



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 06:51 AM BST

PDB ID : 2WQY  
Title : Remodelling of carboxin binding to the Q-site of avian respiratory complex II  
Authors : Ruprecht, J.; Iwata, S.; Cecchini, G.  
Deposited on : 2009-08-27  
Resolution : 2.10 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](mailto: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.

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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

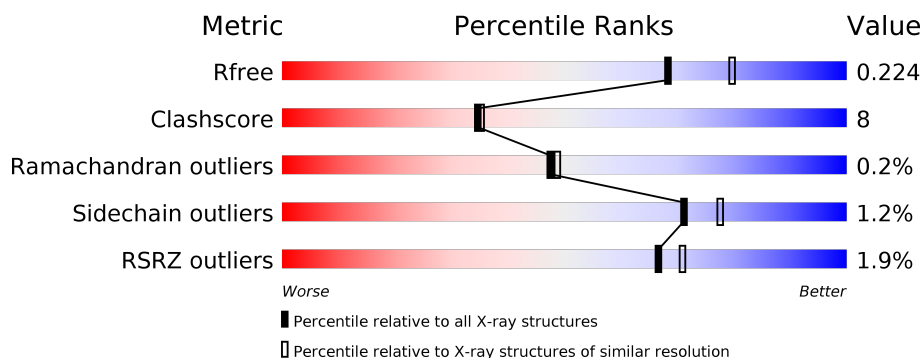
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	N	621	<div> <div>85%</div> <div>13%</div> <div>•</div> </div>
2	B	252	<div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div>
2	O	252	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>• 5%</div> </div>
3	C	141	<div> <div>7%</div> <div>74%</div> <div>23%</div> <div>••</div> </div>
3	P	141	<div> <div>7%</div> <div>74%</div> <div>24%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	103	
4	Q	103	

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
13	GOL	P	208	-	-	-	X
14	BHG	C	142	X	-	-	-
14	BHG	P	204	X	-	-	-
17	PEE	D	109	-	-	-	X
17	PEE	Q	210	-	-	-	X
5	UNL	A	1003	-	-	X	-
5	UNL	A	1004	-	-	X	-
5	UNL	A	1005	-	-	-	X
5	UNL	A	1007	-	-	-	X
5	UNL	A	1008	-	-	-	X
5	UNL	A	1010	-	-	-	X
5	UNL	A	1011	-	-	-	X
5	UNL	A	1012	-	-	-	X
5	UNL	A	1015	-	-	-	X
5	UNL	A	1023	-	-	-	X
5	UNL	B	1005	-	-	X	-
5	UNL	B	1006	-	-	-	X
5	UNL	B	1007	-	-	-	X
5	UNL	B	1009	-	-	-	X
5	UNL	B	268	-	-	-	X
5	UNL	C	145	-	-	X	-
5	UNL	C	214	-	-	X	-
5	UNL	C	235	-	-	-	X
5	UNL	C	248	-	-	-	X
5	UNL	C	254	-	-	-	X
5	UNL	C	259	-	-	-	X
5	UNL	C	292	-	-	-	X
5	UNL	C	293	-	-	-	X
5	UNL	D	245	-	-	X	-
5	UNL	D	247	-	-	-	X
5	UNL	D	263	-	-	-	X
5	UNL	D	265	-	-	-	X
5	UNL	D	266	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	UNL	D	291	-	-	-	X
5	UNL	N	1003	-	-	X	-
5	UNL	N	1005	-	-	-	X
5	UNL	N	1006	-	-	-	X
5	UNL	N	1012	-	-	-	X
5	UNL	N	1014	-	-	-	X
5	UNL	N	1016	-	-	-	X
5	UNL	N	1018	-	-	-	X
5	UNL	N	1022	-	-	-	X
5	UNL	O	1005	-	-	X	-
5	UNL	O	276	-	-	-	X
5	UNL	P	211	-	-	X	X
5	UNL	P	224	-	-	-	X
5	UNL	P	274	-	-	-	X
5	UNL	Q	287	-	-	-	X
5	UNL	Q	288	-	-	-	X
9	OAA	A	1002	-	-	X	-
9	OAA	N	1002	-	-	X	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 19490 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4731	2959	844	899	29			
1	N	612	Total	C	N	O	S	0	0	0
			4725	2956	843	897	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
			1918	1213	325	358	22			
2	O	239	Total	C	N	O	S	0	0	0
			1918	1213	325	358	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	0
			1078	708	179	187	4			
3	P	140	Total	C	N	O	S	0	0	0
			1078	708	179	187	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
			765	505	121	136	3			
4	Q	101	Total	C	N	O	S	0	0	0
			765	505	121	136	3			

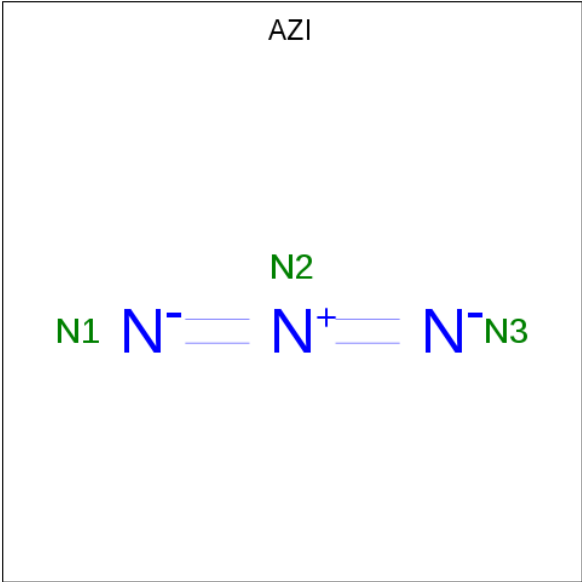
- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	7	Total	C	O	0	0
			11	6	5		
5	Q	6	Total	C		0	0
			6	6			
5	D	9	Total	C		0	0
			9	9			
5	B	10	Total	C	O	0	0
			14	9	5		
5	C	15	Total	C	O	0	0
			22	13	9		
5	A	21	Total	C	O	0	0
			29	19	10		
5	N	21	Total	C	O	0	0
			24	20	4		
5	O	6	Total	C	O	0	0
			10	5	5		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

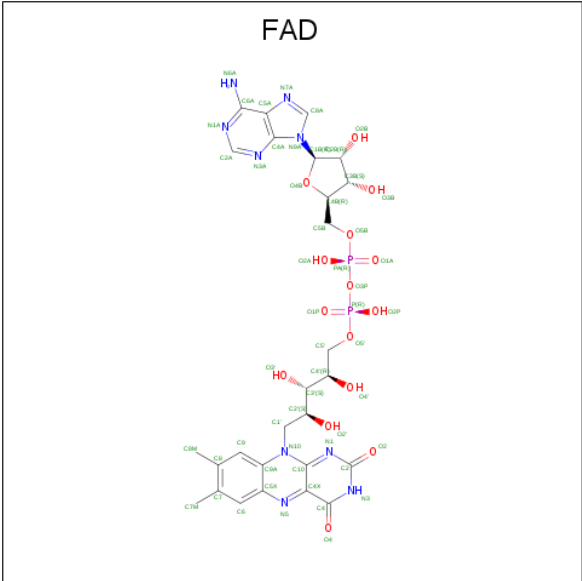
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		
6	A	1	Total	K	0	0
			1	1		
6	N	1	Total	K	0	0
			1	1		

- Molecule 7 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



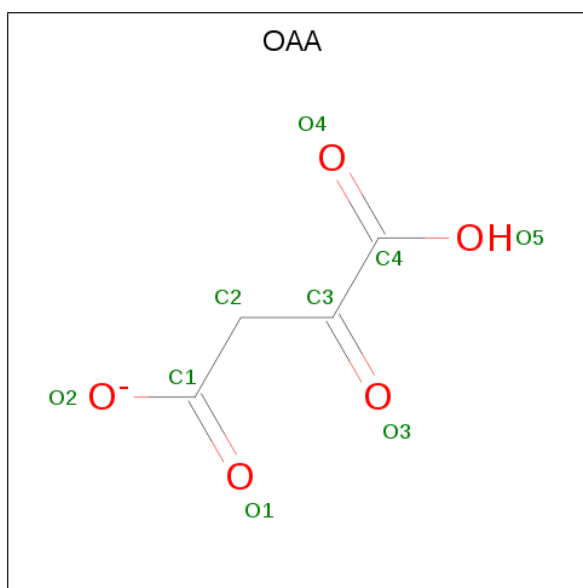
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 3 3	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



