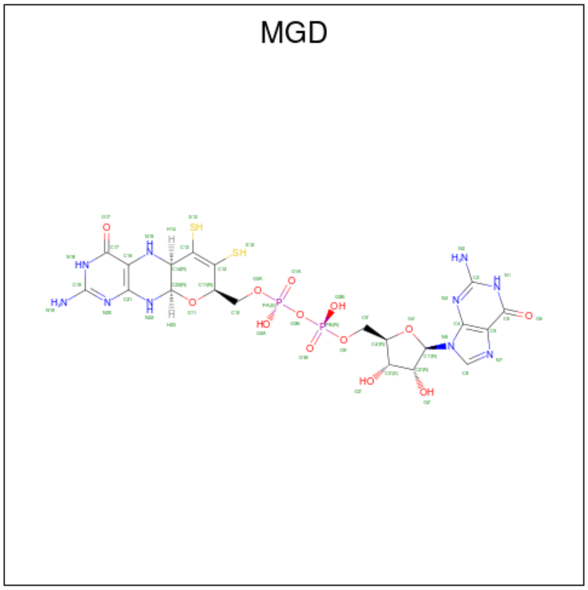
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
4	A	1	1	1	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



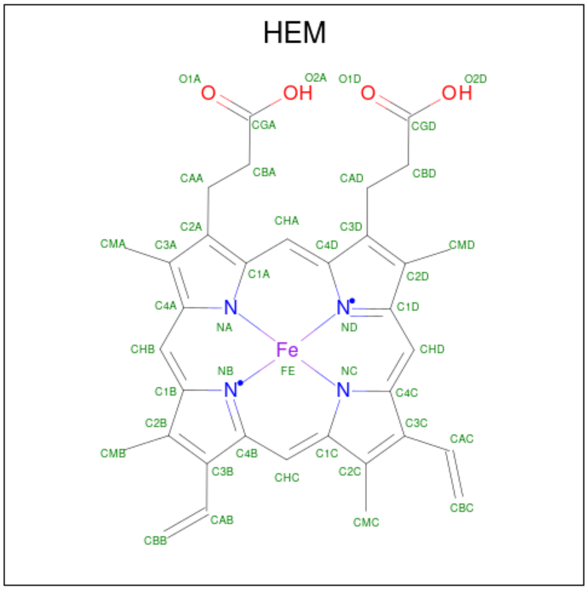
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0
5	B	1	Total Fe S 8 4 4	0	0

- Molecule 6 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P S 47 20 10 13 2 2	0	0
6	A	1	Total C N O P S 47 20 10 13 2 2	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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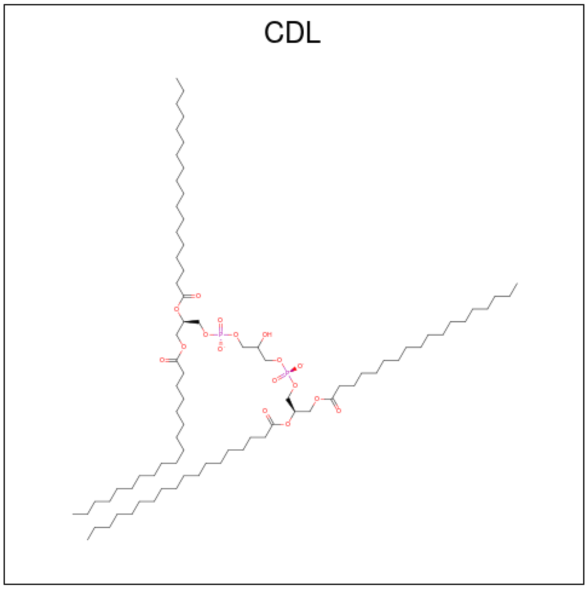
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0

- Molecule 8 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
8	C	1	70	51	17	2	0	0

- Molecule 9 is water.

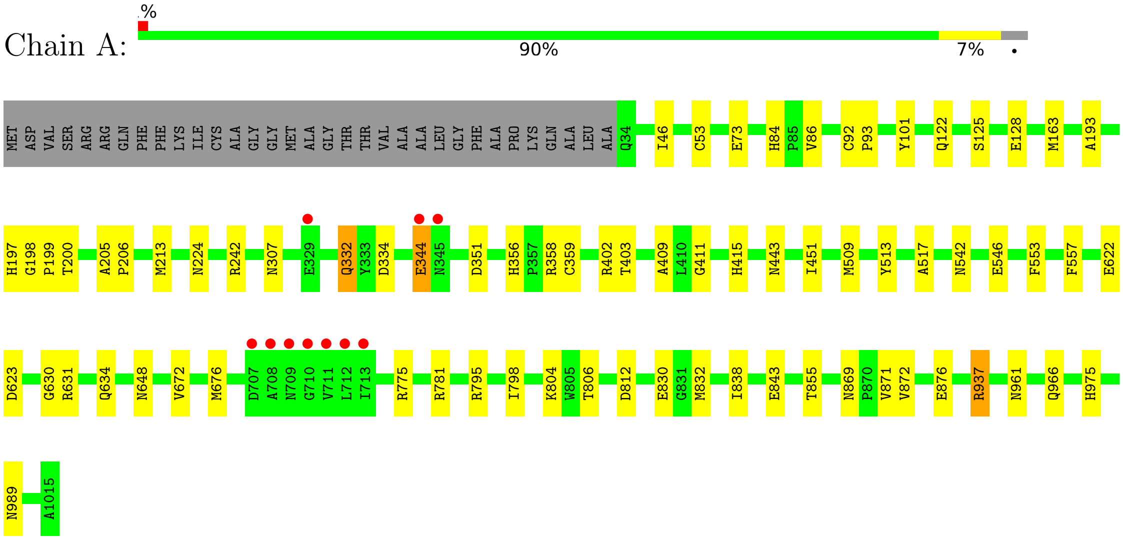
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	1497	1497	1497	0	0
9	B	399	399	399	0	0
9	C	93	93	93	0	0

3 Residue-property plots

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.

