



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:04 PM BST

PDB ID : 4QI7
Title : Cellobiose dehydrogenase from *Neurospora crassa*, NcCDH
Authors : Tan, T.C.; Gandini, R.; Sygmund, C.; Kittl, R.; Haltrich, D.; Ludwig, R.;
Hallberg, B.M.; Divne, C.
Deposited on : 2014-05-30
Resolution : 2.90 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 : 2.13.1
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) : 2.13.1

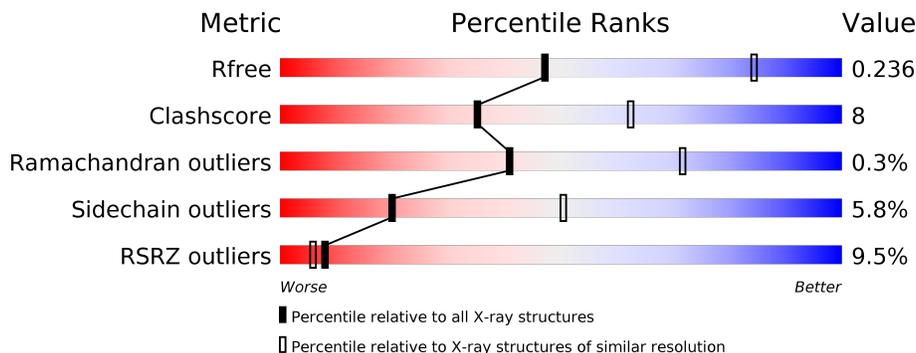
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

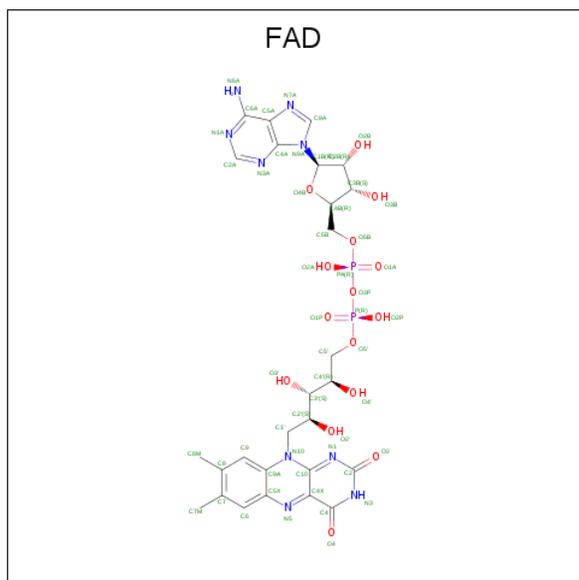
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	806	
1	B	806	

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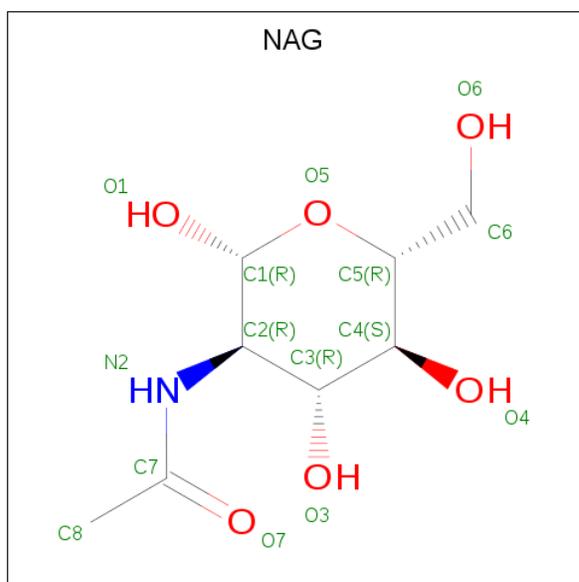
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



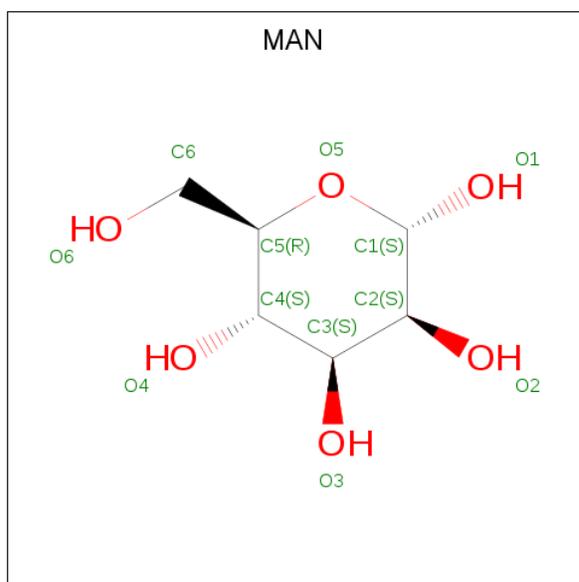
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0

- Molecule 6 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	8	Total Pt 8 8	0	0
6	A	12	Total Pt 12 12	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	A	3	Total Mg 3 3	0	0