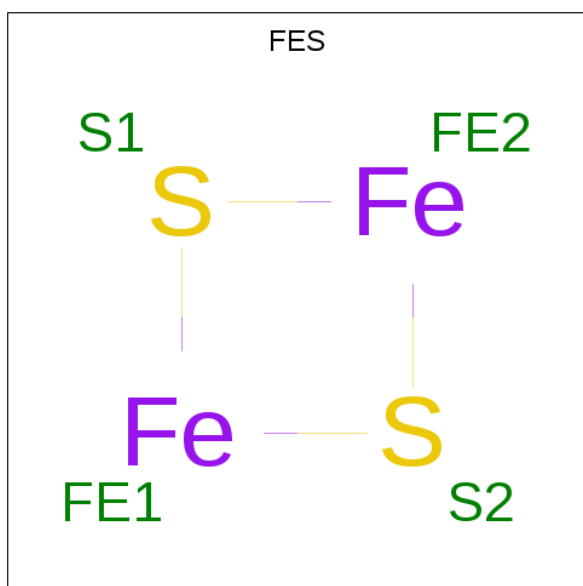
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O P 53 27 9 15 2	0	0
8	N	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 9 is OXALOACETATE ION (three-letter code: OAA) (formula:  $C_4H_3O_5$ ).



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

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

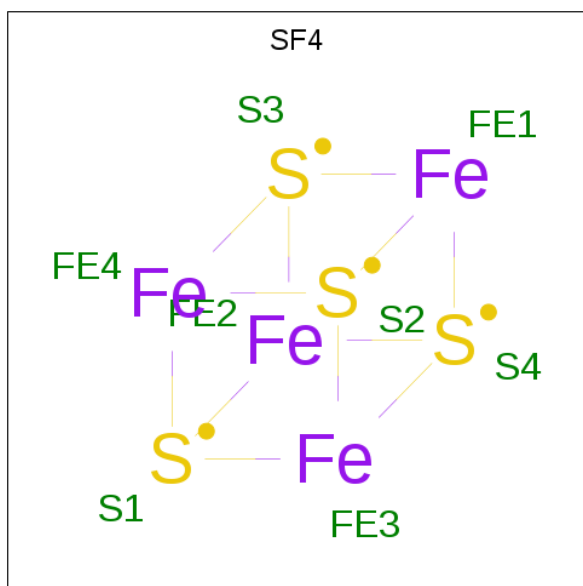
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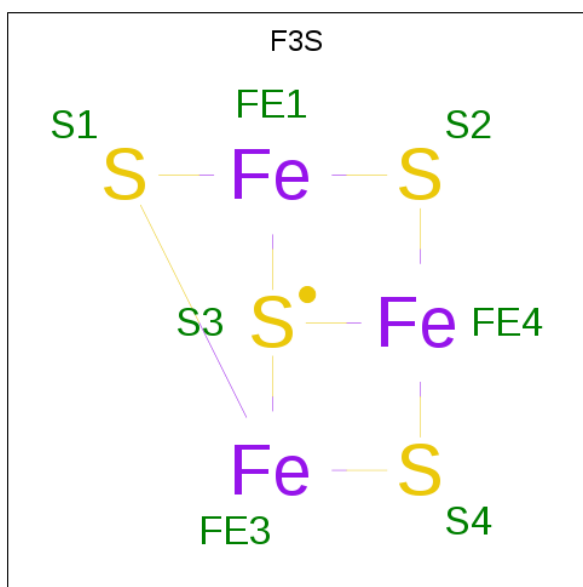
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	O	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



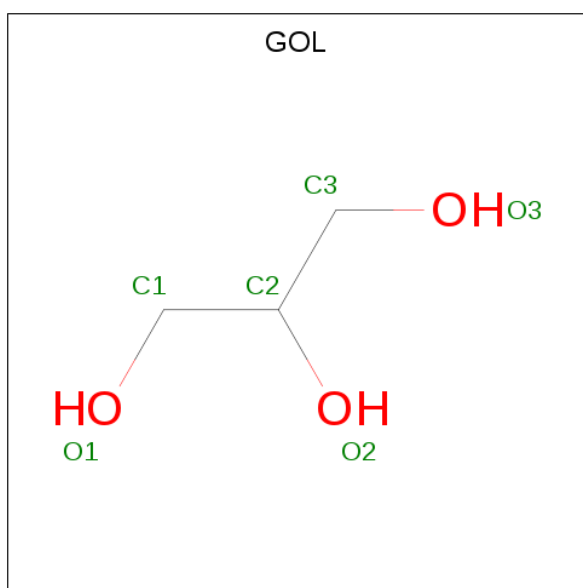
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



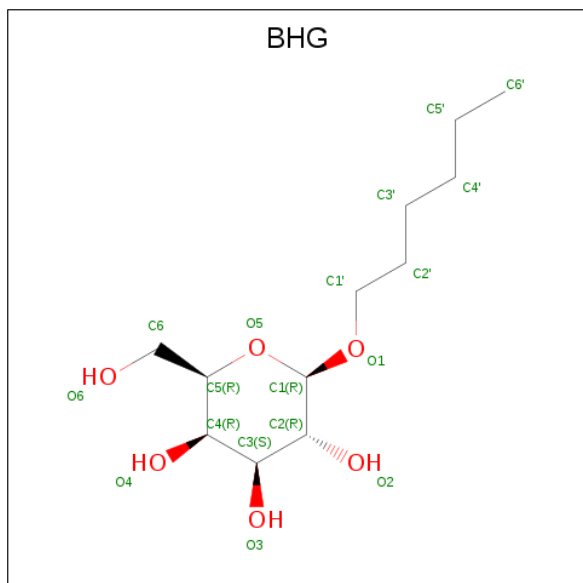
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			6	3	3		
13	C	1	Total	C	O	0	0
			6	3	3		

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

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



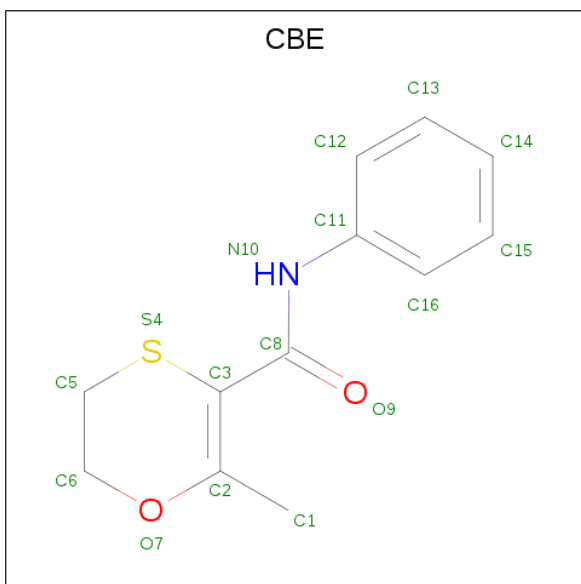
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			18	12	6		
14	P	1	Total	C	O	0	0
			18	12	6		

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 16 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula:  $C_{12}H_{13}NO_2S$ ).



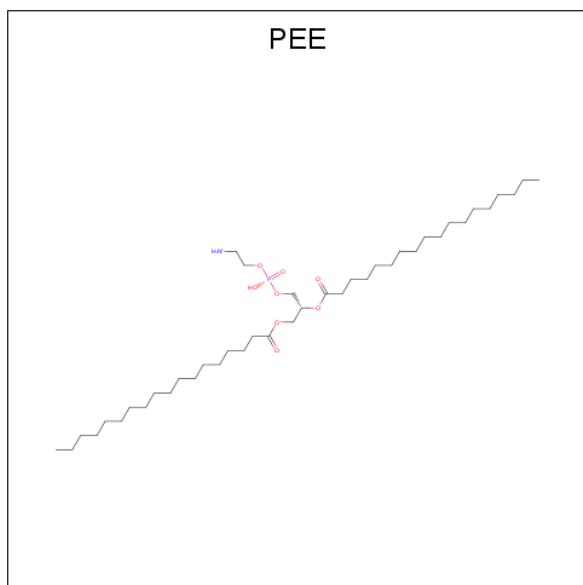
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	P	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 17 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total	C	0	0
			24	24		
17	Q	1	Total	C	0	0
			24	24		

- Molecule 18 is water.