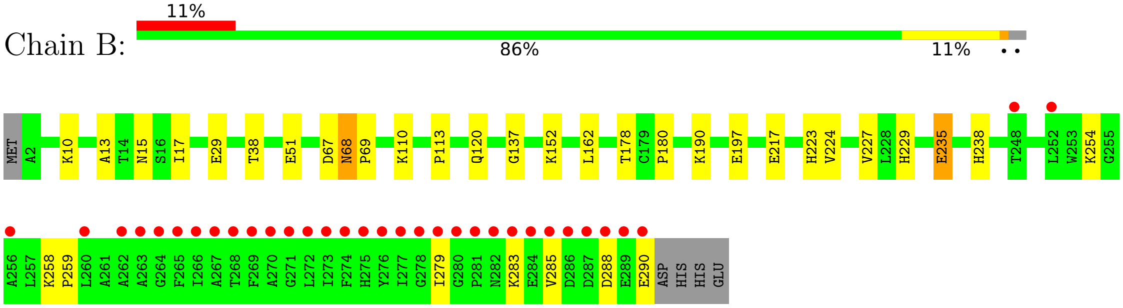
- Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

Chain A:



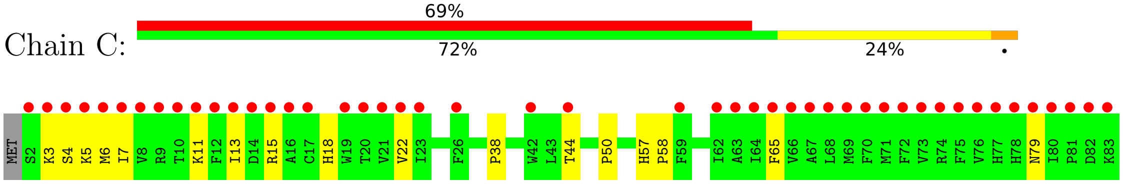
- Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT

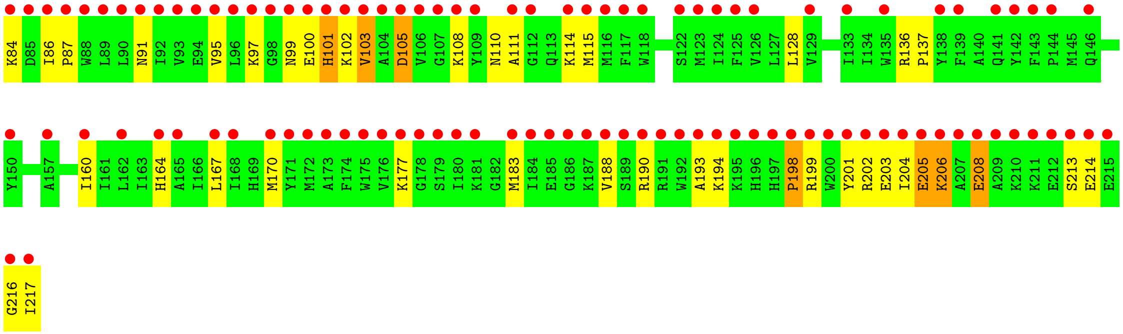
Chain B:



- Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT

Chain C:




K84
D85
I86
P87
W88
L89
L90
N91
I92
V93
E94
V95
L96
K97
G98
N99
E100
H101
K102
V103
A104
D105
V106
G107
K108
Y109
N110
A111
G112
Q113
K114
M115
M116
F117
W118
S122
M123
I124
F125
V126
L127
L128
V129
I133
I134
W135
R136
P137
Y138
F139
A140
Q141
Y142
F143
P144
M145
Q146
Y150
A157
I160
I161
L162
I163
H164
A165
I166
L167
I168
H169
M170
Y171
M172
A173
F174
W175
V176
K177
G178
S179
I180
K181
G182
M183
I184
E185
G186
K187
V188
S189
R190
R191
W192
A193
K194
K195
H196
H197
P198
R199
W200
Y201
R202
E203
I204
E205
K206
A207
E208
A209
K210
K211
E212
S213
E214
E215
G216
I217

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	203.00Å 203.00Å 203.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 39.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-1.60) 94.1 (39.81-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.195 0.183 , 0.196	Depositor DCC
R_{free} test set	3446 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13989	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SEC, CDL, SF4, 6MO, HEM, MGD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.34	0/7910	0.69	2/10749 (0.0%)
2	B	0.32	0/2255	0.68	2/3056 (0.1%)
3	C	0.33	0/1840	0.62	0/2483
All	All	0.33	0/12005	0.68	4/16288 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASP	N-CA-C	-6.00	94.79	111.00
2	B	227	VAL	N-CA-C	-5.85	95.21	111.00
1	A	975	HIS	N-CA-C	5.28	125.26	111.00
2	B	224	VAL	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7719	0	7457	60	0
2	B	2207	0	2140	21	0
3	C	1783	0	1836	57	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	0	0	0
5	B	32	0	0	0	0
6	A	94	0	44	1	0
7	C	86	0	60	2	0
8	C	70	0	83	0	0
9	A	1497	0	0	16	2
9	B	399	0	0	6	0
9	C	93	0	0	10	0
All	All	13989	0	11620	132	2

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 6.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:CYS:HB3	9:A:1672:HOH:O	1.66	0.95
1:A:356:HIS:HD2	1:A:358:ARG:H	1.15	0.93
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.52	0.91
1:A:224:ASN:HD22	1:A:403:THR:H	1.16	0.88
1:A:622:GLU:OE1	1:A:648:ASN:HB2	1.73	0.86

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2324:HOH:O	9:A:2324:HOH:O[6_456]	1.12	1.08
9:A:1746:HOH:O	9:A:1746:HOH:O[6_456]	1.25	0.95

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	979/1015 (96%)	951 (97%)	26 (3%)	2 (0%)	47	26
2	B	287/294 (98%)	278 (97%)	9 (3%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	17	4
All	All	1480/1526 (97%)	1435 (97%)	41 (3%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	409	ALA
1	A	838	ILE
3	C	198	PRO