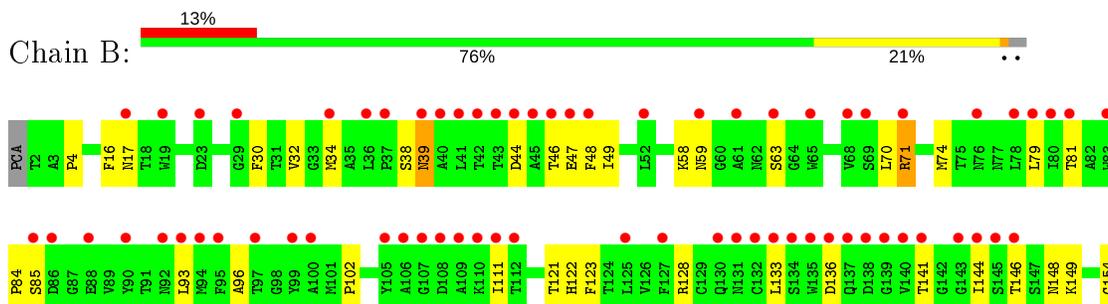
3 Residue-property plots [i](#)

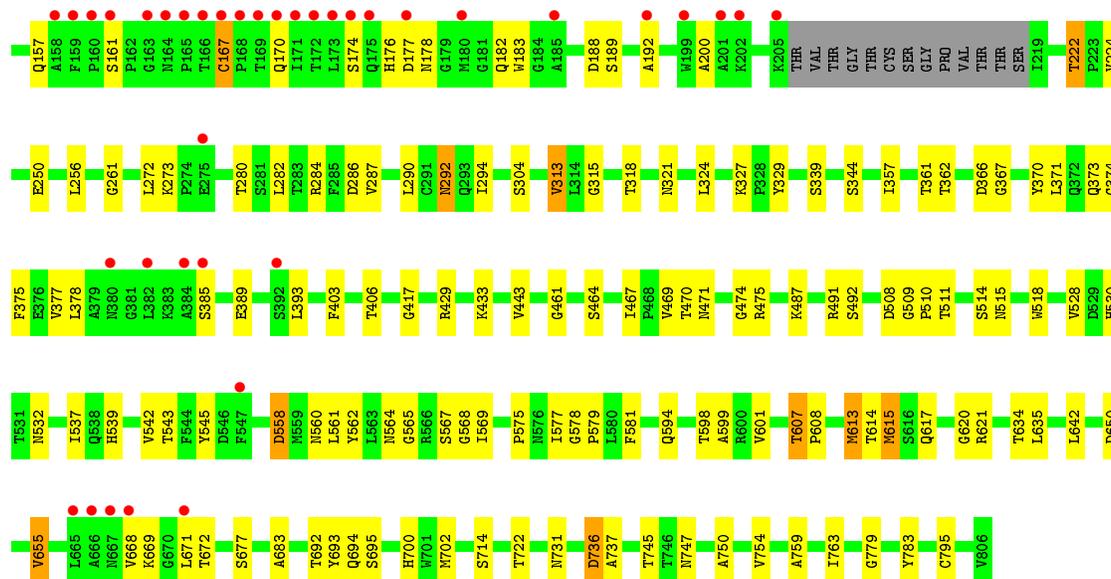
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cellobiose dehydrogenase



- Molecule 1: Cellobiose dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.60Å 141.85Å 147.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.04 – 2.90 58.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.04-2.90) 99.9 (58.64-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1477)	Depositor
R, R_{free}	0.185 , 0.235 0.188 , 0.236	Depositor DCC
R_{free} test set	1995 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.068 for -h,l,k	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12482	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: MG, NAG, PT, HEM, FAD, MAN

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	0.47	0/6214	0.67	0/8481
1	B	0.46	1/6130 (0.0%)	0.66	0/8362
All	All	0.47	1/12344 (0.0%)	0.66	0/16843

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	THR	C-N	-5.71	1.23	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	SER	Peptide
1	B	470	THR	Peptide

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	6061	0	5828	99	0
1	B	5979	0	5749	100	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
3	A	53	0	31	5	0
3	B	53	0	31	3	0
4	A	98	0	91	5	0
4	B	84	0	78	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
6	A	12	0	0	0	0
6	B	8	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
All	All	12482	0	11908	201	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 201 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:B:4:PRO:HB2	1:B:17:ASN:HD22	1.41	0.83
1:B:176:HIS:CE1	2:B:901:HEM:NA	2.48	0.81
1:A:79:LEU:HD22	2:A:901:HEM:HAC	1.67	0.76
1:A:63:SER:HA	1:A:161:SER:HB3	1.67	0.76
1:B:133:LEU:HD22	1:B:144:ILE:HD11	1.68	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	803/806 (100%)	766 (95%)	35 (4%)	2 (0%)	47	78
1	B	788/806 (98%)	752 (95%)	34 (4%)	2 (0%)	41	71
All	All	1591/1612 (99%)	1518 (95%)	69 (4%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	ASN
1	A	605	PHE
1	B	736	ASP
1	A	219	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	643/643 (100%)	610 (95%)	33 (5%)	24	56
1	B	632/643 (98%)	591 (94%)	41 (6%)	17	45
All	All	1275/1286 (99%)	1201 (94%)	74 (6%)	20	50