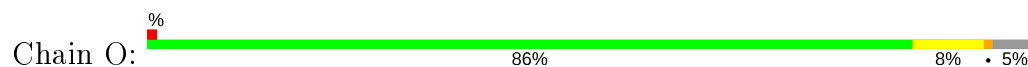
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	548	Total	O	0	0
			548	548		
18	B	297	Total	O	0	0
			297	297		
18	C	102	Total	O	0	0
			102	102		
18	D	60	Total	O	0	0
			60	60		
18	N	558	Total	O	0	0
			558	558		
18	O	287	Total	O	0	0
			287	287		

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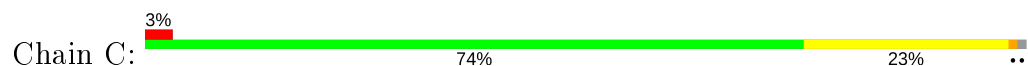
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	P	82	Total	O	0	0
			82	82		
18	Q	62	Total	O	0	0
			62	62		

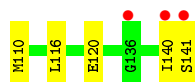
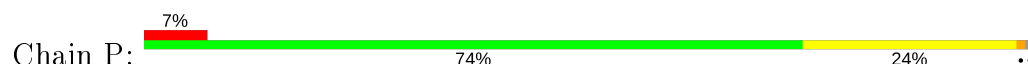




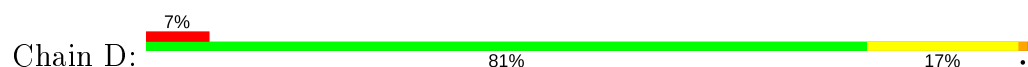
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



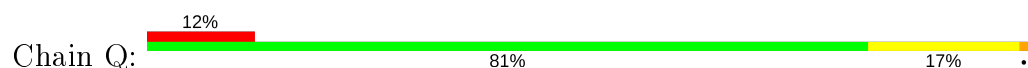
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT



• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.70Å 200.75Å 67.63Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.09 – 2.10 64.09 – 2.06	Depositor EDS
% Data completeness (in resolution range)	88.3 (64.09-2.10) 85.1 (64.09-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.62 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.184 , 0.223 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	8237 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.287 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, OAA, CBE, SF4, BHG, F3S, FES, PEE, HEM, UNL, K, FAD

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	0.65	0/4832	0.81	5/6543 (0.1%)
1	N	0.66	0/4826	0.81	5/6535 (0.1%)
2	B	0.66	0/1959	0.81	2/2641 (0.1%)
2	O	0.64	0/1959	0.80	2/2641 (0.1%)
3	C	0.51	0/1107	0.60	0/1506
3	P	0.49	0/1107	0.60	0/1506
4	D	0.44	0/788	0.60	0/1082
4	Q	0.43	0/788	0.59	0/1082
All	All	0.62	0/17366	0.77	14/23536 (0.1%)

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
3	C	0	1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	N	469	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	O	18	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	469	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	O	18	ARG	NE-CZ-NH1	5.97	123.29	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	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	4731	0	4614	57	0
1	N	4725	0	4609	65	0
2	B	1918	0	1910	27	0
2	O	1918	0	1909	27	0
3	C	1078	0	1118	35	0
3	P	1078	0	1118	36	0
4	D	765	0	761	19	0
4	Q	765	0	761	15	0
5	A	29	0	0	10	0
5	B	14	0	0	4	0
5	C	22	0	0	4	0
5	D	9	0	0	2	0
5	N	24	0	0	3	0
5	O	10	0	0	3	0
5	P	11	0	0	2	0
5	Q	6	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	A	3	0	0	0	0
8	A	53	0	29	4	0
8	N	53	0	29	4	0
9	A	9	0	2	6	0
9	N	9	0	2	5	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	0	0
13	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	O	6	0	8	2	0
13	P	6	0	8	0	0
14	C	18	0	24	0	0
14	P	18	0	24	0	0
15	C	41	0	24	1	0
15	P	41	0	24	0	0
16	C	16	0	13	3	0
16	P	16	0	13	3	0
17	D	24	0	40	0	0
17	Q	24	0	40	2	0
18	A	548	0	0	9	0
18	B	297	0	0	6	0
18	C	102	0	0	4	0
18	D	60	0	0	1	0
18	N	558	0	0	18	0
18	O	287	0	0	6	0
18	P	82	0	0	4	0
18	Q	62	0	0	1	0
All	All	19490	0	17096	286	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 286 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)
5:B:1005:UNL:O5	5:B:1005:UNL:O6	1.55	1.25
5:A:1003:UNL:O5	5:A:1003:UNL:O6	1.54	1.25
5:O:1005:UNL:O6	5:O:1005:UNL:O5	1.54	1.24
5:A:1004:UNL:O5	5:A:1004:UNL:O6	1.55	1.23
5:P:211:UNL:O5	5:P:211:UNL:O1	1.57	1.22

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	611/621 (98%)	590 (97%)	21 (3%)	0	100	100
1	N	610/621 (98%)	590 (97%)	20 (3%)	0	100	100
2	B	237/252 (94%)	228 (96%)	8 (3%)	1 (0%)	34	32
2	O	237/252 (94%)	229 (97%)	7 (3%)	1 (0%)	34	32
3	C	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	22	18
3	P	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	22	18
4	D	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
4	Q	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
All	All	2169/2234 (97%)	2101 (97%)	64 (3%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG
3	C	140	ILE
3	P	140	ILE

### 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	498/506 (98%)	495 (99%)	3 (1%)	86	90
1	N	497/506 (98%)	493 (99%)	4 (1%)	81	86
2	B	214/219 (98%)	211 (99%)	3 (1%)	67	73
2	O	214/219 (98%)	211 (99%)	3 (1%)	67	73
3	C	118/119 (99%)	117 (99%)	1 (1%)	81	86
3	P	118/119 (99%)	117 (99%)	1 (1%)	81	86
4	D	78/79 (99%)	75 (96%)	3 (4%)	33	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	78/79 (99%)	75 (96%)	3 (4%)	33	34
All	All	1815/1846 (98%)	1794 (99%)	21 (1%)	71	77