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	A	815/837 (97%)	807 (99%)	8 (1%)	76	61
2	B	238/243 (98%)	229 (96%)	9 (4%)	33	10
3	C	188/189 (100%)	182 (97%)	6 (3%)	39	15
All	All	1241/1269 (98%)	1218 (98%)	23 (2%)	57	34

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	229	HIS
3	C	101	HIS
2	B	290	GLU
3	C	103	VAL
1	A	855	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	185	HIS
3	C	79	ASN
3	C	196	HIS
3	C	101	HIS
2	B	238	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	MGD	A	1019	4	41,52,52	2.53	10 (24%)	40,81,81	1.89	9 (22%)
5	SF4	B	808	2	0,12,12	-	-	-		
7	HEM	C	810	3	41,50,50	1.64	8 (19%)	45,82,82	1.46	8 (17%)
6	MGD	A	1018	4	41,52,52	2.16	10 (24%)	40,81,81	2.70	10 (25%)
5	SF4	B	806	2	0,12,12	-	-	-		
5	SF4	B	805	2	0,12,12	-	-	-		
8	CDL	C	812	-	69,69,99	2.93	21 (30%)	75,81,111	2.62	16 (21%)
5	SF4	A	1017	1	0,12,12	-	-	-		
7	HEM	C	809	3	41,50,50	1.81	9 (21%)	45,82,82	1.49	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SF4	B	807	2	0,12,12	-	-	-		

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
6	MGD	A	1019	4	-	8/18/66/66	0/6/6/6
5	SF4	B	808	2	-	-	0/6/5/5
7	HEM	C	810	3	-	3/12/54/54	-
6	MGD	A	1018	4	-	6/18/66/66	0/6/6/6
5	SF4	B	806	2	-	-	0/6/5/5
5	SF4	B	805	2	-	-	0/6/5/5
8	CDL	C	812	-	-	38/80/80/110	-
5	SF4	A	1017	1	-	-	0/6/5/5
7	HEM	C	809	3	-	6/12/54/54	-
5	SF4	B	807	2	-	-	0/6/5/5

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	CDL	OB8-CB6	-14.51	1.12	1.45
6	A	1018	MGD	O3A-C10	-9.94	1.06	1.44
6	A	1019	MGD	O3A-C10	-9.74	1.07	1.44
8	C	812	CDL	OA6-CA5	9.73	1.61	1.34
8	C	812	CDL	OB6-CB5	7.65	1.55	1.34

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	812	CDL	OB6-CB5-C51	13.86	141.36	111.50
6	A	1018	MGD	O11-C23-C14	8.99	114.96	108.96
6	A	1018	MGD	O4'-C1'-C2'	-7.53	95.92	106.93
8	C	812	CDL	CB6-OB8-CB7	-7.36	89.86	117.12
8	C	812	CDL	CA6-CA4-CA3	-7.13	94.93	111.79

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1018	MGD	C10-O3A-PA-O1A
6	A	1018	MGD	O4'-C4'-C5'-O5'
6	A	1019	MGD	C5'-O5'-PB-O1B
6	A	1019	MGD	C5'-O5'-PB-O2B
6	A	1019	MGD	C5'-O5'-PB-O3B

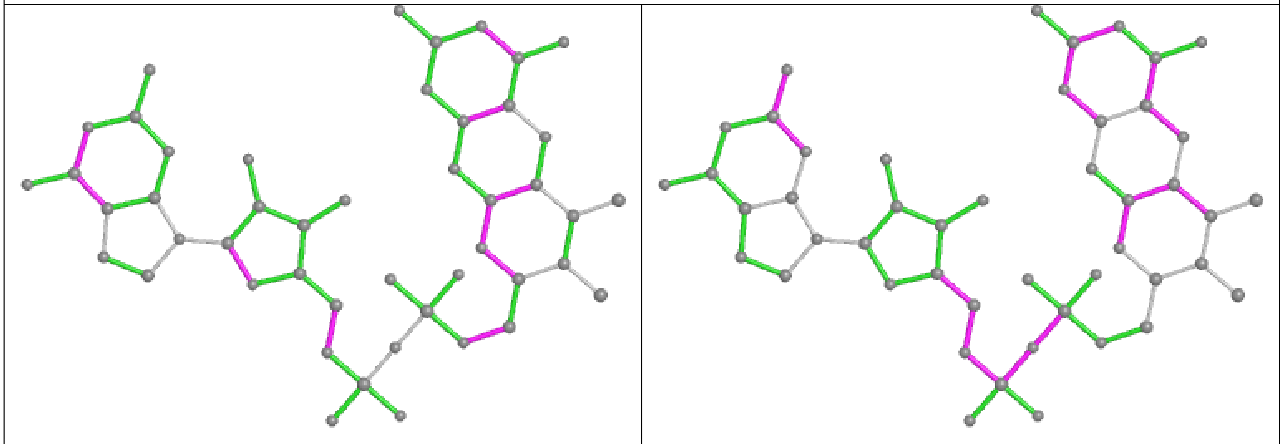
There are no ring outliers.

2 monomers are involved in 3 short contacts:

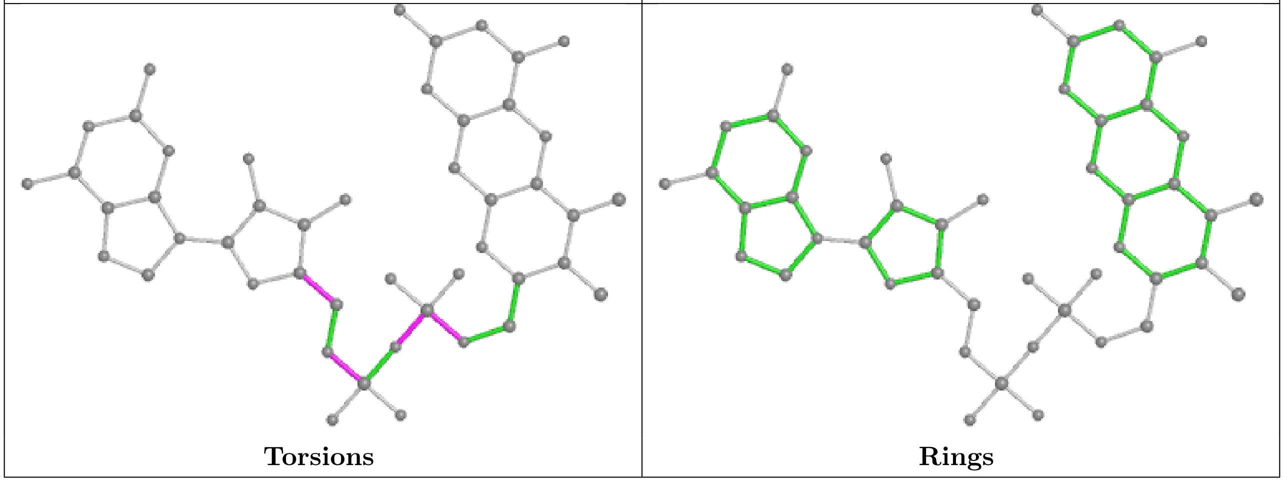
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	810	HEM	2	0
6	A	1018	MGD	1	0

