



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 2H88 / pdb_00002h88
Title : Avian Mitochondrial Respiratory Complex II at 1.8 Angstrom Resolution
Authors : Huang, L.S.; Shen, J.T.; Wang, A.C.; Berry, E.A.
Deposited on : 2006-06-06
Resolution : 1.74 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

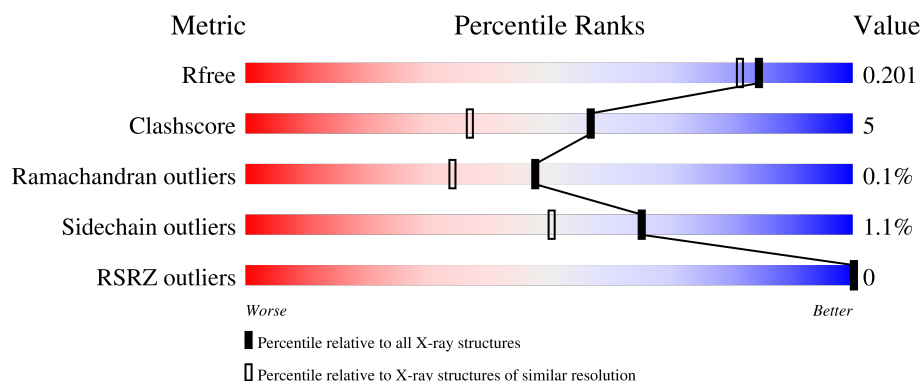
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. 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	621	 86% 12% ..
1	N	621	 86% 12% .
2	B	252	 85% 8% . 5%
2	O	252	 86% 9% 5%
3	C	140	 79% 19% ..

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Mol	Chain	Length	Quality of chain
3	P	140	 80%19%..
4	D	103	 83%15%.
4	Q	103	 85%13%.

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
14	BHG	C	141	X	-	-	-
14	BHG	P	205	X	-	-	-
6	AZI	A	623	-	X	-	-
6	AZI	N	623	-	X	-	-
8	TEO	A	1002	X	-	-	-
8	TEO	N	1002	X	-	-	-
9	UNL	N	1007	-	-	X	-
9	UNL	O	1006	-	-	X	-
9	UNL	P	208	-	-	X	-
9	UNL	P	209	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 19414 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 SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			
1	N	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ARG	CYS	conflict	UNP Q9YHT1
A	556	LEU	PHE	conflict	UNP Q9YHT1
A	560	GLU	ASP	conflict	UNP Q9YHT1
N	501	ARG	CYS	conflict	UNP Q9YHT1
N	556	LEU	PHE	conflict	UNP Q9YHT1
N	560	GLU	ASP	conflict	UNP Q9YHT1

- Molecule 2 is a protein called Succinate dehydrogenase Ip subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1916	1213	325	356	22			
2	O	239	Total	C	N	O	S	0	0	0
			1916	1213	325	356	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			
3	P	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			

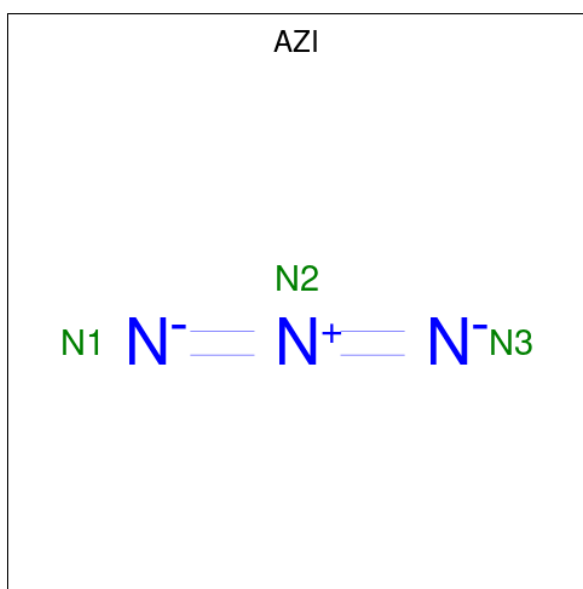
- Molecule 4 is a protein called Succinate dehydrogenase cytochrome B, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			
4	Q	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

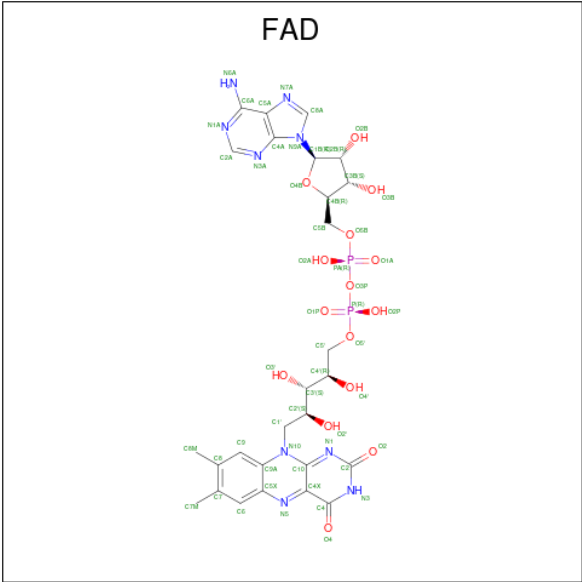
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	N	1	Total K 1 1	0	0
5	O	1	Total K 1 1	0	0

- Molecule 6 is AZIDE ION (CCD ID: AZI) (formula: N₃).



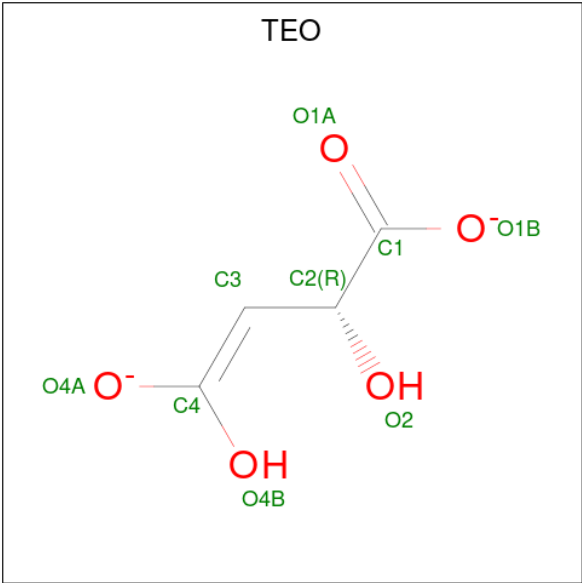
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N 3 3	0	0
6	N	1	Total N 3 3	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 8 is MALATE LIKE INTERMEDIATE (CCD ID: TEO) (formula: C₄H₄O₅).

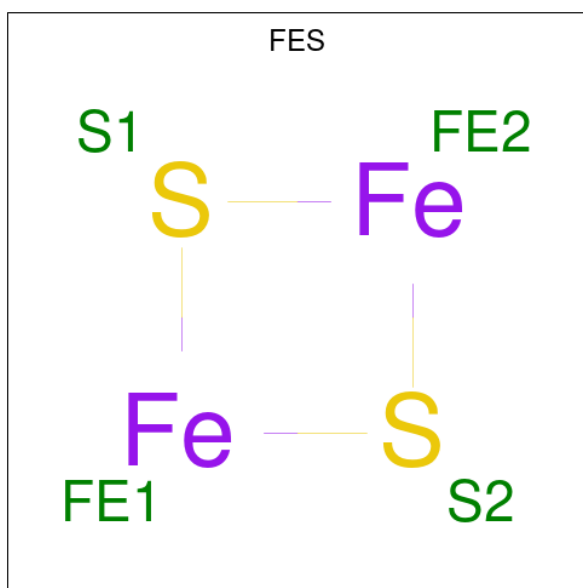


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			9	4	5		
8	N	1	Total	C	O	0	0
			9	4	5		