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	101	TRP
1	N	72	GLU
3	P	11	ARG
4	D	36	ASP
4	Q	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	101	ASN
1	N	112	ASN
3	P	101	ASN
4	D	9	HIS
4	D	53	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 95 are unknown and 4 are monoatomic - leaving 23 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$
12	F3S	B	1004	2	0,9,9	0.00	-	-		
14	BHG	P	204	-	18,18,18	1.58	3 (16%)	23,23,23	0.68	0
15	HEM	C	143	3,4	26,48,50	1.75	4 (15%)	21,80,82	1.40	3 (14%)
17	PEE	D	109	-	22,22,50	0.89	1 (4%)	20,20,55	1.00	2 (10%)
8	FAD	N	1001	1	51,58,58	2.37	21 (41%)	60,89,89	2.17	15 (25%)
15	HEM	P	201	3,4	26,48,50	1.89	6 (23%)	21,80,82	1.35	2 (9%)
10	FES	B	1002	2	0,4,4	0.00	-	-		
13	GOL	O	1009	-	5,5,5	1.05	0	5,5,5	0.58	0
16	CBE	C	144	-	16,17,17	1.07	1 (6%)	16,22,22	1.86	2 (12%)
13	GOL	P	208	-	5,5,5	1.27	0	5,5,5	0.61	0
16	CBE	P	202	-	16,17,17	1.06	1 (6%)	16,22,22	1.86	2 (12%)
14	BHG	C	142	-	18,18,18	1.92	5 (27%)	23,23,23	0.76	0
12	F3S	O	1004	2	0,9,9	0.00	-	-		
7	AZI	A	623	-	0,2,2	0.00	-	0,1,1	0.00	-
9	OAA	A	1002	-	2,8,8	11.52	2 (100%)	2,10,10	1.81	1 (50%)
13	GOL	C	294	-	5,5,5	1.21	0	5,5,5	0.59	0
17	PEE	Q	210	-	22,22,50	0.90	1 (4%)	20,20,55	0.97	2 (10%)
11	SF4	B	1003	2	0,12,12	0.00	-	-		
10	FES	O	1002	2	0,4,4	0.00	-	-		
9	OAA	N	1002	-	2,8,8	13.43	2 (100%)	2,10,10	2.08	1 (50%)
13	GOL	B	1010	-	5,5,5	1.09	0	5,5,5	0.52	0
8	FAD	A	1001	1	51,58,58	2.34	18 (35%)	60,89,89	2.18	16 (26%)
11	SF4	O	1003	2	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	F3S	B	1004	2	-	-	0/3/3/3
14	BHG	P	204	-	1/1/5/5	2/9/29/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	C	143	3,4	-	0/6/50/54	-
11	SF4	O	1003	2	-	-	0/6/5/5
8	FAD	N	1001	1	-	10/30/50/50	0/6/6/6
15	HEM	P	201	3,4	-	0/6/50/54	-
10	FES	B	1002	2	-	-	0/1/1/1
13	GOL	O	1009	-	-	4/4/4/4	-
16	CBE	C	144	-	-	2/6/19/19	0/1/2/2
17	PEE	D	109	-	-	11/18/18/54	-
13	GOL	P	208	-	-	2/4/4/4	-
16	CBE	P	202	-	-	2/6/19/19	0/1/2/2
12	F3S	O	1004	2	-	-	0/3/3/3
9	OAA	A	1002	-	-	0/2/8/8	-
13	GOL	C	294	-	-	2/4/4/4	-
17	PEE	Q	210	-	-	13/18/18/54	-
11	SF4	B	1003	2	-	-	0/6/5/5
10	FES	O	1002	2	-	-	0/1/1/1
9	OAA	N	1002	-	-	0/2/8/8	-
13	GOL	B	1010	-	-	1/4/4/4	-
8	FAD	A	1001	1	-	9/30/50/50	0/6/6/6
14	BHG	C	142	-	1/1/5/5	3/9/29/29	0/1/1/1

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	1002	OAA	O3-C3	18.07	1.51	1.22
9	A	1002	OAA	O3-C3	15.76	1.47	1.22
8	A	1001	FAD	C4X-N5	5.92	1.41	1.33
15	P	201	HEM	CAB-C3B	-5.82	1.39	1.51
9	N	1002	OAA	C2-C3	-5.81	1.46	1.51

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	FAD	C4X-N5-C5X	7.25	124.02	116.77
8	N	1001	FAD	C4X-N5-C5X	7.17	123.93	116.77
8	A	1001	FAD	N3A-C2A-N1A	-5.99	119.32	128.68
8	N	1001	FAD	C4-N3-C2	5.89	120.12	115.14
8	A	1001	FAD	C4-N3-C2	5.86	120.09	115.14

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
14	P	204	BHG	C4
14	C	142	BHG	C4

5 of 61 torsion outliers are listed below:

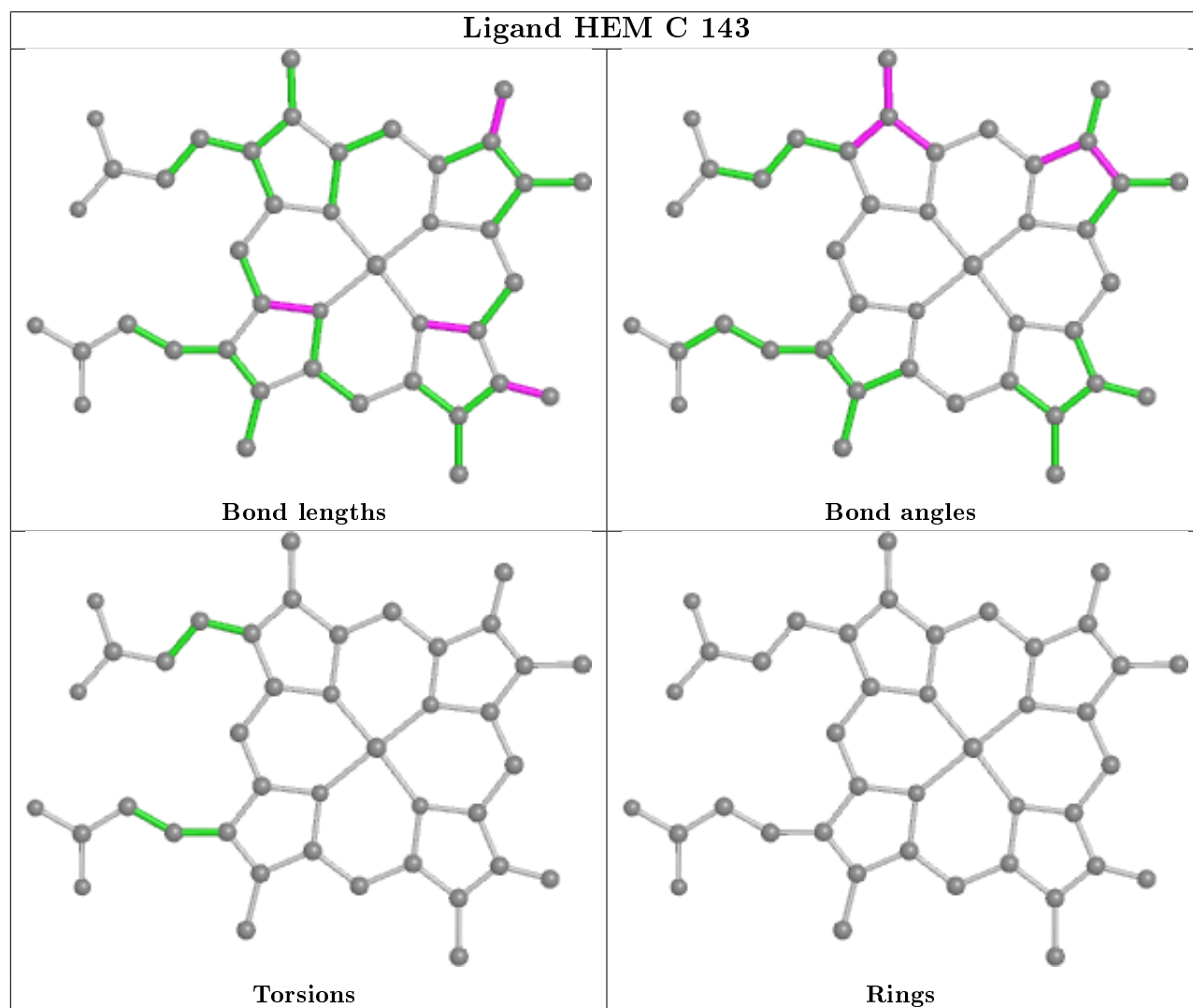
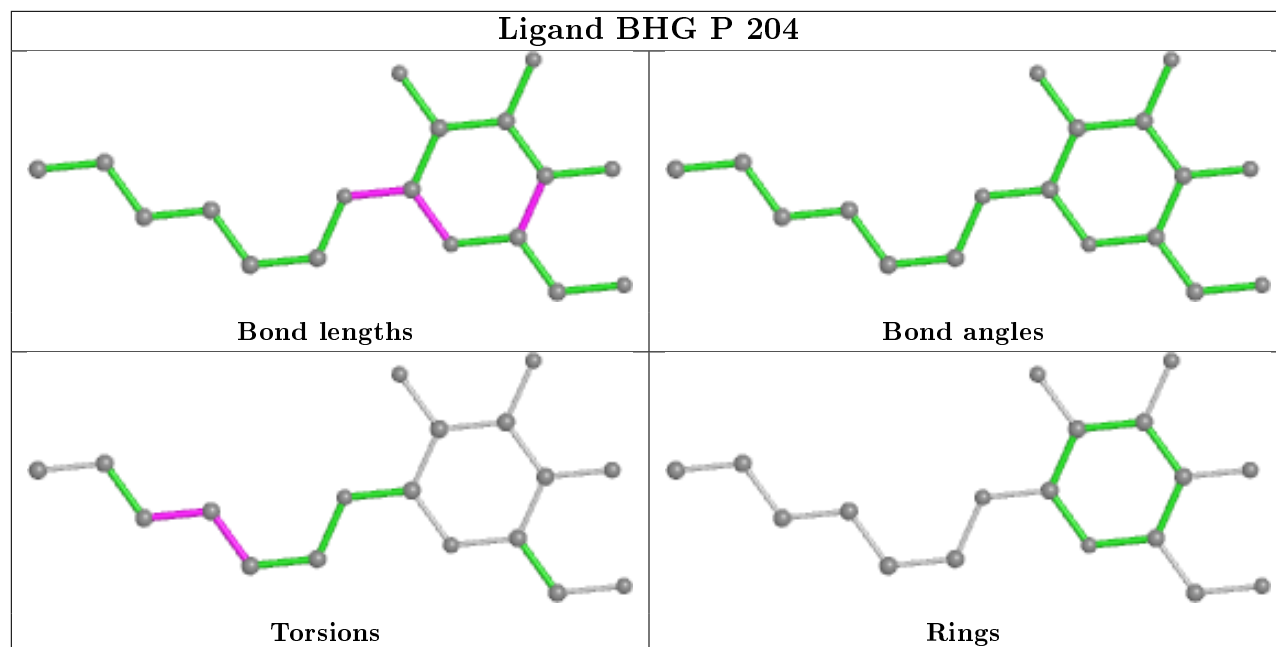
Mol	Chain	Res	Type	Atoms
13	C	294	GOL	C1-C2-C3-O3
8	N	1001	FAD	N10-C1'-C2'-O2'
8	N	1001	FAD	N10-C1'-C2'-C3'
8	N	1001	FAD	O4'-C4'-C5'-O5'
8	N	1001	FAD	C5'-O5'-P-O1P