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

Ligand MGD A 1019

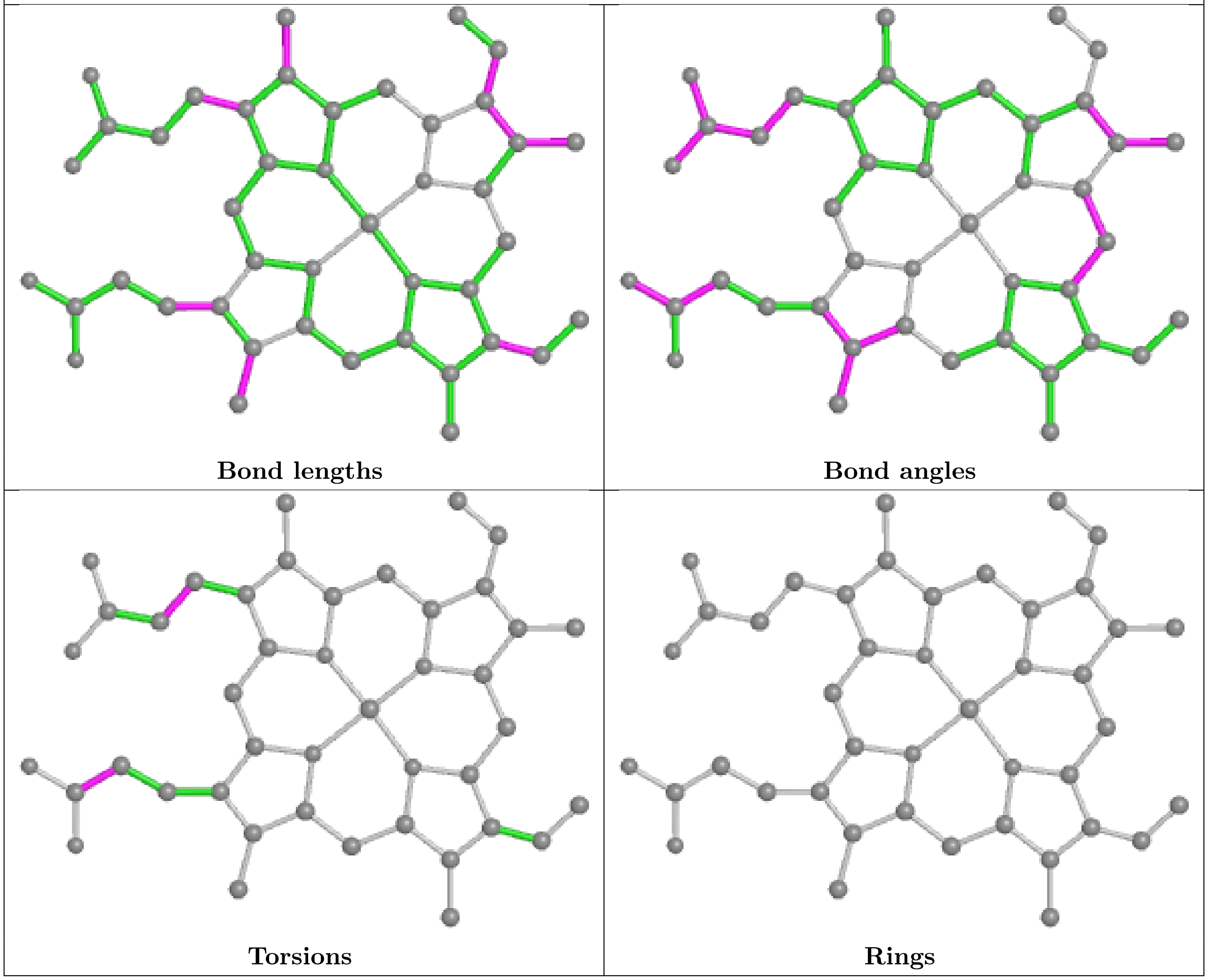


Bond lengths **Bond angles**



Torsions **Rings**

Ligand HEM C 810



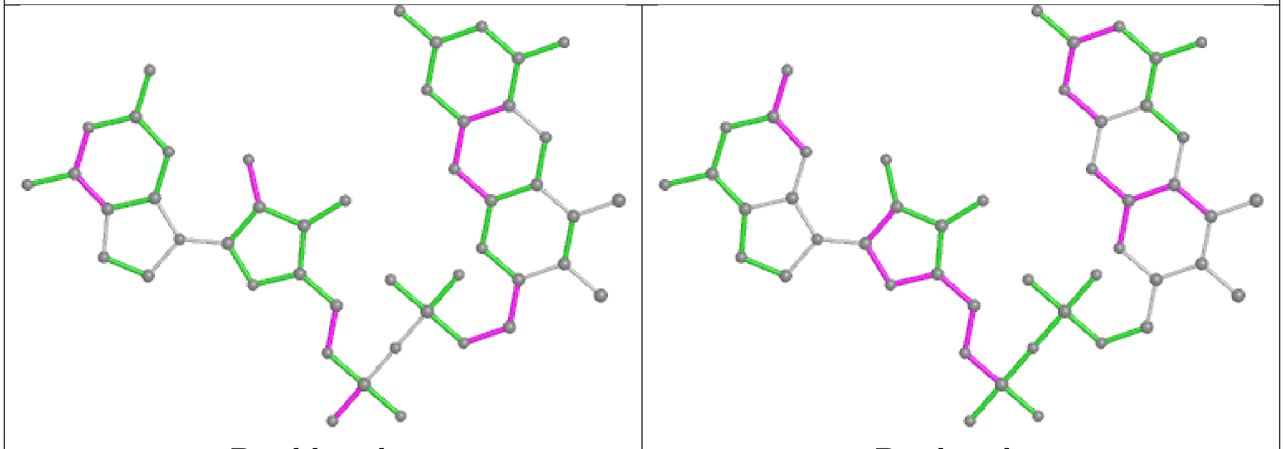
Bond lengths

Bond angles

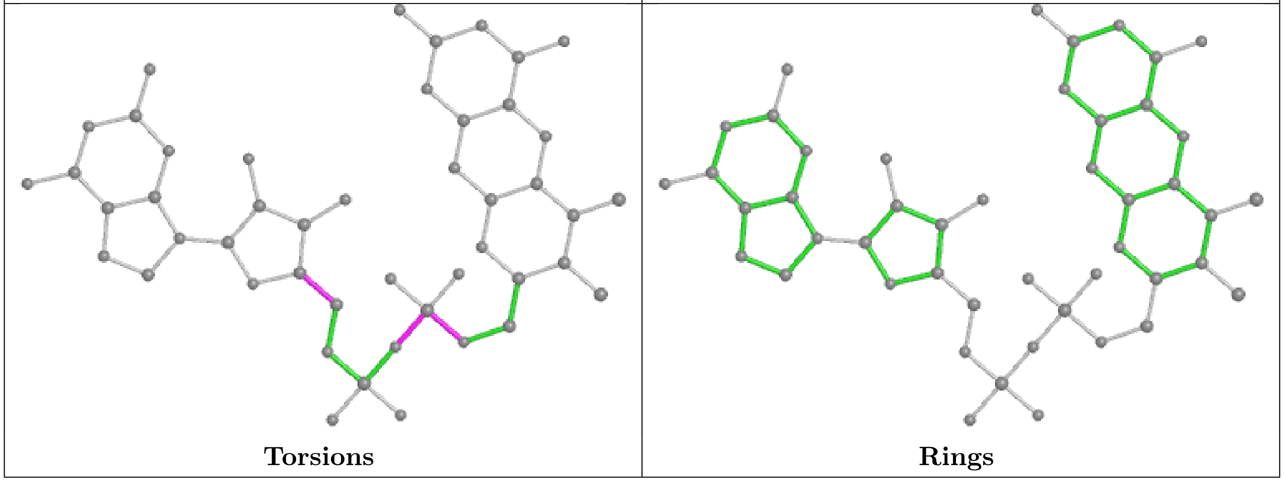
Torsions

Rings

Ligand MGD A 1018

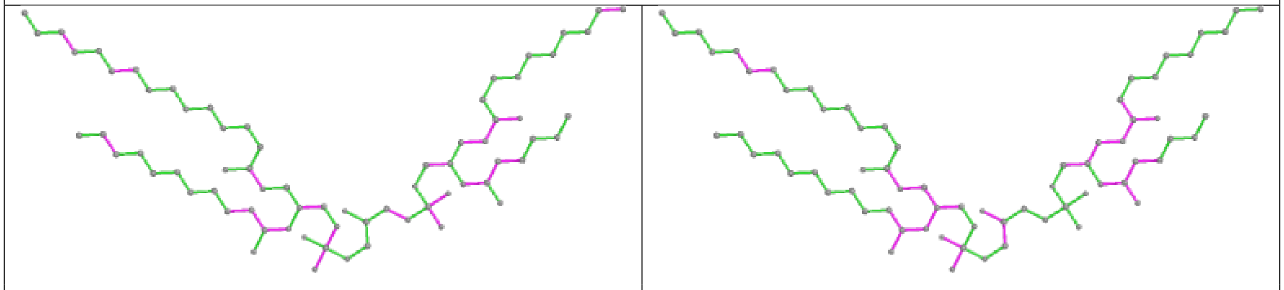


Bond lengths **Bond angles**

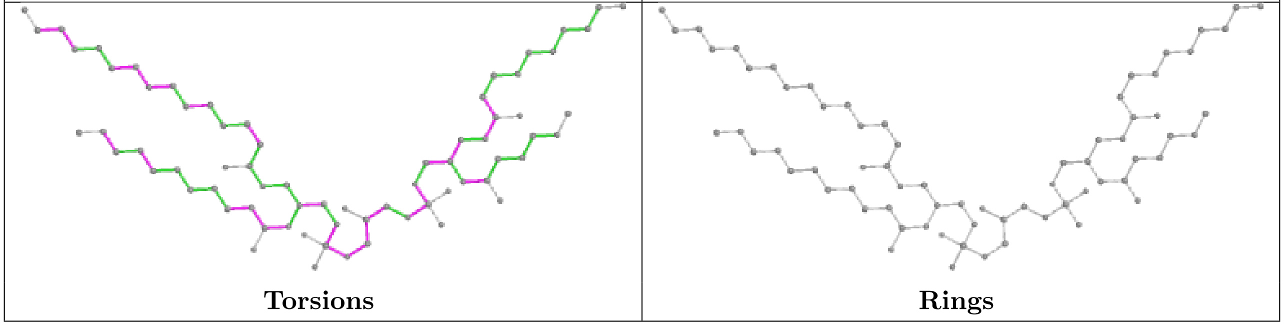


Torsions **Rings**

Ligand CDL C 812

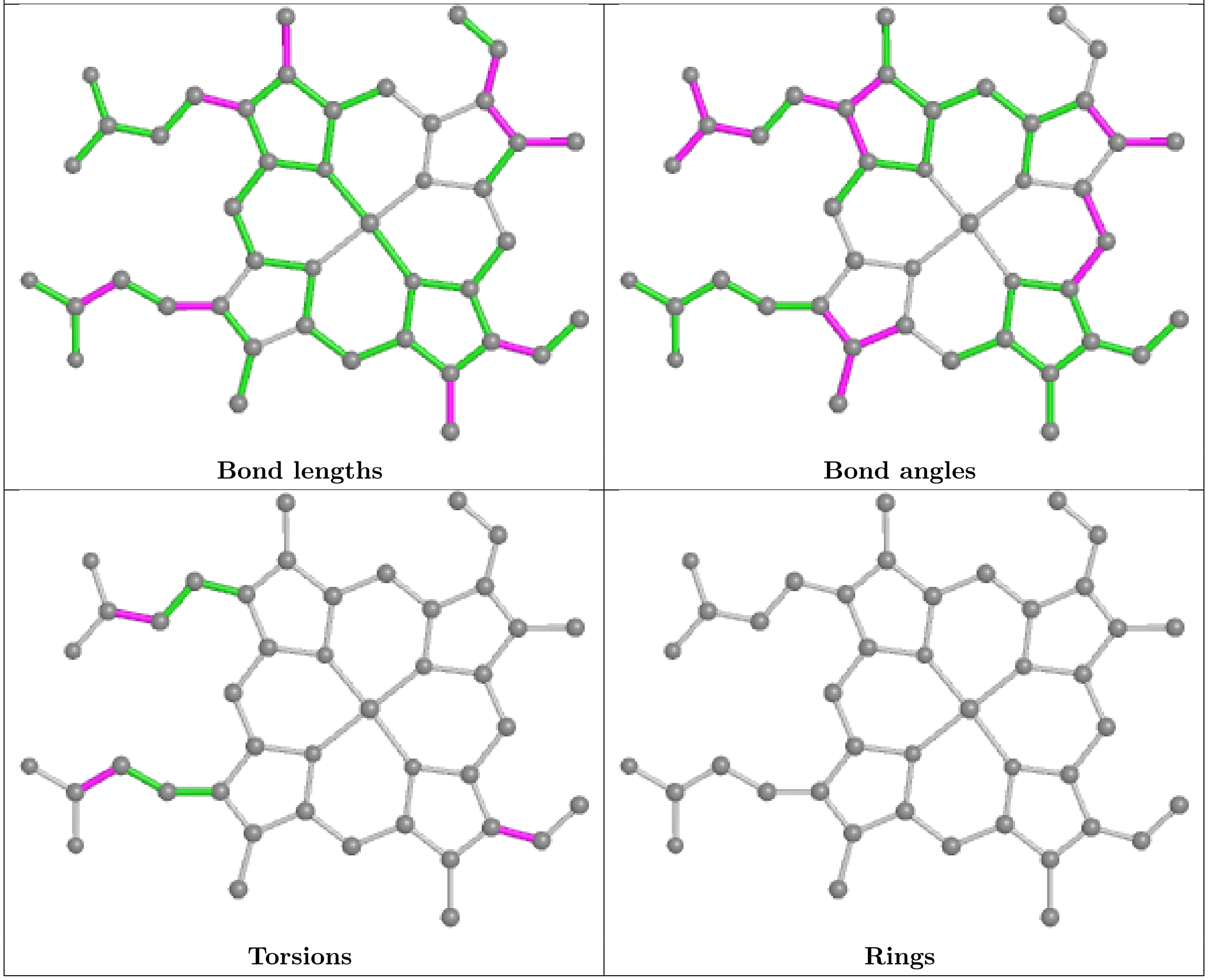


Bond lengths **Bond angles**



Torsions **Rings**

Ligand HEM C 809