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	32	VAL
1	B	222	THR

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Mol	Chain	Res	Type
1	B	669	LYS
1	B	34	MET
1	B	85	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	705	ASN
1	B	17	ASN
1	B	182	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 24 are monoatomic - leaving 21 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	MAN	B	909	1	11,11,12	1.99	2 (18%)	15,15,17	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	908	1	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
5	MAN	B	910	1	11,11,12	2.45	6 (54%)	15,15,17	1.23	1 (6%)
4	NAG	B	907	1	14,14,15	0.54	0	17,19,21	0.64	0
4	NAG	A	907	1	14,14,15	0.26	0	17,19,21	0.83	1 (5%)
4	NAG	A	903	1	14,14,15	0.33	0	17,19,21	0.32	0
2	HEM	A	901	1	27,50,50	2.49	10 (37%)	17,82,82	3.09	10 (58%)
4	NAG	A	904	1	14,14,15	0.33	0	17,19,21	0.58	0
5	MAN	A	911	1	11,11,12	1.94	5 (45%)	15,15,17	1.01	0
4	NAG	B	905	1	14,14,15	0.36	0	17,19,21	0.46	0
4	NAG	B	904	1	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	B	903	1	14,14,15	0.22	0	17,19,21	0.67	0
4	NAG	B	908	1	14,14,15	0.63	1 (7%)	17,19,21	0.60	0
5	MAN	A	910	1	11,11,12	1.11	2 (18%)	15,15,17	1.56	3 (20%)
3	FAD	B	902	-	51,58,58	1.34	5 (9%)	60,89,89	1.66	12 (20%)
4	NAG	B	906	1	14,14,15	0.21	0	17,19,21	0.73	1 (5%)
3	FAD	A	902	-	51,58,58	1.42	7 (13%)	60,89,89	1.57	10 (16%)
2	HEM	B	901	1	27,50,50	2.71	9 (33%)	17,82,82	2.98	7 (41%)
4	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	A	906	1	14,14,15	0.87	1 (7%)	17,19,21	1.49	1 (5%)
4	NAG	A	909	1	14,14,15	0.30	0	17,19,21	0.50	0

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	MAN	B	909	1	-	2/2/19/22	0/1/1/1
4	NAG	A	908	1	-	2/6/23/26	0/1/1/1
5	MAN	B	910	1	-	2/2/19/22	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	2/6/23/26	0/1/1/1
4	NAG	A	903	1	-	2/6/23/26	0/1/1/1
2	HEM	A	901	1	-	3/6/54/54	-
4	NAG	A	904	1	-	4/6/23/26	0/1/1/1
5	MAN	A	911	1	-	2/2/19/22	0/1/1/1
4	NAG	B	905	1	-	2/6/23/26	0/1/1/1
4	NAG	B	904	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1
5	MAN	A	910	1	-	2/2/19/22	0/1/1/1
3	FAD	B	902	-	-	4/30/50/50	0/6/6/6
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
3	FAD	A	902	-	-	7/30/50/50	0/6/6/6
2	HEM	B	901	1	-	0/6/54/54	-
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	906	1	-	4/6/23/26	0/1/1/1
4	NAG	A	909	1	-	0/6/23/26	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C1A-NA	6.41	1.49	1.36
2	B	901	HEM	C4A-NA	6.36	1.49	1.36
2	A	901	HEM	C1A-NA	6.09	1.48	1.36
2	B	901	HEM	C3C-C2C	6.02	1.48	1.40
2	A	901	HEM	C4A-NA	5.46	1.47	1.36

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	HEM	C1D-C2D-C3D	-8.06	101.39	107.00
2	A	901	HEM	C1D-C2D-C3D	-7.83	101.55	107.00
3	A	902	FAD	C4-N3-C2	6.23	120.41	115.14
3	B	902	FAD	C4-N3-C2	6.17	120.35	115.14
2	B	901	HEM	C3B-C4B-NB	5.23	115.97	109.21

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

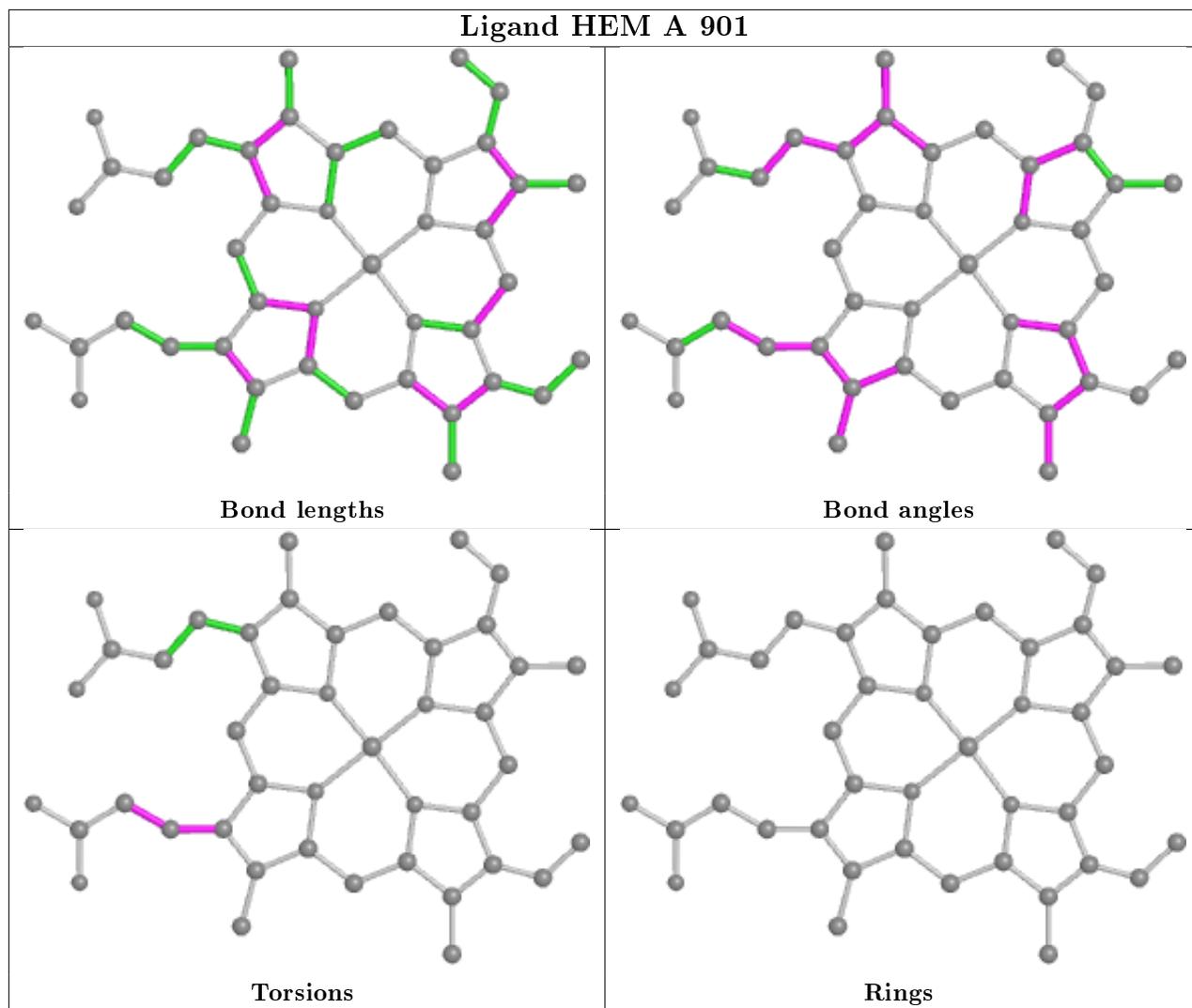
Mol	Chain	Res	Type	Atoms
3	B	902	FAD	C2'-C1'-N10-C9A
3	B	902	FAD	N10-C1'-C2'-O2'
3	A	902	FAD	C2'-C1'-N10-C9A
3	A	902	FAD	N10-C1'-C2'-O2'
3	A	902	FAD	N10-C1'-C2'-C3'