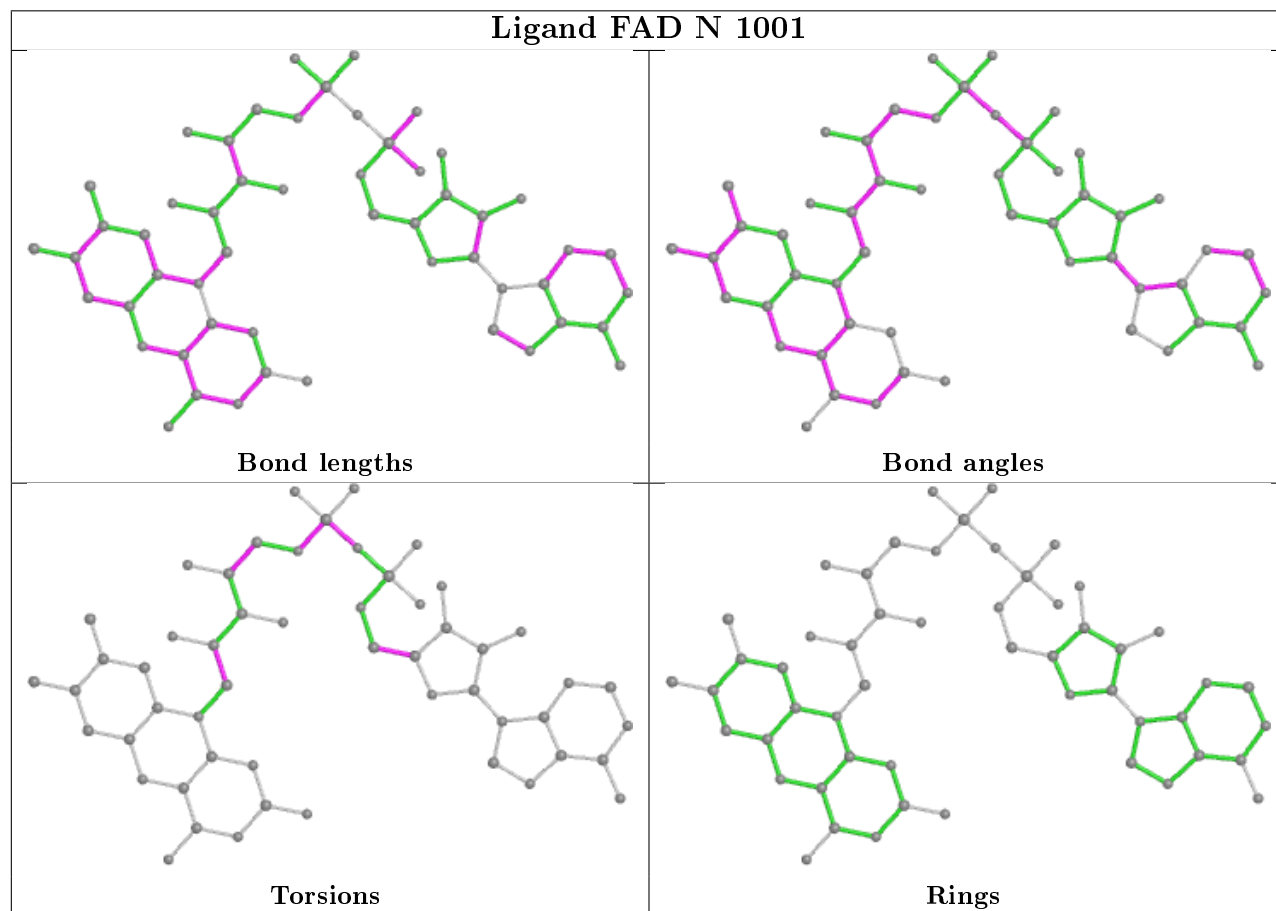
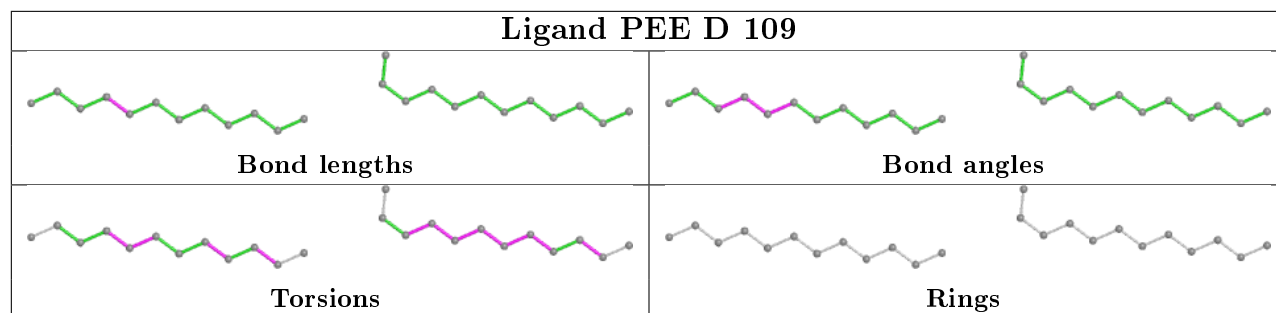
There are no ring outliers.