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	981/1015 (96%)	-0.20	10 (1%) 82 82	11, 18, 30, 56	0
2	B	289/294 (98%)	0.47	33 (11%) 5 4	11, 18, 52, 67	0
3	C	216/217 (99%)	3.97	150 (69%) 0 0	30, 49, 63, 65	0
All	All	1486/1526 (97%)	0.54	193 (12%) 3 2	11, 19, 54, 67	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	217	ILE	18.4
3	C	207	ALA	14.5
2	B	285	VAL	13.5
3	C	209	ALA	12.2
3	C	216	GLY	12.1

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 monosaccharides in this entry.

6.4 Ligands

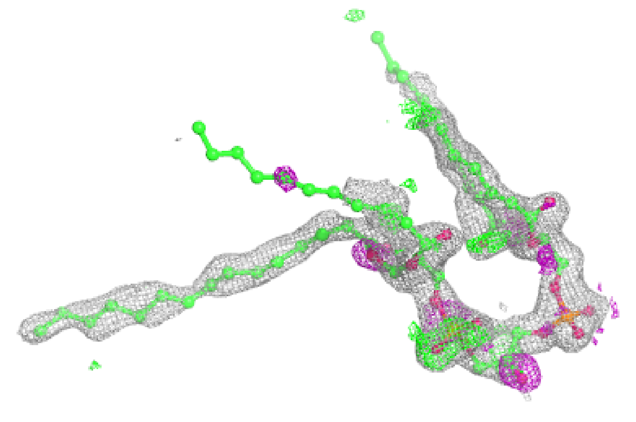
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