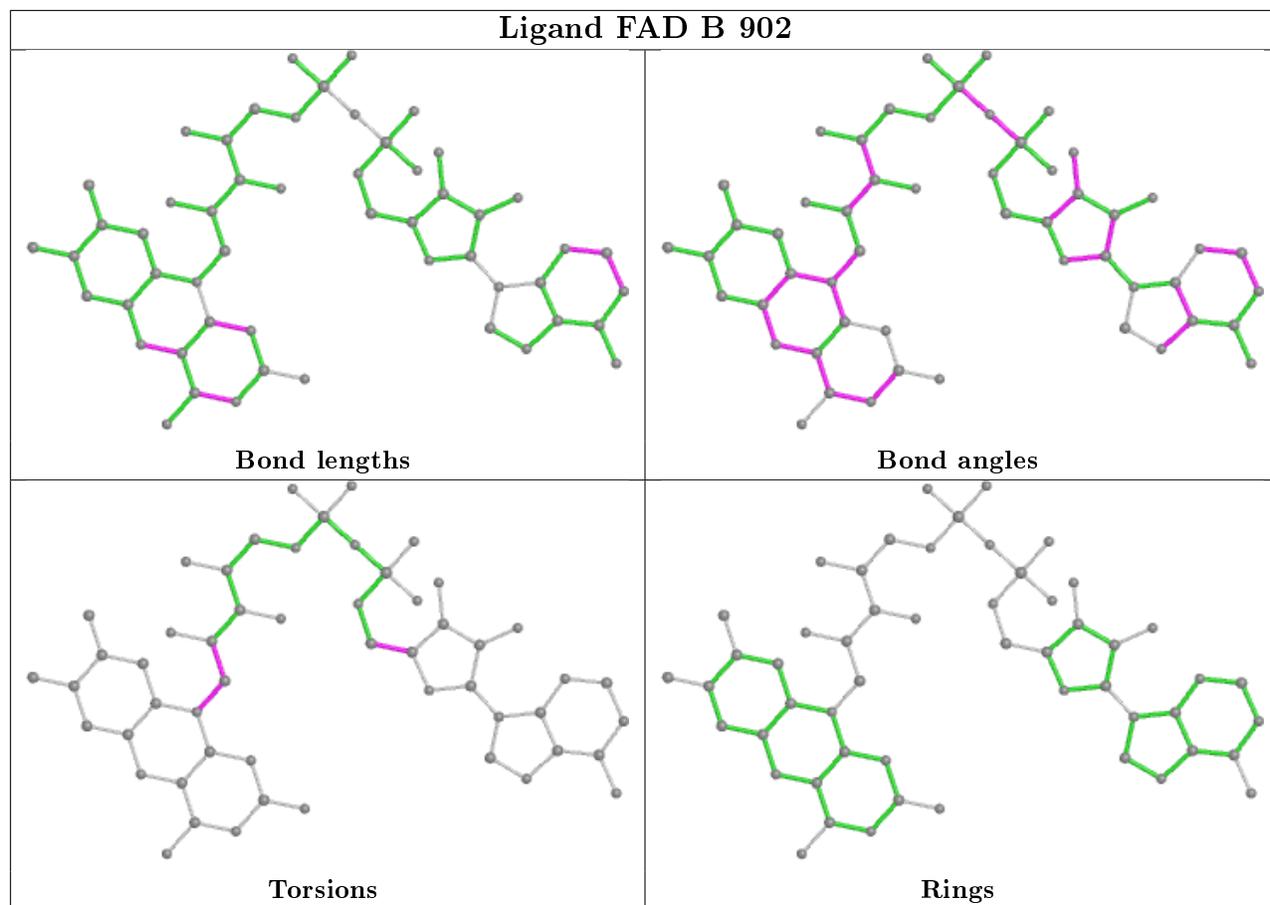
There are no ring outliers.