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

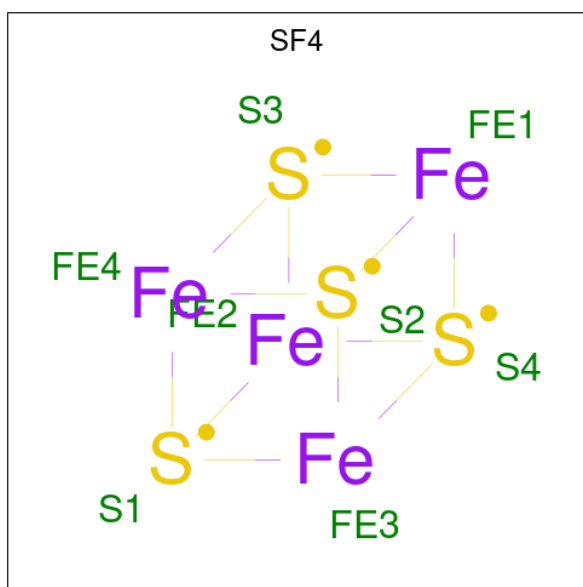
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	6	Total O 7 7	0	0
9	B	4	Total O 4 4	0	0
9	C	9	Total C O 16 6 10	0	0
9	D	11	Total C O 32 21 11	0	0
9	N	10	Total O 11 11	0	0
9	O	4	Total O 4 4	0	0
9	P	14	Total C O 22 6 16	0	0
9	Q	6	Total C O 16 12 4	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



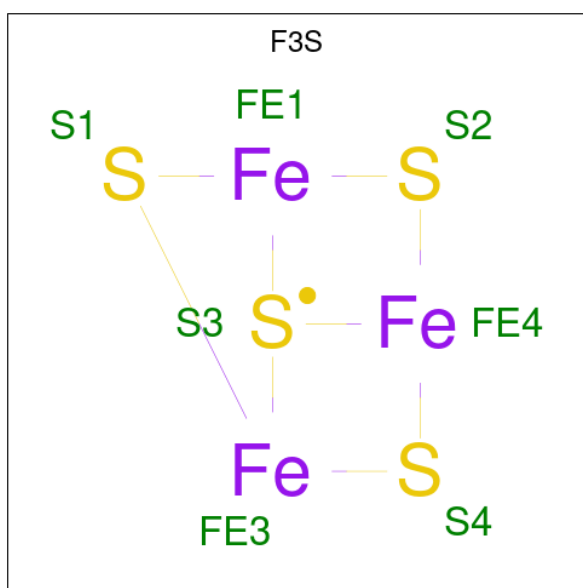
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 4 2 2	0	0
10	O	1	Total Fe S 4 2 2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



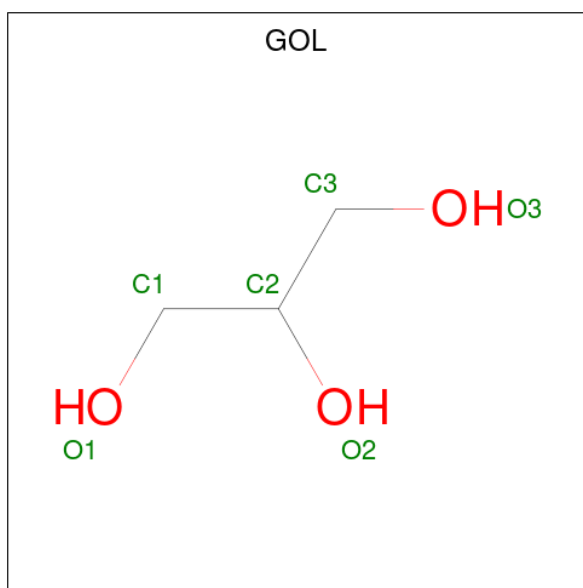
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



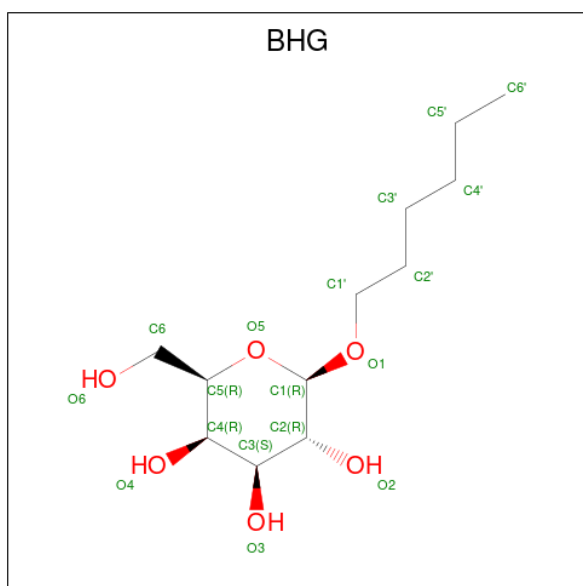
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		
12	O	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			6	3	3		
13	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 14 is hexyl beta-D-galactopyranoside (CCD ID: BHG) (formula: $C_{12}H_{24}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			18	12	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	P	1	Total	C	O	0	0
			18	12	6		

- # HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 41	C 32	Fe 1	N 4	O 4	0	0
15	P	1	Total 41	C 32	Fe 1	N 4	O 4	0	0

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 16 | A | 579 | Total O
579 579 | 0 | 0 |
| 16 | B | 296 | Total O
296 296 | 0 | 0 |
| 16 | C | 104 | Total O
104 104 | 0 | 0 |
| 16 | D | 51 | Total O
51 51 | 0 | 0 |
| 16 | N | 569 | Total O
569 569 | 0 | 0 |
| 16 | O | 281 | Total O
281 281 | 0 | 0 |

WORLDWIDE
PDB
PROTEIN DATA BANK

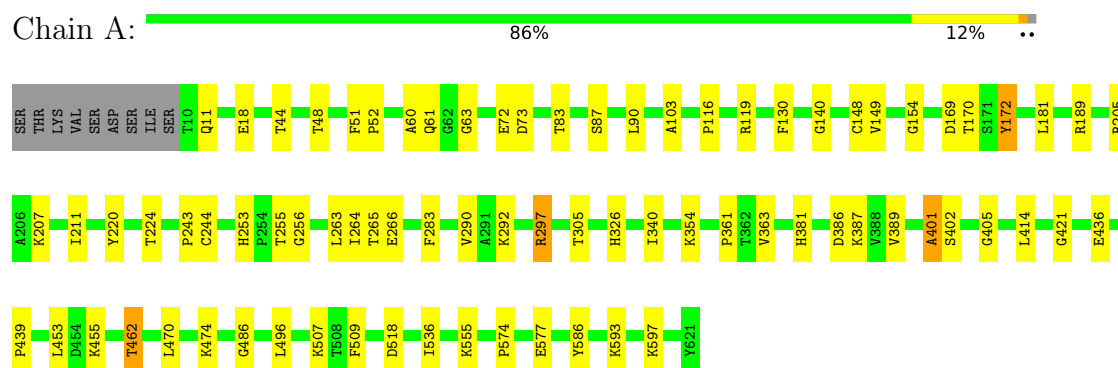
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	99	Total 99	O 99	0	0
16	Q	51	Total 51	O 51	0	0

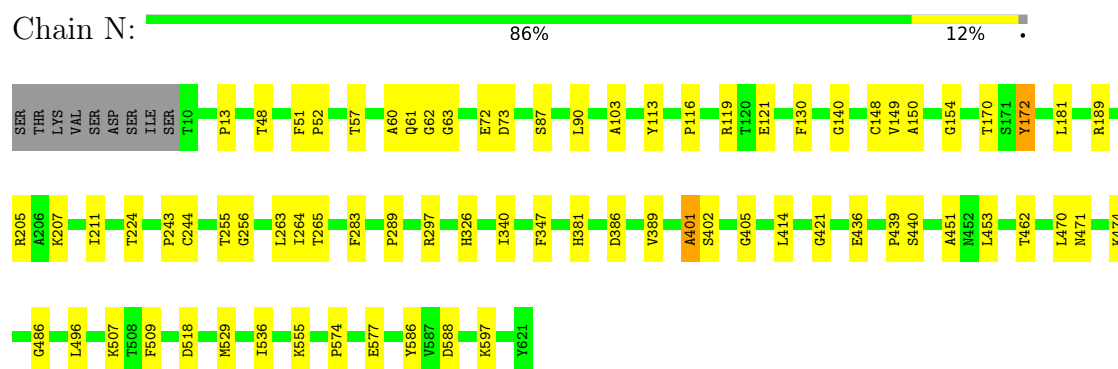
3 Residue-property plots

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.