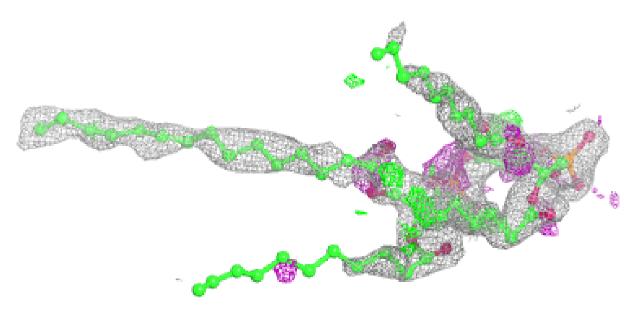
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
8	CDL	C	812	70/100	0.76	0.26	44,56,61,61	0
7	HEM	C	810	43/43	0.87	0.25	44,45,48,49	0
7	HEM	C	809	43/43	0.92	0.15	29,33,35,37	0
6	MGD	A	1019	47/47	0.96	0.12	11,14,16,18	0
6	MGD	A	1018	47/47	0.96	0.11	11,13,14,15	0
5	SF4	B	808	8/8	0.98	0.07	16,18,19,19	0
5	SF4	B	807	8/8	0.98	0.08	14,15,16,16	0
5	SF4	B	806	8/8	0.99	0.09	12,13,13,13	0
4	6MO	A	1016	1/1	0.99	0.09	16,16,16,16	0
5	SF4	A	1017	8/8	0.99	0.10	11,12,12,12	0
5	SF4	B	805	8/8	0.99	0.09	12,13,13,14	0

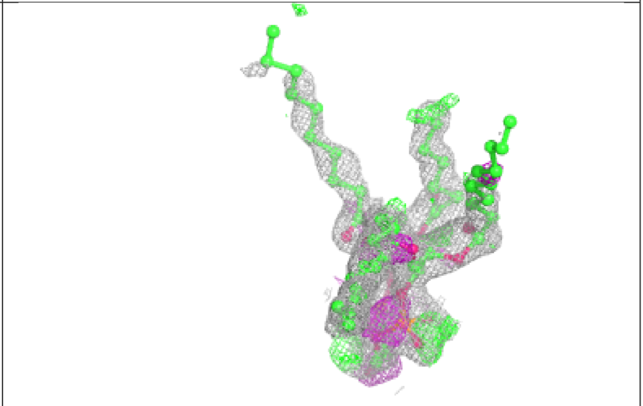
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL C 812:

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

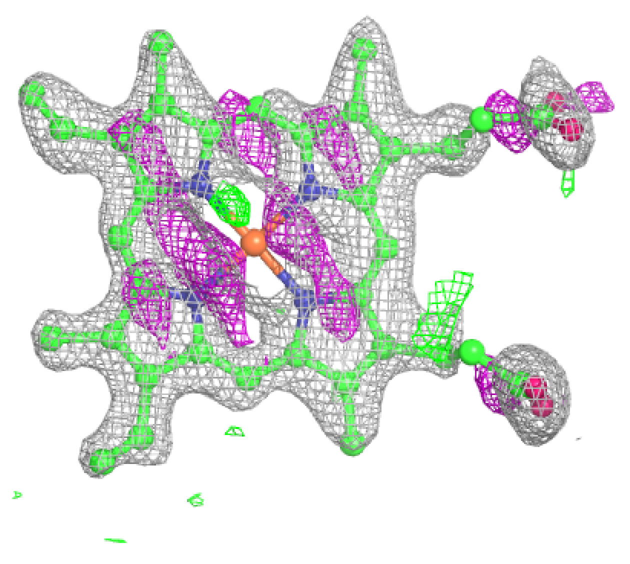


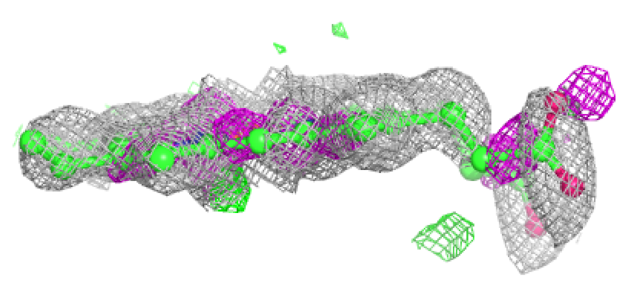


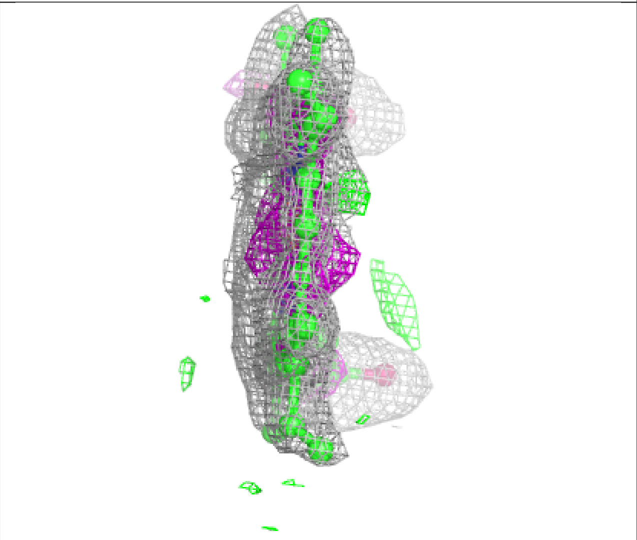


Electron density around HEM C 810:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