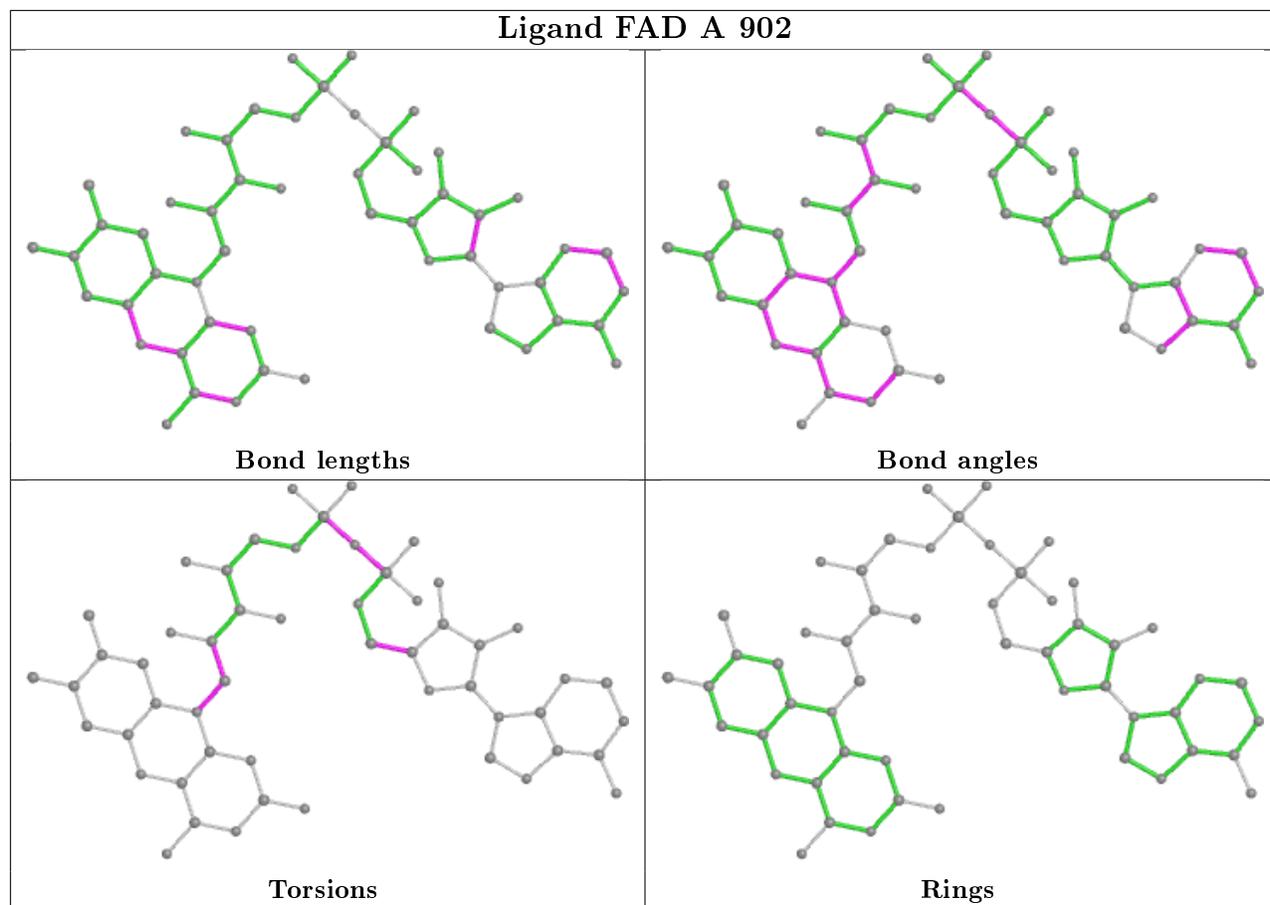
8 monomers are involved in 28 short contacts:

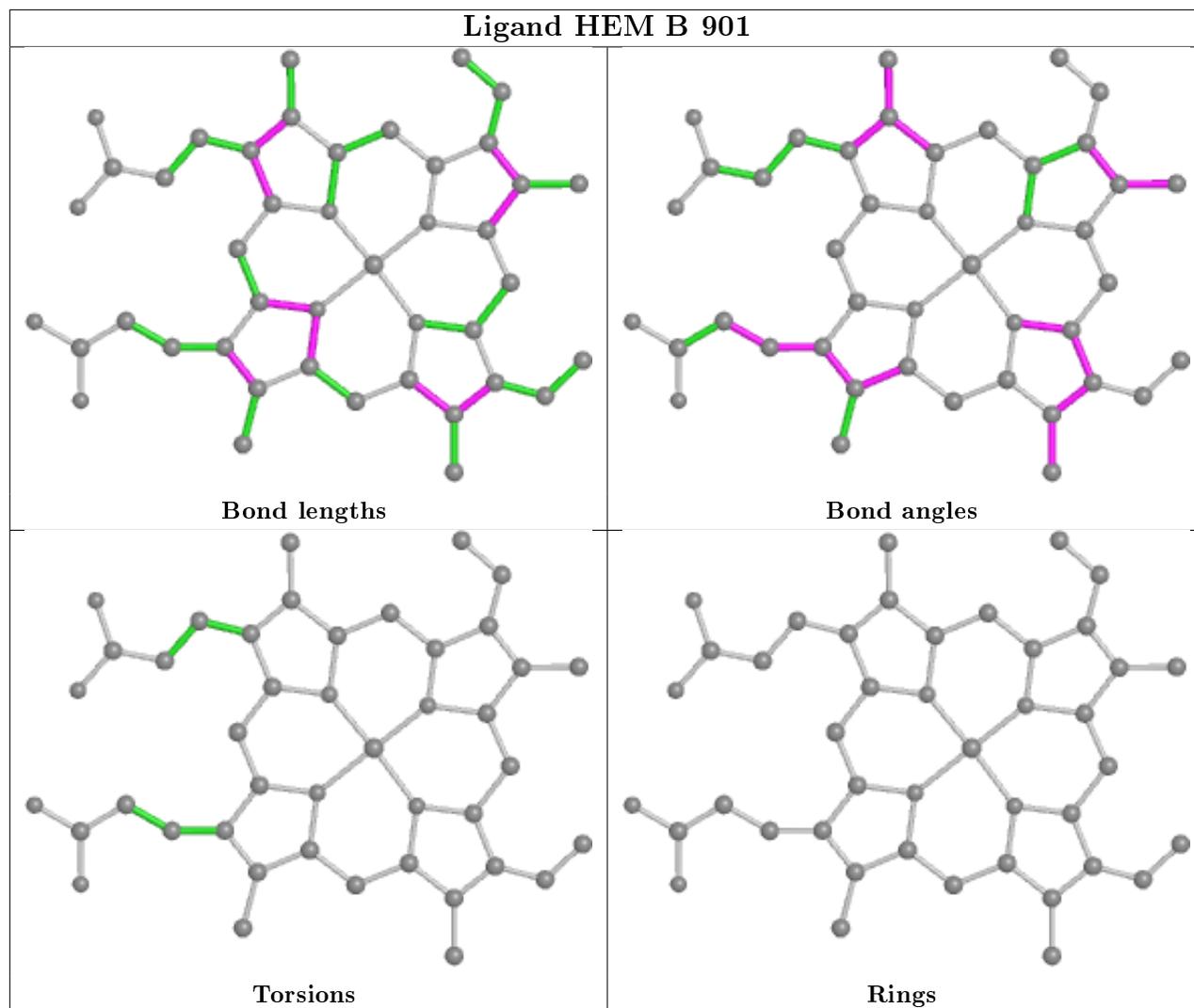
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	NAG	1	0
4	A	903	NAG	2	0
2	A	901	HEM	6	0
4	A	904	NAG	1	0
3	B	902	FAD	3	0
3	A	902	FAD	5	0
2	B	901	HEM	9	0
4	A	906	NAG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	805/806 (99%)	0.27	47 (5%) 23 19	22, 69, 122, 179	0
1	B	792/806 (98%)	0.61	105 (13%) 3 2	25, 75, 149, 196	0
All	All	1597/1612 (99%)	0.44	152 (9%) 8 6	22, 71, 138, 196	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	8.0
1	B	136	ASP	6.6
1	B	132	CYS	6.2
1	B	171	ILE	6.1
1	B	140	VAL	5.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