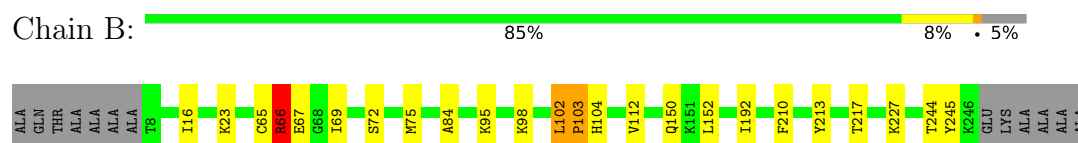
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



• Molecule 2: Succinate dehydrogenase Ip subunit



• Molecule 2: Succinate dehydrogenase Ip subunit





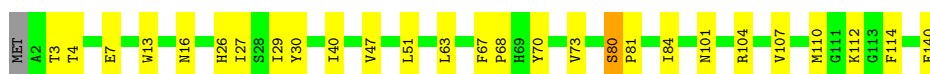
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT

Chain C: 79% 19% ..



- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT

Chain P: 80% 19% ..



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit

Chain D: 83% 15% .



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit

Chain Q: 85% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.97Å 199.39Å 68.06Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	45.14 – 1.74 45.14 – 1.74	Depositor EDS
% Data completeness (in resolution range)	89.2 (45.14-1.74) 88.9 (45.14-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.206 0.175 , 0.201	Depositor DCC
R_{free} test set	15106 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.227 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19414	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: F3S, UNL, FAD, BHG, FES, TEO, SF4, GOL, HEM, K, AZI

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	1.16	3/4827 (0.1%)	1.14	27/6535 (0.4%)
1	N	1.19	5/4827 (0.1%)	1.14	27/6535 (0.4%)
2	B	1.18	5/1958 (0.3%)	1.11	11/2640 (0.4%)
2	O	1.23	6/1958 (0.3%)	1.13	12/2640 (0.5%)
3	C	0.86	1/1106 (0.1%)	0.95	3/1503 (0.2%)
3	P	0.83	1/1106 (0.1%)	0.99	6/1503 (0.4%)
4	D	0.73	0/789	0.96	2/1082 (0.2%)
4	Q	0.69	0/789	0.93	2/1082 (0.2%)
All	All	1.11	21/17360 (0.1%)	1.10	90/23520 (0.4%)

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	N	0	1
3	C	0	1
3	P	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	66	ARG	CA-C	8.18	1.63	1.52
1	A	103	ALA	CA-CB	8.03	1.65	1.53
2	B	66	ARG	CA-C	7.89	1.63	1.52
2	O	112	VAL	CA-CB	7.78	1.61	1.53
2	O	84	ALA	CA-CB	7.66	1.65	1.53

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	255	THR	N-CA-C	10.41	123.21	108.54
1	A	255	THR	N-CA-C	10.12	122.80	108.54
1	A	401	ALA	N-CA-C	8.73	121.95	111.82
1	N	401	ALA	N-CA-C	8.70	121.91	111.82
1	N	265	THR	N-CA-C	8.01	121.54	110.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain
3	C	30	TYR	Sidechain
1	N	172	TYR	Sidechain
3	P	30	TYR	Sidechain

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	4726	0	4609	37	0
1	N	4726	0	4609	35	0
2	B	1916	0	1913	11	0
2	O	1916	0	1913	8	0
3	C	1077	0	1112	25	0
3	P	1077	0	1112	21	0
4	D	766	0	761	12	0
4	Q	766	0	761	10	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
6	A	3	0	0	0	0
6	N	3	0	0	0	0
7	A	53	0	30	3	0
7	N	53	0	30	3	0
8	A	9	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	9	0	2	1	0
9	A	7	0	0	0	0
9	B	4	0	0	1	0
9	C	16	0	0	0	0
9	D	32	0	0	1	0
9	N	11	0	0	3	0
9	O	4	0	0	2	0
9	P	22	0	0	4	0
9	Q	16	0	0	0	0
10	B	4	0	0	0	0
10	O	4	0	0	0	0
11	B	8	0	0	0	0
11	O	8	0	0	0	0
12	B	7	0	0	0	0
12	O	7	0	0	0	0
13	B	6	0	8	1	0
13	O	6	0	8	1	0
14	C	18	0	24	0	0
14	P	18	0	24	0	0
15	C	41	0	24	0	0
15	P	41	0	24	0	0
16	A	579	0	0	8	0
16	B	296	0	0	4	0
16	C	104	0	0	3	0
16	D	51	0	0	1	0
16	N	569	0	0	7	0
16	O	281	0	0	0	0
16	P	99	0	0	0	0
16	Q	51	0	0	0	0
All	All	19414	0	16966	157	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 5.

The worst 5 of 157 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)
9:O:1005:UNL:O1	9:O:1006:UNL:O1	1.69	1.09
1:N:13:PRO:O	9:N:1011:UNL:O1	1.75	1.04
9:B:1005:UNL:O1	9:B:1006:UNL:O1	1.84	0.96
4:Q:91:VAL:HG11	4:Q:99:MET:HE1	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:ASN:HD21	3:P:104:ARG:HH11	1.27	0.82

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	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
1	N	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
2	B	237/252 (94%)	231 (98%)	5 (2%)	1 (0%)	30	16
2	O	237/252 (94%)	232 (98%)	4 (2%)	1 (0%)	30	16
3	C	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
3	P	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
4	D	99/103 (96%)	98 (99%)	1 (1%)	0	100	100
4	Q	99/103 (96%)	98 (99%)	1 (1%)	0	100	100
All	All	2166/2232 (97%)	2113 (98%)	51 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG

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	497/506 (98%)	492 (99%)	5 (1%)	68	54
1	N	497/506 (98%)	492 (99%)	5 (1%)	68	54
2	B	214/219 (98%)	211 (99%)	3 (1%)	59	41
2	O	214/219 (98%)	210 (98%)	4 (2%)	50	28
3	C	118/119 (99%)	117 (99%)	1 (1%)	73	64
3	P	118/119 (99%)	118 (100%)	0	100	100
4	D	78/79 (99%)	77 (99%)	1 (1%)	61	43
4	Q	78/79 (99%)	77 (99%)	1 (1%)	61	43
All	All	1814/1846 (98%)	1794 (99%)	20 (1%)	65	50

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	462	THR
2	O	217	THR
4	Q	14	ARG
2	O	224	THR
2	B	67	GLU

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	O	121	GLN
3	P	26	HIS
4	Q	69	ASN
3	P	66	GLN
2	O	144	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 4 are monoatomic and 64 are unknown - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GOL	B	1009	-	5,5,5	1.20	0	5,5,5	0.54	0
10	FES	B	1002	2	0,4,4	-	-	-		
12	F3S	O	1004	2	0,9,9	-	-	-		
14	BHG	C	141	-	18,18,18	1.80	4 (22%)	23,23,23	0.80	1 (4%)
6	AZI	A	623	-	2,2,2	3.36	2 (100%)	0,1,1	-	-
7	FAD	N	1001	1	58,58,58	2.48	17 (29%)	85,89,89	1.76	21 (24%)
6	AZI	N	623	-	2,2,2	3.23	2 (100%)	0,1,1	-	-
8	TEO	A	1002	-	5,8,8	3.29	2 (40%)	4,10,10	3.41	2 (50%)
7	FAD	A	1001	1	58,58,58	2.34	18 (31%)	85,89,89	1.81	22 (25%)
8	TEO	N	1002	-	5,8,8	3.50	3 (60%)	4,10,10	3.71	3 (75%)
15	HEM	C	142	3,4	48,48,50	1.53	9 (18%)	66,80,82	1.47	12 (18%)
10	FES	O	1002	2	0,4,4	-	-	-		
11	SF4	O	1003	2	0,12,12	-	-	-		
12	F3S	B	1004	2	0,9,9	-	-	-		
13	GOL	O	1009	-	5,5,5	1.23	0	5,5,5	0.70	0
14	BHG	P	205	-	18,18,18	1.39	2 (11%)	23,23,23	0.65	0
11	SF4	B	1003	2	0,12,12	-	-	-		
15	HEM	P	201	3,4	48,48,50	1.44	7 (14%)	66,80,82	1.46	13 (19%)