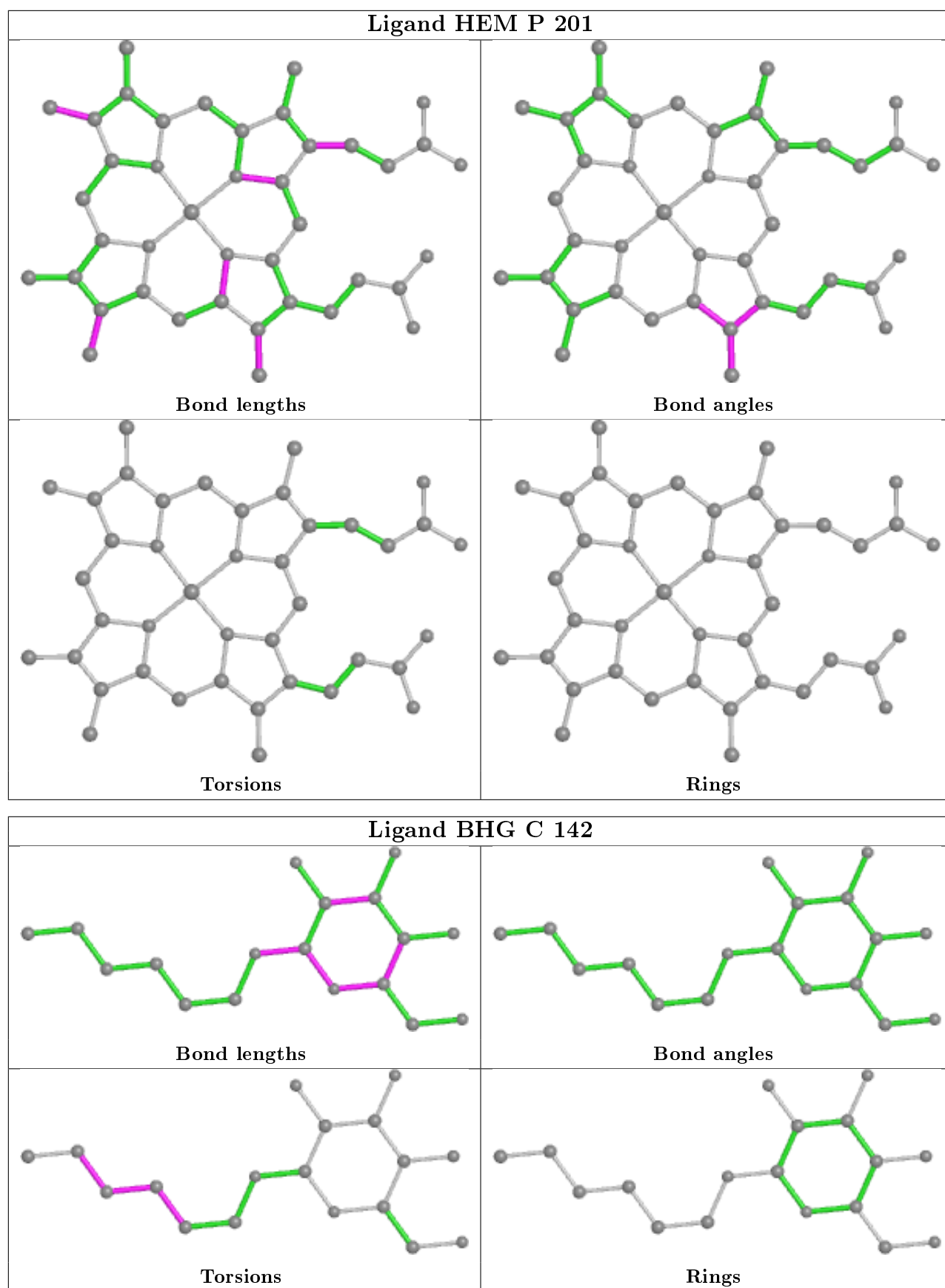
10 monomers are involved in 29 short contacts:

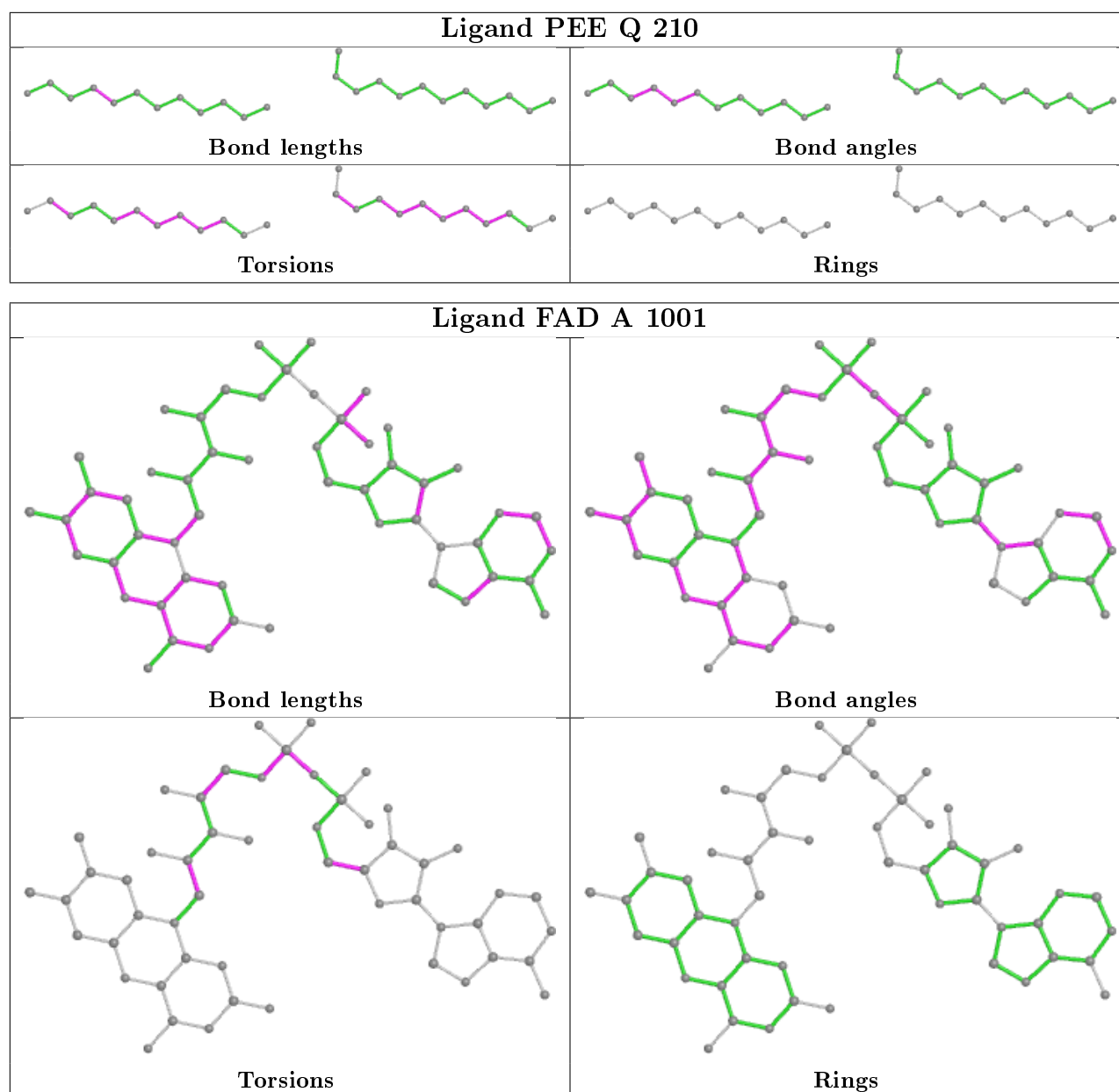
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	143	HEM	1	0
8	N	1001	FAD	4	0
13	O	1009	GOL	2	0
16	C	144	CBE	3	0
16	P	202	CBE	3	0
9	A	1002	OAA	6	0
13	C	294	GOL	1	0
17	Q	210	PEE	2	0
9	N	1002	OAA	5	0
8	A	1001	FAD	4	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/621 (98%)	-0.13	3 (0%) 91 92	11, 23, 45, 85	0
1	N	612/621 (98%)	-0.11	2 (0%) 94 94	10, 22, 42, 81	0
2	B	239/252 (94%)	-0.16	1 (0%) 92 93	15, 22, 38, 67	0
2	O	239/252 (94%)	-0.16	2 (0%) 86 88	13, 22, 37, 68	0
3	C	140/141 (99%)	0.15	4 (2%) 51 57	19, 34, 52, 75	0
3	P	140/141 (99%)	0.47	10 (7%) 16 20	18, 37, 77, 87	0
4	D	101/103 (98%)	0.43	7 (6%) 16 21	21, 41, 59, 62	0
4	Q	101/103 (98%)	0.64	12 (11%) 4 5	26, 47, 67, 75	0
All	All	2185/2234 (97%)	-0.01	41 (1%) 66 71	10, 24, 53, 87	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	10	THR	9.6
3	P	141	SER	7.4
3	P	140	ILE	6.9
3	C	140	ILE	6.3
1	A	9	SER	5.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	UNL	N	1005	1/-	-0.09	1.73	76,76,76,76	0
5	UNL	B	1007	1/-	0.11	0.89	74,74,74,74	0
5	UNL	N	1012	1/-	0.14	1.01	94,94,94,94	0
5	UNL	Q	287	1/-	0.16	0.77	75,75,75,75	0
5	UNL	C	259	1/-	0.20	0.49	64,64,64,64	0
5	UNL	B	1006	1/-	0.24	1.25	76,76,76,76	0
5	UNL	N	1014	1/-	0.32	0.61	76,76,76,76	0
5	UNL	A	1005	1/-	0.33	1.31	66,66,66,66	0
13	GOL	P	208	6/6	0.35	1.64	155,156,156,157	0
5	UNL	N	1022	1/-	0.42	0.64	72,72,72,72	0
5	UNL	O	276	1/-	0.46	0.45	65,65,65,65	0
5	UNL	P	211	5/-	0.47	0.96	119,119,120,121	0
5	UNL	A	1022	1/-	0.47	0.35	51,51,51,51	0
5	UNL	D	265	1/-	0.50	1.14	103,103,103,103	0
5	UNL	B	1005	5/-	0.53	0.39	92,93,93,94	0
5	UNL	N	1016	1/-	0.53	0.40	62,62,62,62	0
5	UNL	D	266	1/-	0.54	0.56	62,62,62,62	0
5	UNL	P	224	1/-	0.55	0.66	71,71,71,71	0
5	UNL	N	1006	1/-	0.58	0.53	52,52,52,52	0
5	UNL	A	1007	1/-	0.60	0.56	66,66,66,66	0
17	PEE	Q	210	24/51	0.60	0.56	70,82,95,95	0
5	UNL	B	1009	1/-	0.61	0.62	73,73,73,73	0
5	UNL	N	1018	1/-	0.61	0.48	46,46,46,46	0
5	UNL	C	235	1/-	0.63	0.52	71,71,71,71	0
5	UNL	C	214	5/-	0.64	0.37	90,91,92,93	0
5	UNL	A	1015	1/-	0.64	1.04	69,69,69,69	0
17	PEE	D	109	24/51	0.64	0.40	48,64,74,75	0
5	UNL	C	248	1/-	0.64	0.70	57,57,57,57	0
5	UNL	D	247	1/-	0.64	0.41	68,68,68,68	0
5	UNL	N	1023	1/-	0.65	0.32	45,45,45,45	0
5	UNL	A	1003	6/-	0.65	0.26	135,136,136,137	0
5	UNL	A	1010	1/-	0.67	0.66	67,67,67,67	0
5	UNL	C	254	1/-	0.67	0.45	55,55,55,55	0
5	UNL	A	1023	1/-	0.69	0.45	53,53,53,53	0
5	UNL	C	292	1/-	0.69	0.57	64,64,64,64	0
5	UNL	O	1005	5/-	0.71	0.37	146,146,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UNL	D	291	1/-	0.71	0.43	58,58,58,58	0
5	UNL	B	277	1/-	0.73	0.23	46,46,46,46	0
5	UNL	B	268	1/-	0.74	0.49	51,51,51,51	0
5	UNL	A	1004	4/-	0.75	0.21	55,60,60,61	0
5	UNL	N	1021	1/-	0.75	0.29	42,42,42,42	0
5	UNL	A	1013	1/-	0.75	0.27	39,39,39,39	0
5	UNL	N	1013	1/-	0.76	0.30	57,57,57,57	0
5	UNL	C	293	1/-	0.76	0.50	62,62,62,62	0
5	UNL	P	274	1/-	0.76	0.52	56,56,56,56	0
5	UNL	N	1009	1/-	0.76	0.32	50,50,50,50	0
5	UNL	A	1012	1/-	0.77	0.69	69,69,69,69	0
5	UNL	A	1011	1/-	0.77	0.44	55,55,55,55	0
5	UNL	P	285	1/-	0.77	0.35	50,50,50,50	0
5	UNL	D	263	1/-	0.77	0.51	53,53,53,53	0
5	UNL	A	1008	1/-	0.78	1.00	62,62,62,62	0
5	UNL	Q	288	1/-	0.78	0.45	44,44,44,44	0
5	UNL	O	282	1/-	0.78	0.28	52,52,52,52	0
5	UNL	N	1007	1/-	0.79	0.38	59,59,59,59	0
5	UNL	B	280	1/-	0.80	0.40	53,53,53,53	0
5	UNL	Q	237	1/-	0.81	0.38	47,47,47,47	0
5	UNL	D	262	1/-	0.81	0.47	59,59,59,59	0
7	AZI	A	623	3/3	0.81	0.19	56,56,64,64	0
14	BHG	C	142	18/18	0.81	0.37	49,67,79,79	0
5	UNL	P	233	1/-	0.82	0.40	44,44,44,44	0
5	UNL	C	251	1/-	0.82	0.49	53,53,53,53	0
5	UNL	O	1007	1/-	0.83	0.31	69,69,69,69	0
5	UNL	B	258	1/-	0.83	0.37	57,57,57,57	0
5	UNL	A	1016	1/-	0.83	0.62	50,50,50,50	0
5	UNL	A	1014	1/-	0.83	0.47	47,47,47,47	0
5	UNL	A	1009	1/-	0.83	0.30	50,50,50,50	0
5	UNL	O	1006	1/-	0.83	0.48	66,66,66,66	0
13	GOL	C	294	6/6	0.84	0.64	132,132,133,133	0
5	UNL	C	289	1/-	0.84	0.33	57,57,57,57	0
5	UNL	A	1021	1/-	0.85	0.31	37,37,37,37	0
5	UNL	C	145	4/-	0.85	0.11	70,70,70,70	0
5	UNL	Q	221	1/-	0.85	0.49	56,56,56,56	0
5	UNL	O	1008	1/-	0.85	0.29	47,47,47,47	0
5	UNL	B	297	1/-	0.85	0.26	51,51,51,51	0
5	UNL	B	1008	1/-	0.86	0.69	61,61,61,61	0
5	UNL	P	218	1/-	0.86	0.44	57,57,57,57	0
5	UNL	C	267	1/-	0.86	0.48	52,52,52,52	0
5	UNL	N	1020	1/-	0.87	0.27	56,56,56,56	0