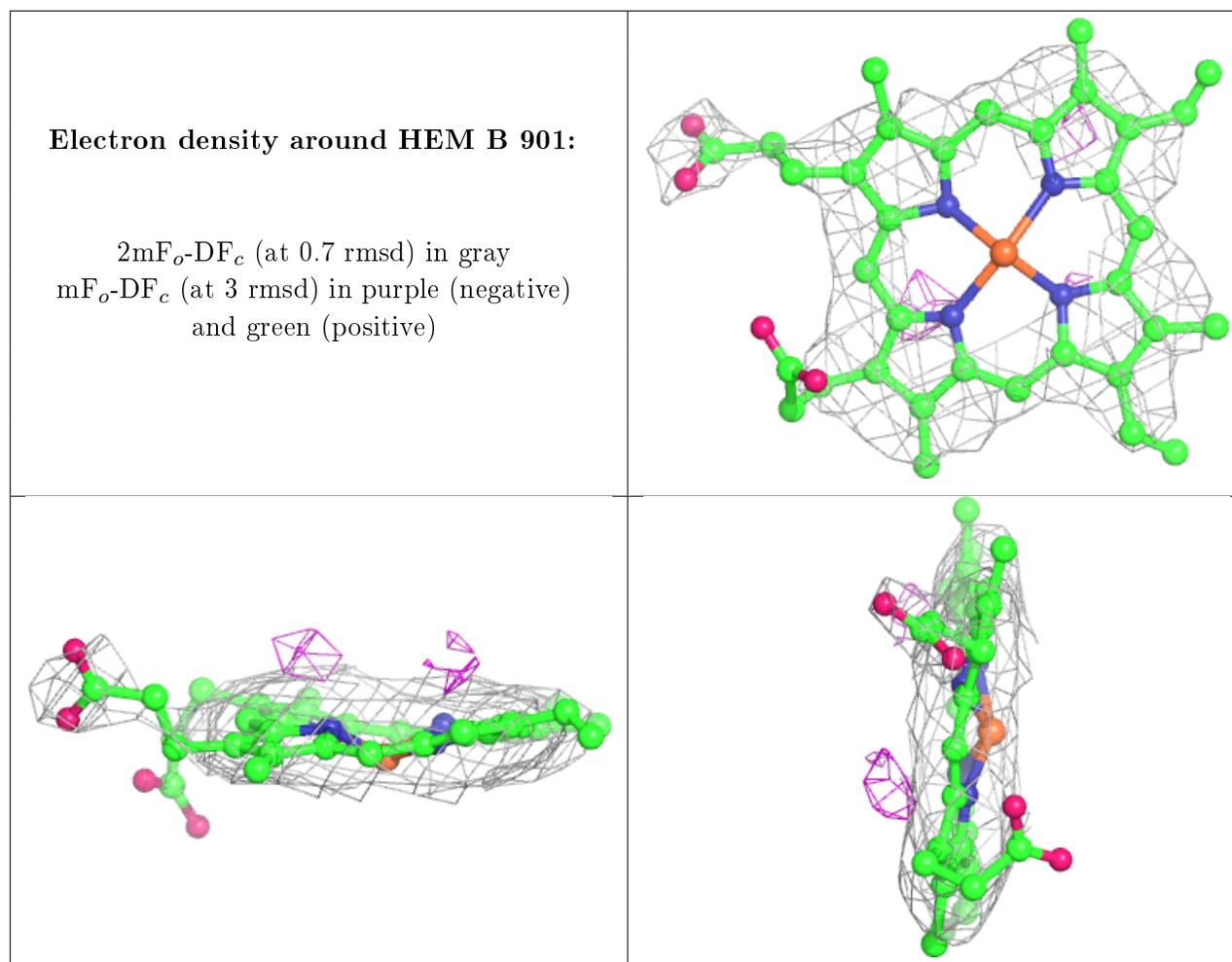
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	906	14/15	0.76	0.37	72,105,123,124	0
6	PT	B	915	1/1	0.78	0.15	164,164,164,164	1
7	MG	A	924	1/1	0.82	0.62	73,73,73,73	0
4	NAG	A	904	14/15	0.84	0.41	90,104,121,121	0
4	NAG	B	903	14/15	0.84	0.22	98,111,115,117	0
6	PT	B	912	1/1	0.84	0.21	147,147,147,147	1
5	MAN	B	910	11/12	0.86	0.30	61,92,106,106	0
4	NAG	B	907	14/15	0.86	0.28	86,119,129,129	0
4	NAG	B	904	14/15	0.86	0.24	85,104,111,123	0
6	PT	A	921	1/1	0.87	0.42	282,282,282,282	0
5	MAN	B	909	11/12	0.88	0.29	73,81,96,96	0
6	PT	A	914	1/1	0.89	0.19	156,156,156,156	1
4	NAG	A	903	14/15	0.90	0.30	96,105,116,123	0
5	MAN	A	911	11/12	0.90	0.30	89,101,108,109	0
6	PT	A	915	1/1	0.90	0.07	155,155,155,155	1
4	NAG	B	908	14/15	0.90	0.22	75,91,103,106	0
5	MAN	A	910	11/12	0.91	0.17	91,100,115,119	0
4	NAG	A	908	14/15	0.91	0.25	83,106,124,129	0
7	MG	B	919	1/1	0.92	0.24	54,54,54,54	0
6	PT	A	920	1/1	0.92	0.15	114,114,114,114	1
6	PT	B	913	1/1	0.93	0.07	146,146,146,146	1
4	NAG	B	906	14/15	0.94	0.15	59,75,109,118	0
7	MG	A	925	1/1	0.94	0.43	54,54,54,54	0
6	PT	A	918	1/1	0.95	0.17	123,123,123,123	1
4	NAG	B	905	14/15	0.95	0.22	81,99,103,107	0
6	PT	B	914	1/1	0.95	0.15	134,134,134,134	1
4	NAG	A	907	14/15	0.95	0.12	63,76,109,116	0
4	NAG	A	909	14/15	0.95	0.27	66,83,98,100	0
7	MG	A	926	1/1	0.95	0.25	56,56,56,56	0
6	PT	A	913	1/1	0.95	0.19	120,120,120,120	0
6	PT	B	918	1/1	0.95	0.19	132,132,132,132	0
6	PT	A	916	1/1	0.96	0.15	117,117,117,117	1
6	PT	B	916	1/1	0.96	0.18	106,106,106,106	1
2	HEM	B	901	43/43	0.96	0.33	60,86,110,126	0
2	HEM	A	901	43/43	0.96	0.24	55,78,100,129	0
3	FAD	A	902	53/53	0.97	0.19	20,52,93,102	0
3	FAD	B	902	53/53	0.97	0.18	20,54,90,97	0
6	PT	A	917	1/1	0.97	0.14	151,151,151,151	1
4	NAG	A	905	14/15	0.97	0.15	79,96,105,113	0
6	PT	A	922	1/1	0.97	0.23	133,133,133,133	0
6	PT	A	919	1/1	0.98	0.18	107,107,107,107	0
6	PT	B	917	1/1	0.98	0.19	102,102,102,102	0
6	PT	A	912	1/1	0.99	0.25	84,84,84,84	0

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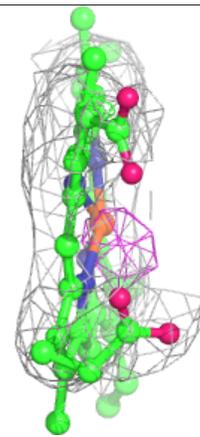
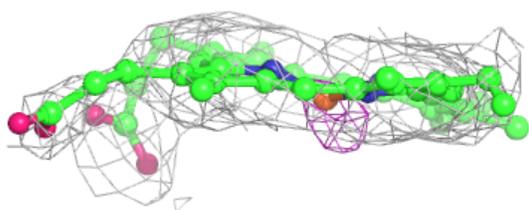
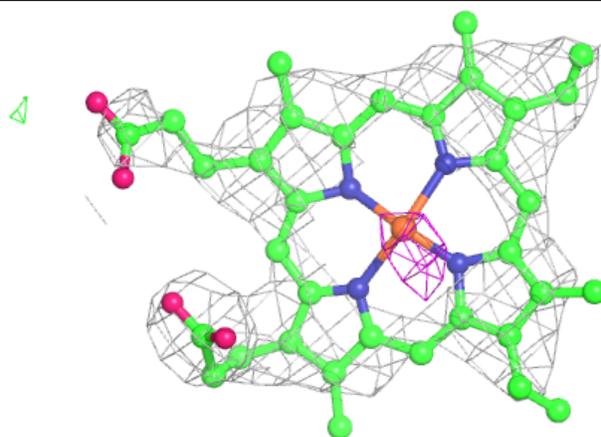
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PT	A	923	1/1	0.99	0.12	92,92,92,92	1
6	PT	B	911	1/1	1.00	0.22	71,71,71,71	0

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.