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
14	BHG	C	141	-	1/1/5/5	1/9/29/29	0/1/1/1
13	GOL	B	1009	-	-	2/4/4/4	-
10	FES	B	1002	2	-	-	0/1/1/1
12	F3S	O	1004	2	-	-	0/3/3/3
7	FAD	N	1001	1	-	8/34/50/50	0/6/6/6
7	FAD	A	1001	1	-	9/34/50/50	0/6/6/6
8	TEO	N	1002	-	1/1/3/4	4/6/8/8	-
8	TEO	A	1002	-	1/1/3/4	4/6/8/8	-
15	HEM	C	142	3,4	-	5/10/50/54	-
10	FES	O	1002	2	-	-	0/1/1/1
11	SF4	O	1003	2	-	-	0/6/5/5
12	F3S	B	1004	2	-	-	0/3/3/3
13	GOL	O	1009	-	-	4/4/4/4	-
14	BHG	P	205	-	1/1/5/5	1/9/29/29	0/1/1/1
11	SF4	B	1003	2	-	-	0/6/5/5
15	HEM	P	201	3,4	-	5/10/50/54	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	FAD	PA-O3P	-10.08	1.48	1.59
7	N	1001	FAD	PA-O3P	-9.71	1.49	1.59
7	N	1001	FAD	P-O3P	6.71	1.66	1.59
8	A	1002	TEO	C2-C1	6.27	1.66	1.54
8	N	1002	TEO	C2-C1	6.17	1.66	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1001	FAD	N3A-C2A-N1A	-6.58	118.62	128.58
7	A	1001	FAD	N3A-C2A-N1A	-6.44	118.84	128.58
8	N	1002	TEO	O1B-C1-O1A	5.97	137.63	124.08
8	A	1002	TEO	O1B-C1-O1A	5.41	136.35	124.08
7	N	1001	FAD	C4'-C3'-C2'	-4.13	106.69	113.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1002	TEO	C2
8	N	1002	TEO	C2
14	C	141	BHG	C4

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Mol	Chain	Res	Type	Atom
14	P	205	BHG	C4

5 of 43 torsion outliers are listed below:

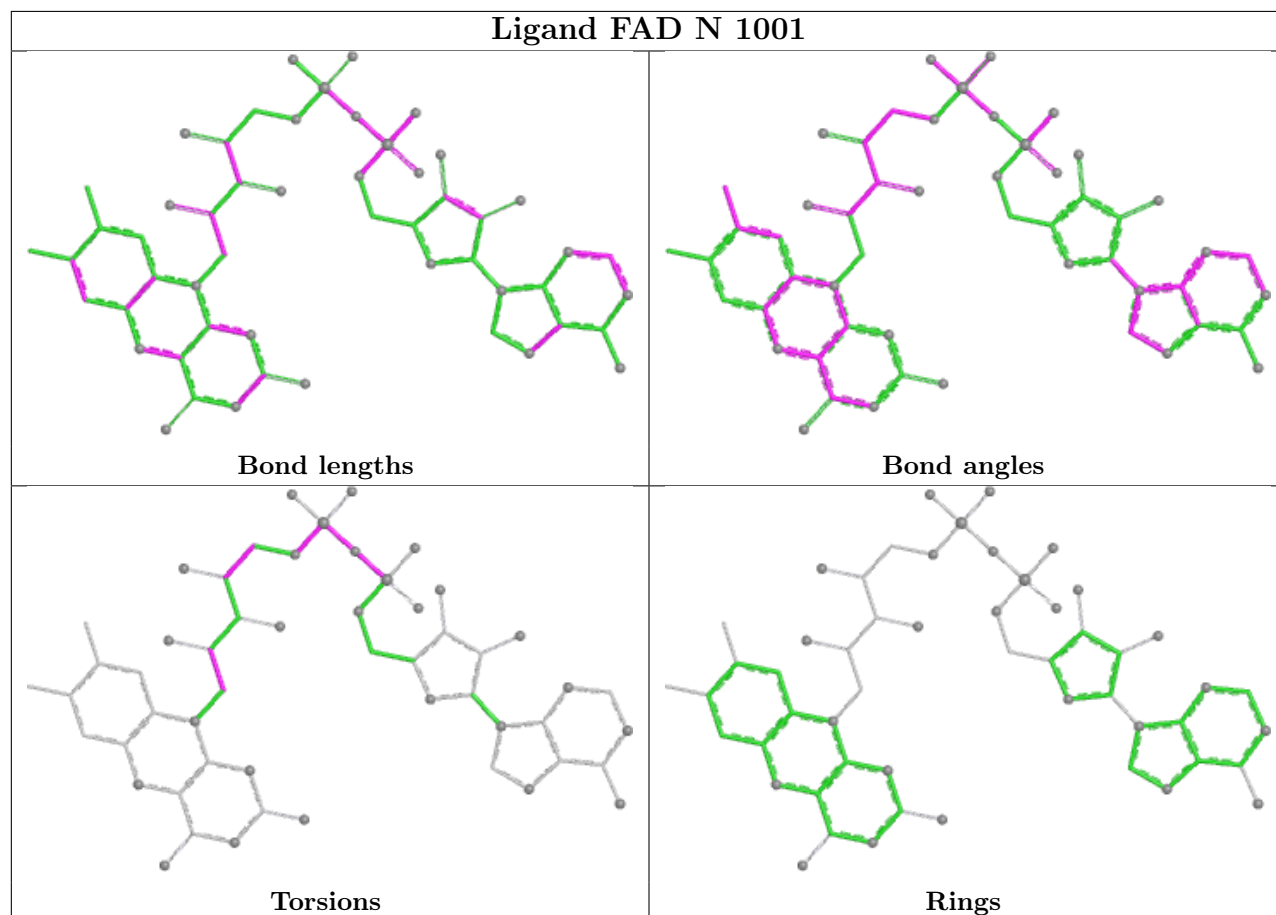
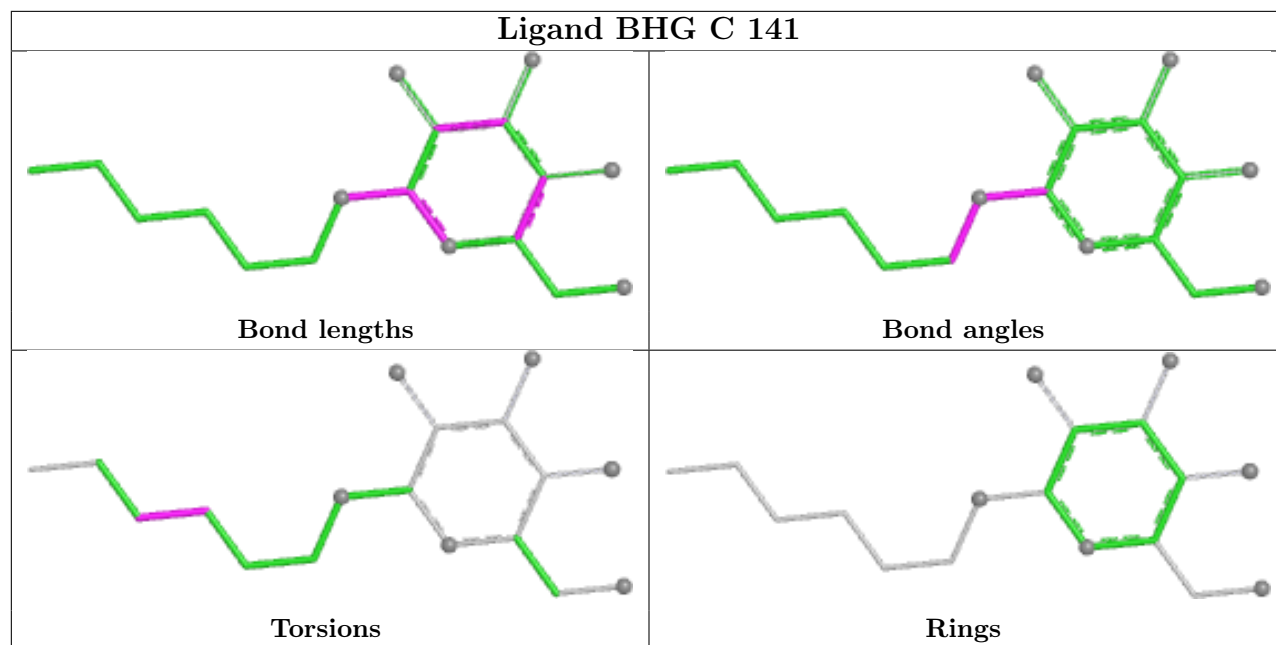
Mol	Chain	Res	Type	Atoms
7	A	1001	FAD	N10-C1'-C2'-O2'
7	A	1001	FAD	O4'-C4'-C5'-O5'
7	A	1001	FAD	C5'-O5'-P-O2P
7	A	1001	FAD	C5'-O5'-P-O3P
7	N	1001	FAD	N10-C1'-C2'-O2'