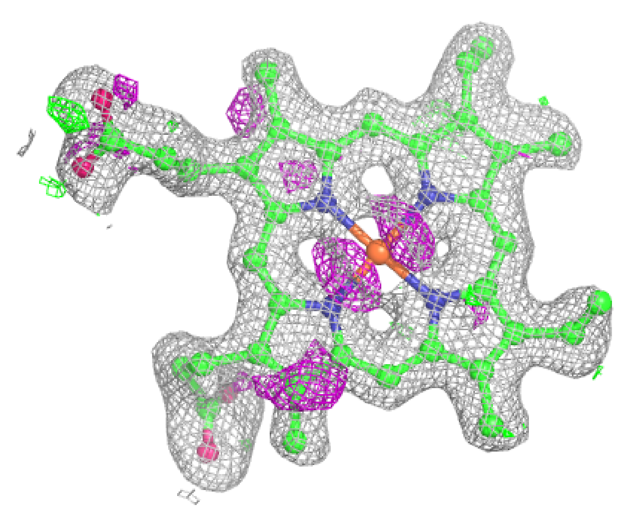


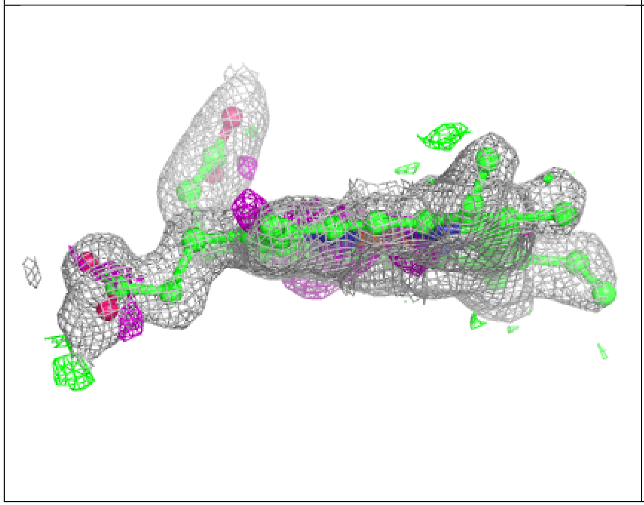


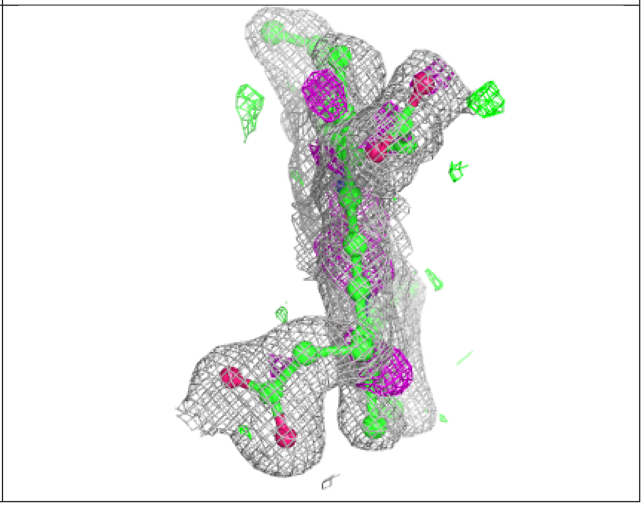


Electron density around HEM C 809:

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

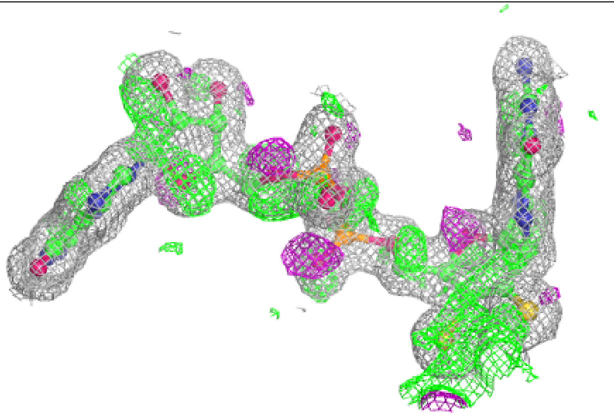


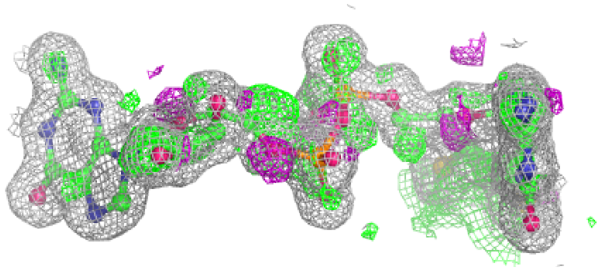


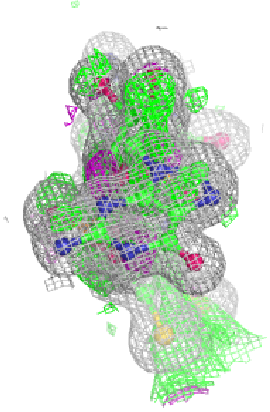


Electron density around MGD A 1019:

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







Electron density around MGD A 1018:

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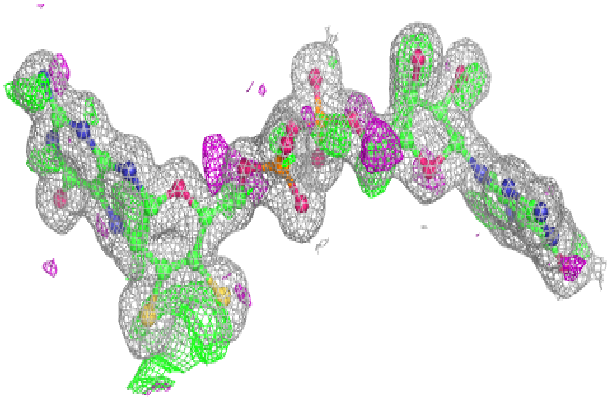
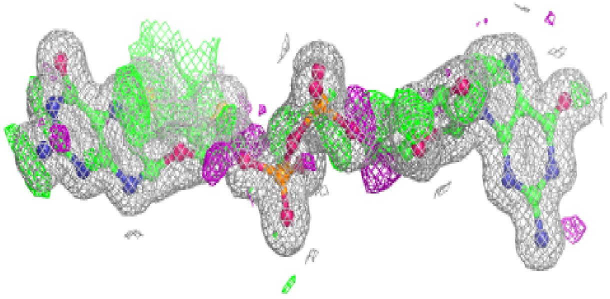
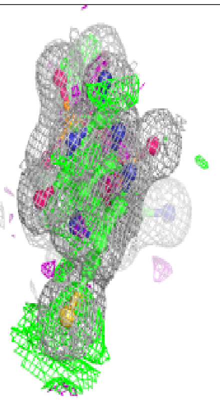
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers ⓘ

There are no such residues in this entry.