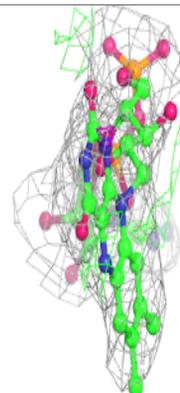
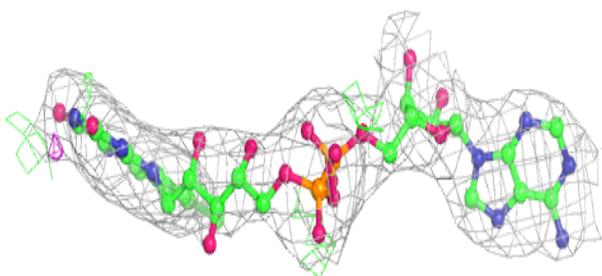
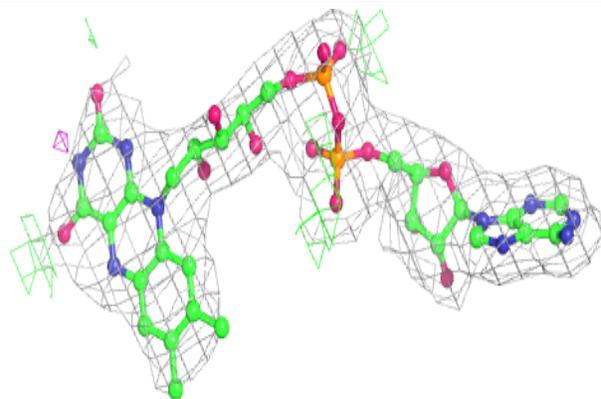


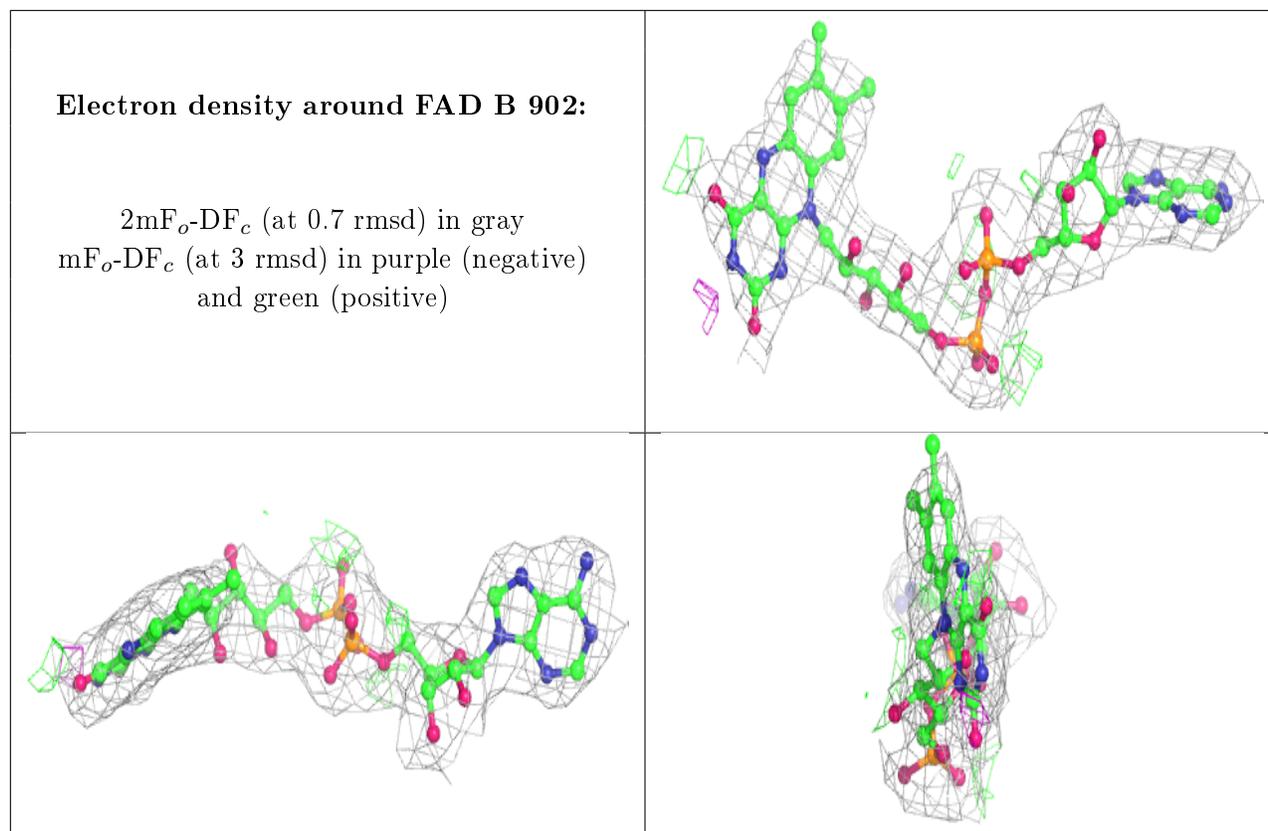
Electron density around HEM A 901:

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

**Electron density around FAD A 902:**

$2mF_o-DF_c$ (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.