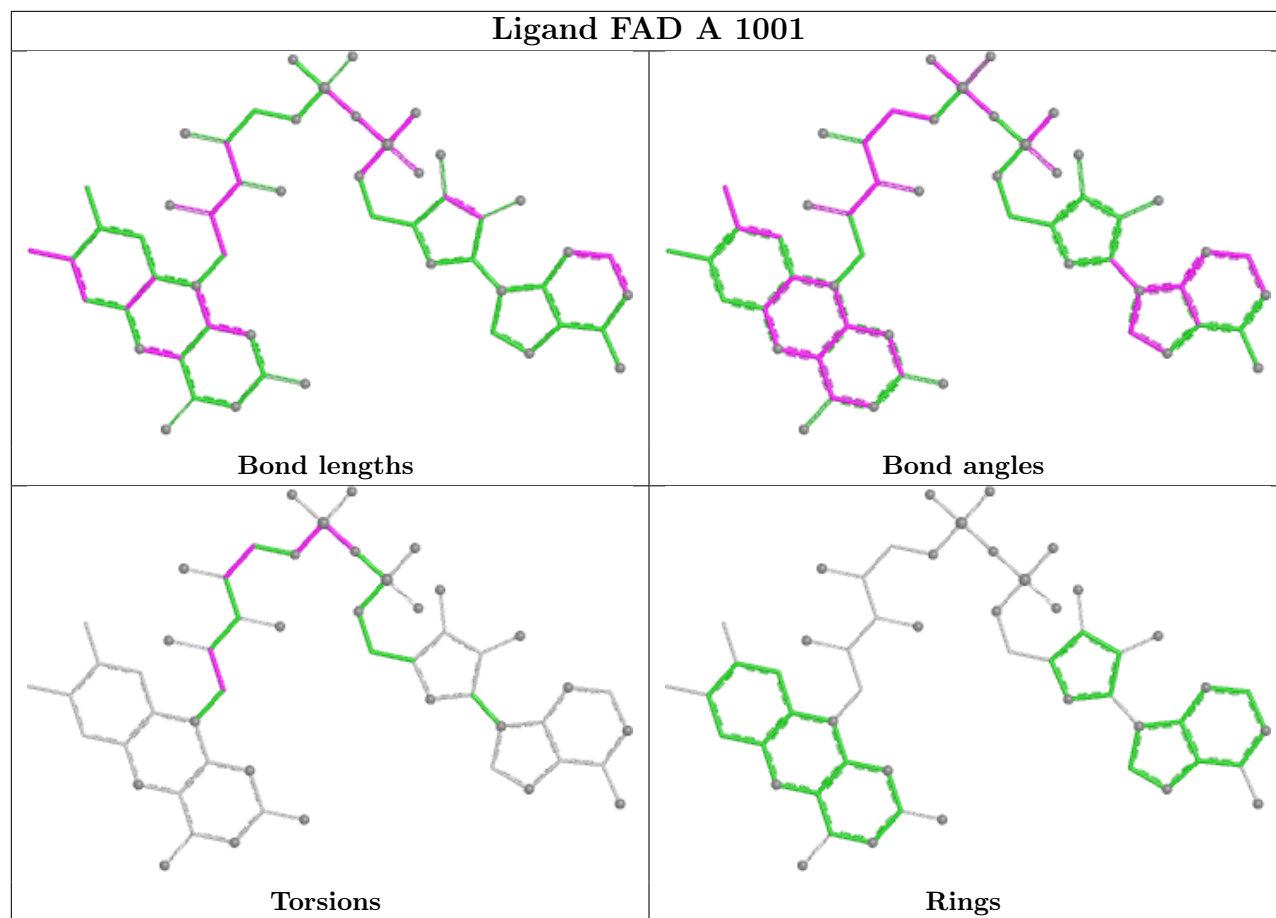
There are no ring outliers.

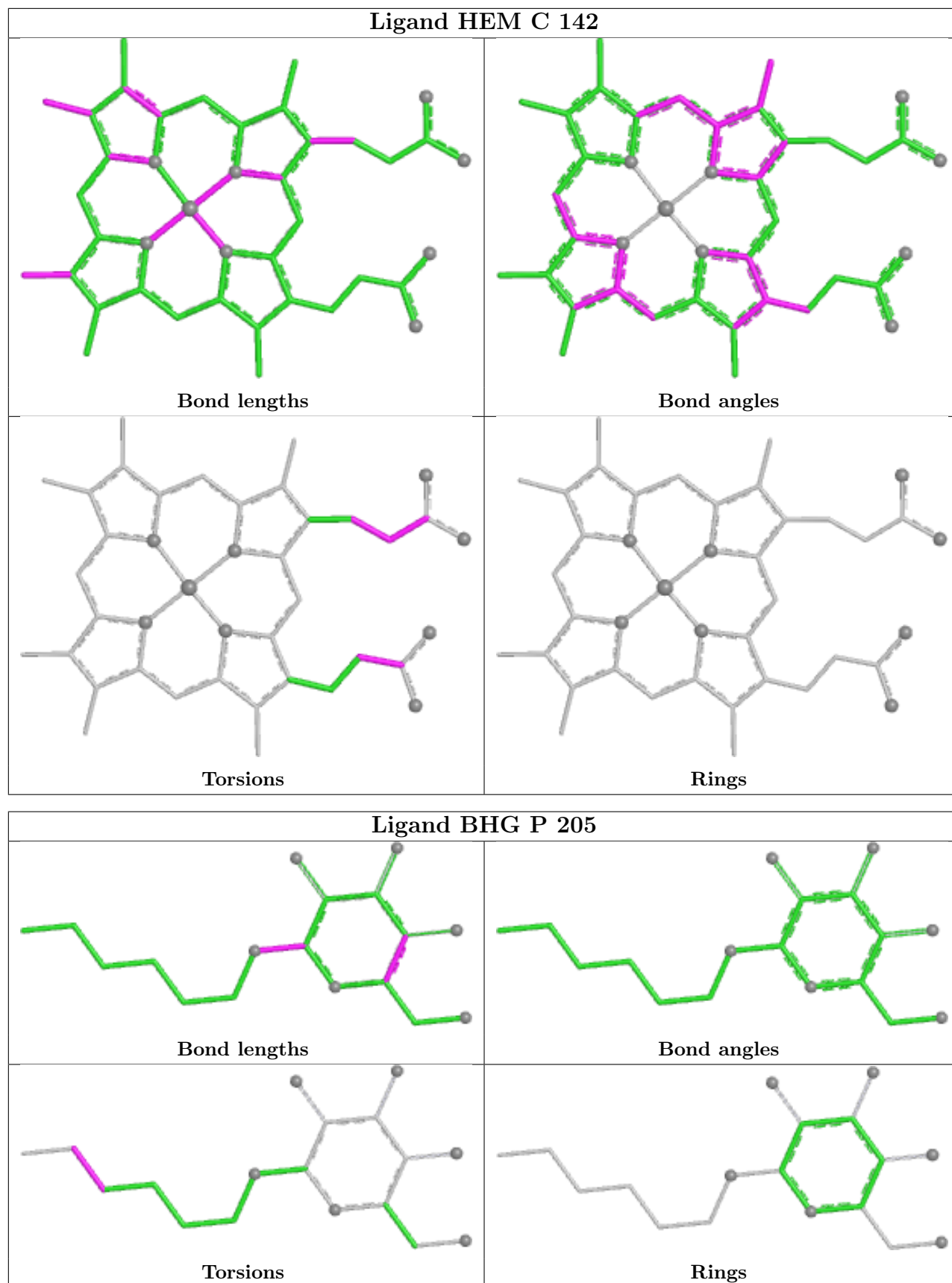
6 monomers are involved in 12 short contacts:

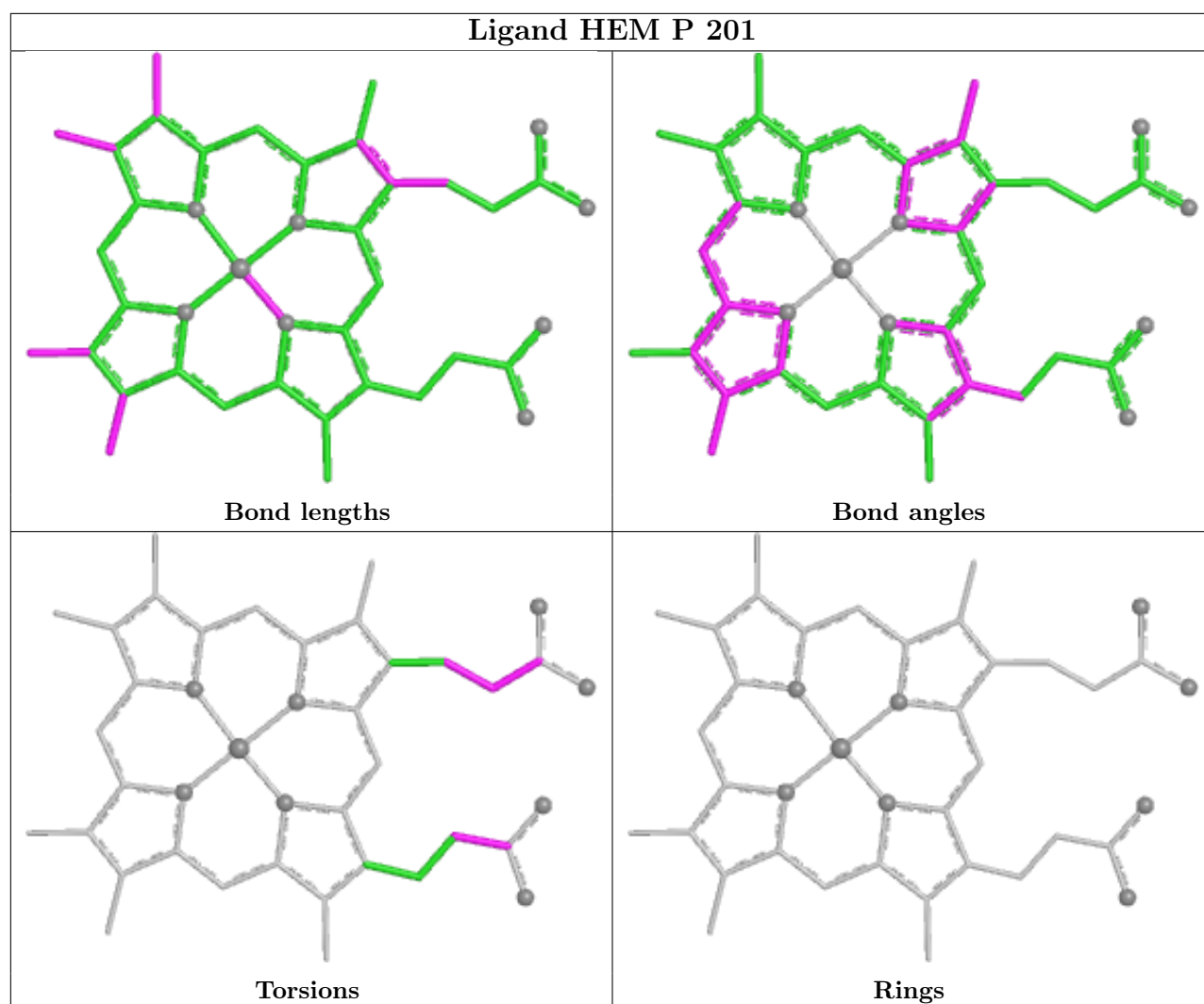
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1009	GOL	1	0
7	N	1001	FAD	3	0
8	A	1002	TEO	3	0
7	A	1001	FAD	3	0
8	N	1002	TEO	1	0
13	O	1009	GOL	1	0

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	612/621 (98%)	-1.26	0 100 100	14, 23, 45, 74	0
1	N	612/621 (98%)	-1.30	0 100 100	12, 22, 43, 69	0
2	B	239/252 (94%)	-1.32	0 100 100	15, 24, 41, 70	0
2	O	239/252 (94%)	-1.36	0 100 100	14, 23, 37, 69	0
3	C	139/140 (99%)	-1.04	0 100 100	21, 35, 50, 61	0
3	P	139/140 (99%)	-0.89	0 100 100	21, 37, 81, 92	0
4	D	101/103 (98%)	-0.87	0 100 100	26, 42, 58, 66	0
4	Q	101/103 (98%)	-0.75	0 100 100	27, 47, 69, 79	0
All	All	2182/2232 (97%)	-1.21	0 100 100	12, 25, 54, 92	0

There are no RSRZ outliers to report.

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 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, 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($\text{\AA}^2$)	Q<0.9
9	UNL	A	1006	1/-	0.94	0.09	63,63,63,63	0
9	UNL	A	1008	1/-	0.94	0.07	64,64,64,64	0
9	UNL	P	217	1/-	0.94	0.06	113,113,113,113	0
9	UNL	C	149	1/-	0.95	0.12	81,81,81,81	0
9	UNL	D	254	1/-	0.95	0.07	67,67,67,67	0
9	UNL	B	1008	1/-	0.95	0.06	69,69,69,69	0
9	UNL	Q	256	1/-	0.95	0.07	84,84,84,84	0
9	UNL	C	237	1/-	0.96	0.06	66,66,66,66	0
9	UNL	D	253	1/-	0.96	0.10	72,72,72,72	0
9	UNL	A	1004	1/-	0.96	0.06	61,61,61,61	0
9	UNL	N	1006	1/-	0.96	0.13	54,54,54,54	0
9	UNL	N	1008	1/-	0.96	0.09	65,65,65,65	0
6	AZI	A	623	3/3	0.96	0.07	62,62,63,64	0
9	UNL	A	1007	2/-	0.96	0.09	65,65,65,66	0
9	UNL	D	251	1/-	0.97	0.06	73,73,73,73	0
9	UNL	D	252	1/-	0.97	0.05	73,73,73,73	0
9	UNL	C	146	4/-	0.97	0.10	108,109,109,109	0
9	UNL	C	148	1/-	0.97	0.07	56,56,56,56	0
9	UNL	N	1003	2/-	0.97	0.07	114,114,114,114	0
9	UNL	N	1004	1/-	0.97	0.11	60,60,60,60	0
9	UNL	N	1005	1/-	0.97	0.07	76,76,76,76	0
9	UNL	B	1007	1/-	0.97	0.10	61,61,61,61	0
6	AZI	N	623	3/3	0.97	0.07	68,68,70,71	0
9	UNL	O	1006	1/-	0.97	0.07	54,54,54,54	0
9	UNL	O	1007	1/-	0.97	0.10	59,59,59,59	0
9	UNL	D	119	1/-	0.97	0.07	63,63,63,63	0
9	UNL	P	230	1/-	0.97	0.10	69,69,69,69	0
9	UNL	P	240	1/-	0.97	0.06	56,56,56,56	0
9	UNL	Q	219	1/-	0.97	0.13	60,60,60,60	0
9	UNL	Q	228	1/-	0.97	0.05	64,64,64,64	0
9	UNL	D	250	1/-	0.97	0.07	73,73,73,73	0
14	BHG	C	141	18/18	0.97	0.07	48,70,75,75	0
9	UNL	N	1007	1/-	0.98	0.10	44,44,44,44	0
9	UNL	D	249	1/-	0.98	0.11	72,72,72,72	0
9	UNL	N	1009	1/-	0.98	0.06	54,54,54,54	0
9	UNL	N	1010	1/-	0.98	0.08	60,60,60,60	0
9	UNL	N	1011	1/-	0.98	0.07	37,37,37,37	0
9	UNL	N	1012	1/-	0.98	0.06	53,53,53,53	0
9	UNL	A	1005	1/-	0.98	0.07	63,63,63,63	0
9	UNL	A	1003	1/-	0.98	0.09	69,69,69,69	0
9	UNL	O	1008	1/-	0.98	0.07	63,63,63,63	0
9	UNL	P	208	1/-	0.98	0.06	44,44,44,44	0
9	UNL	P	209	2/-	0.98	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	UNL	P	214	4/-	0.98	0.10	94,94,94,95	0
9	UNL	P	215	4/-	0.98	0.05	74,74,75,76	0
9	UNL	P	216	1/-	0.98	0.06	53,53,53,53	0
9	UNL	C	144	1/-	0.98	0.11	62,62,62,62	0
9	UNL	P	220	2/-	0.98	0.09	81,81,81,81	0
9	UNL	C	238	1/-	0.98	0.07	59,59,59,59	0
9	UNL	P	231	1/-	0.98	0.07	74,74,74,74	0
9	UNL	P	232	1/-	0.98	0.08	61,61,61,61	0
9	UNL	D	107	6/-	0.98	0.06	66,68,69,70	0
9	UNL	P	241	1/-	0.98	0.08	59,59,59,59	0
9	UNL	P	242	1/-	0.98	0.08	57,57,57,57	0
9	UNL	Q	213	5/-	0.98	0.07	74,74,74,74	0
9	UNL	D	108	1/-	0.98	0.07	63,63,63,63	0
9	UNL	D	114	8/-	0.98	0.07	61,63,64,65	0
9	UNL	D	116	10/-	0.98	0.07	65,66,69,69	0
9	UNL	B	1006	1/-	0.98	0.07	60,60,60,60	0
9	UNL	O	1005	1/-	0.99	0.04	35,35,35,35	0
9	UNL	C	143	2/-	0.99	0.08	65,65,65,65	0
5	K	N	622	1/1	0.99	0.03	25,25,25,25	0
9	UNL	Q	212	7/-	0.99	0.07	74,75,76,76	0
9	UNL	C	145	4/-	0.99	0.07	100,100,100,100	0
9	UNL	Q	218	1/-	0.99	0.03	53,53,53,53	0
9	UNL	P	229	1/-	0.99	0.08	54,54,54,54	0
8	TEO	N	1002	9/9	0.99	0.03	17,18,19,20	1
9	UNL	C	147	1/-	0.99	0.05	59,59,59,59	0
13	GOL	B	1009	6/6	0.99	0.03	33,36,38,38	0
13	GOL	O	1009	6/6	0.99	0.04	35,40,41,43	0
9	UNL	B	1005	1/-	0.99	0.04	39,39,39,39	0
14	BHG	P	205	18/18	0.99	0.05	36,42,59,61	0
15	HEM	C	142	41/43	0.99	0.04	27,32,49,52	0
7	FAD	N	1001	53/53	1.00	0.02	11,14,18,21	0
10	FES	B	1002	4/4	1.00	0.01	14,16,16,16	0
10	FES	O	1002	4/4	1.00	0.01	13,14,14,15	0
11	SF4	B	1003	8/8	1.00	0.01	17,19,19,19	0
11	SF4	O	1003	8/8	1.00	0.01	16,17,18,18	0
12	F3S	B	1004	7/7	1.00	0.01	18,20,21,22	0
12	F3S	O	1004	7/7	1.00	0.01	19,20,21,22	0
8	TEO	A	1002	9/9	1.00	0.02	18,20,23,24	1
5	K	O	253	1/1	1.00	0.08	39,39,39,39	0
5	K	B	253	1/1	1.00	0.07	38,38,38,38	0
5	K	A	622	1/1	1.00	0.03	24,24,24,24	0
7	FAD	A	1001	53/53	1.00	0.02	12,14,18,22	0

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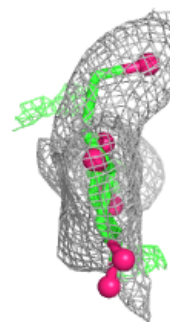
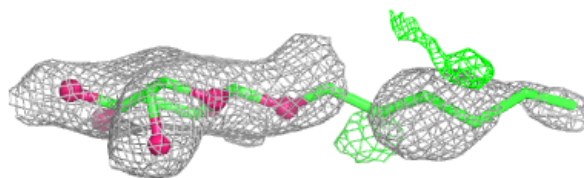
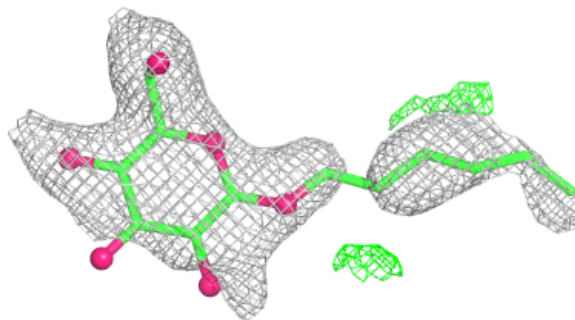
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	HEM	P	201	41/43	1.00	0.04	28,33,50,53	0

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.

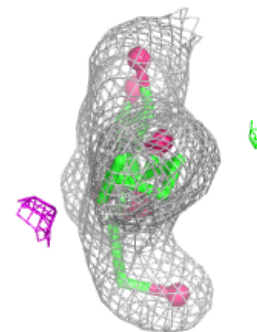
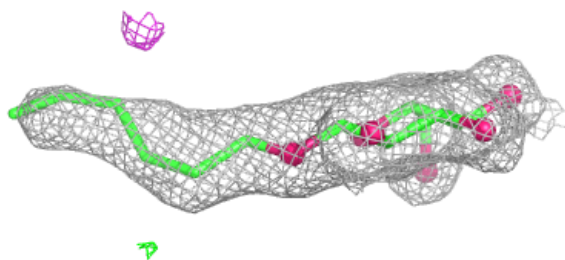
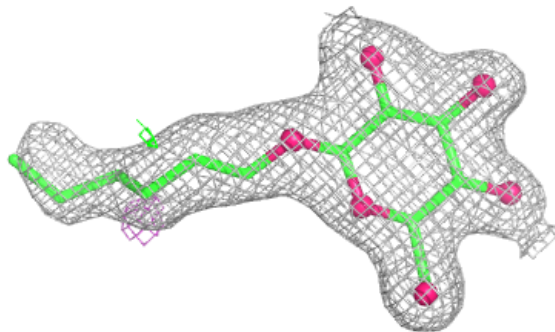
Electron density around BHG C 141:

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



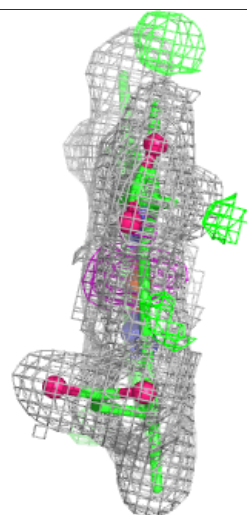
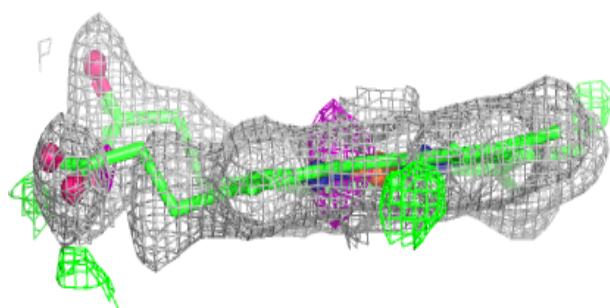
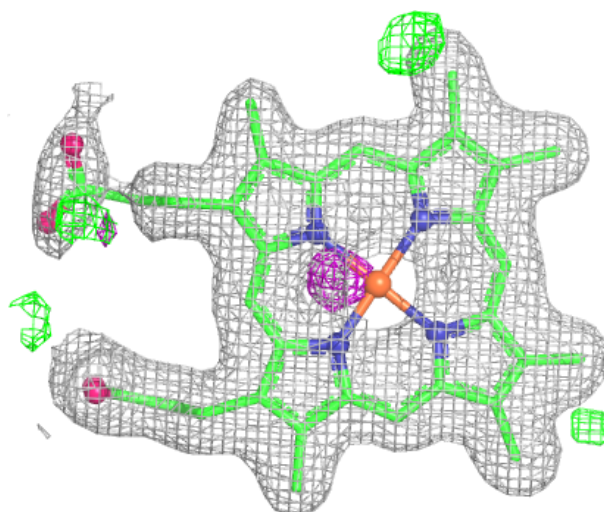
Electron density around BHG P 205:

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



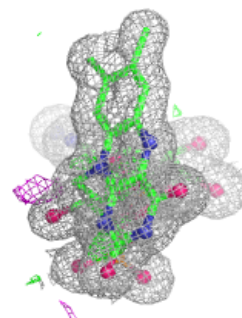
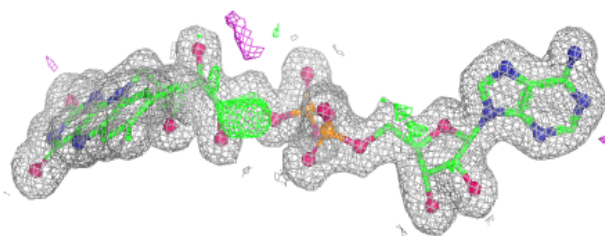
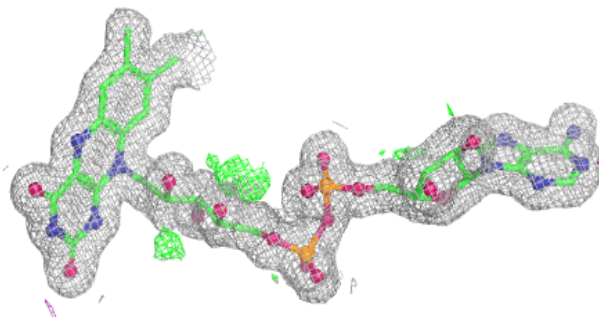
Electron density around HEM C 142:

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

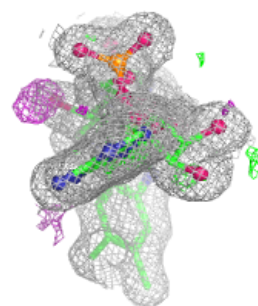
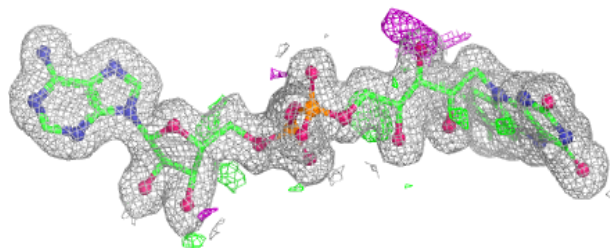
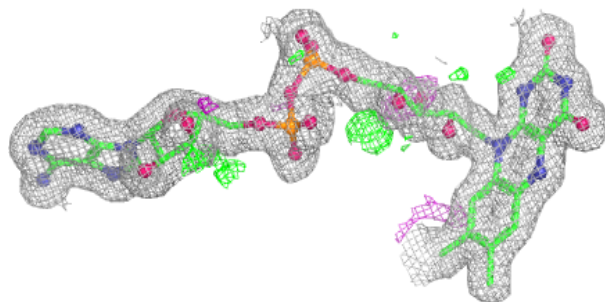


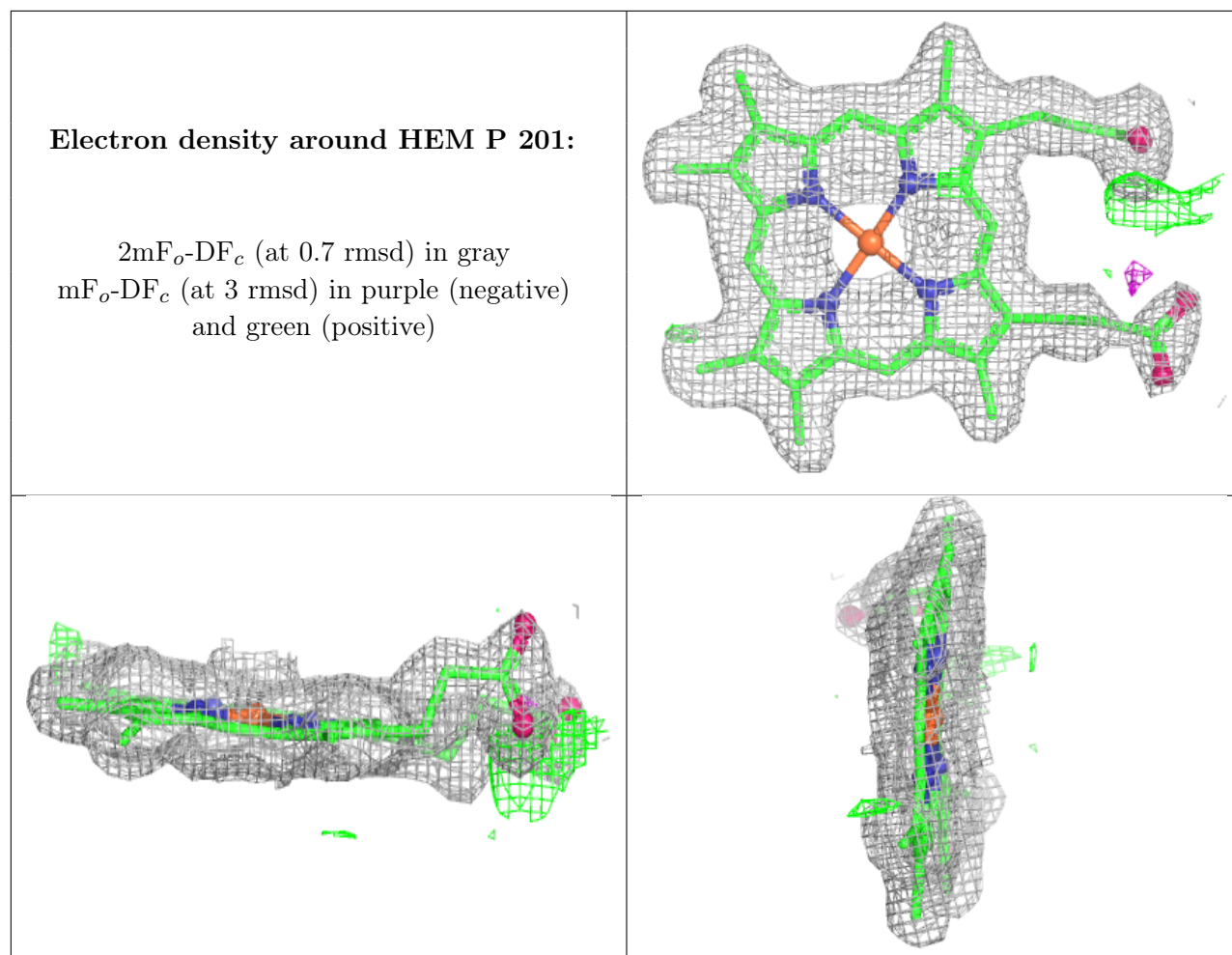
Electron density around FAD N 1001:

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

**Electron density around FAD A 1001:**

$2mF_o-DF_c$ (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.