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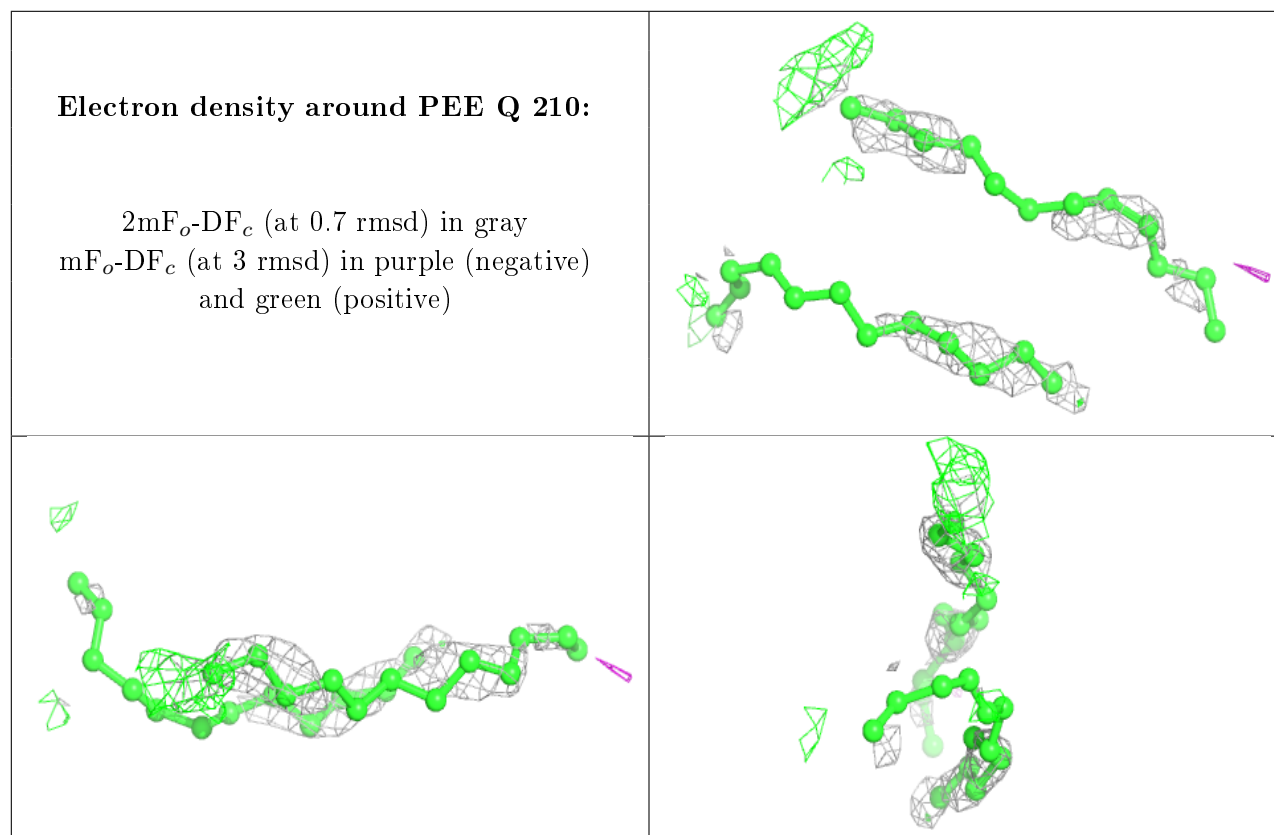
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UNL	P	236	1/-	0.87	0.46	53,53,53,53	0
5	UNL	C	256	1/-	0.87	0.47	61,61,61,61	0
5	UNL	N	1003	4/-	0.88	0.15	57,58,59,59	0
5	UNL	N	1008	1/-	0.88	0.38	39,39,39,39	0
5	UNL	Q	234	1/-	0.89	0.61	53,53,53,53	0
5	UNL	N	1010	1/-	0.89	0.44	63,63,63,63	0
5	UNL	C	240	1/-	0.89	0.38	45,45,45,45	0
5	UNL	N	1019	1/-	0.90	0.46	49,49,49,49	0
5	UNL	N	1011	1/-	0.90	0.30	38,38,38,38	0
5	UNL	C	241	1/-	0.90	0.31	61,61,61,61	0
5	UNL	N	1017	1/-	0.90	0.24	30,30,30,30	0
5	UNL	D	245	1/-	0.90	0.45	58,58,58,58	0
13	GOL	O	1009	6/6	0.90	0.20	29,30,33,33	0
5	UNL	C	272	1/-	0.90	0.43	54,54,54,54	0
5	UNL	N	1004	1/-	0.91	0.33	45,45,45,45	0
5	UNL	A	1017	1/-	0.91	0.18	48,48,48,48	0
5	UNL	D	250	1/-	0.91	0.43	53,53,53,53	0
5	UNL	D	255	1/-	0.92	0.23	35,35,35,35	0
5	UNL	A	1006	1/-	0.92	0.29	47,47,47,47	0
5	UNL	N	1015	1/-	0.92	0.46	42,42,42,42	0
14	BHG	P	204	18/18	0.92	0.17	38,45,58,59	0
5	UNL	A	1018	1/-	0.92	0.41	45,45,45,45	0
5	UNL	Q	219	1/-	0.92	0.34	45,45,45,45	0
5	UNL	A	1020	1/-	0.93	0.30	34,34,34,34	0
5	UNL	A	1019	1/-	0.93	0.28	37,37,37,37	0
16	CBE	C	144	16/16	0.95	0.17	28,32,37,39	0
13	GOL	B	1010	6/6	0.95	0.15	26,29,32,32	0
9	OAA	A	1002	9/9	0.96	0.11	19,21,24,26	0
16	CBE	P	202	16/16	0.96	0.12	25,30,35,35	0
9	OAA	N	1002	9/9	0.96	0.12	13,17,22,23	0
6	K	O	253	1/1	0.96	0.08	39,39,39,39	0
8	FAD	N	1001	53/53	0.97	0.12	4,13,21,24	0
15	HEM	P	201	41/43	0.97	0.13	29,32,43,48	0
15	HEM	C	143	41/43	0.97	0.13	23,32,40,49	0
8	FAD	A	1001	53/53	0.97	0.12	9,14,22,25	0
10	FES	B	1002	4/4	0.99	0.11	14,16,16,17	0
10	FES	O	1002	4/4	0.99	0.10	14,16,16,19	0
11	SF4	B	1003	8/8	0.99	0.10	16,17,19,21	0
6	K	B	253	1/1	0.99	0.06	38,38,38,38	0
6	K	A	622	1/1	0.99	0.09	24,24,24,24	0
12	F3S	B	1004	7/7	0.99	0.11	17,19,20,25	0
11	SF4	O	1003	8/8	0.99	0.11	14,18,20,20	0

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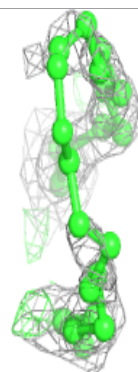
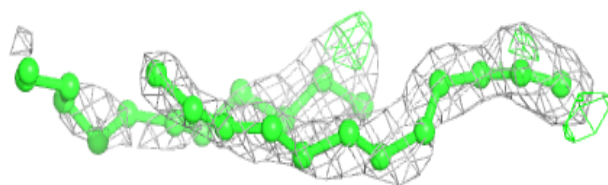
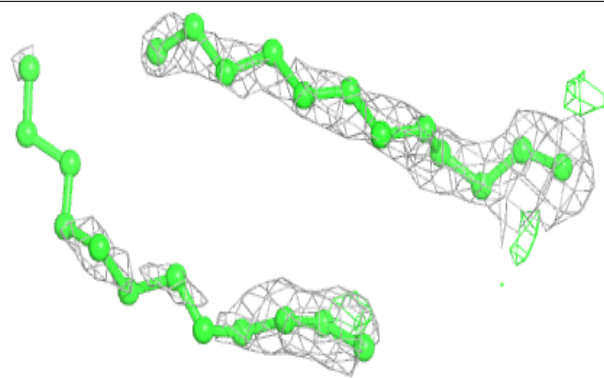
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	F3S	O	1004	7/7	0.99	0.13	15,20,22,22	0
6	K	N	622	1/1	0.99	0.09	19,19,19,19	0

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.

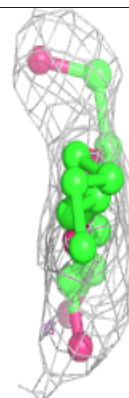
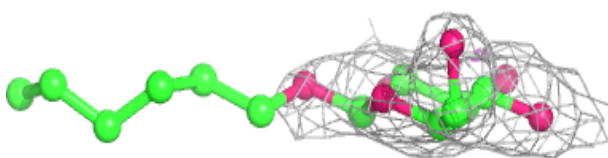
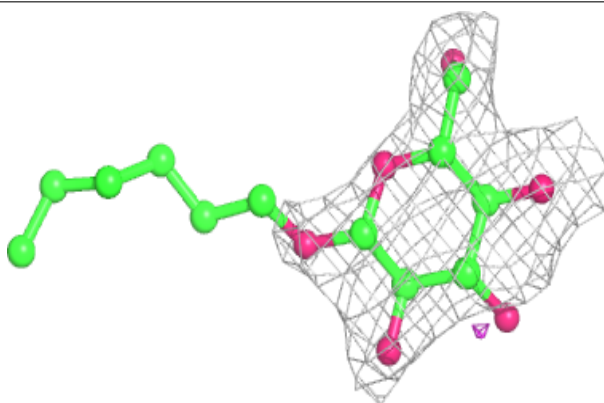


**Electron density around PEE D 109:**

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

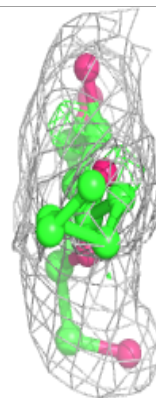
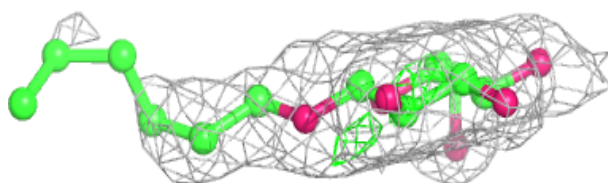
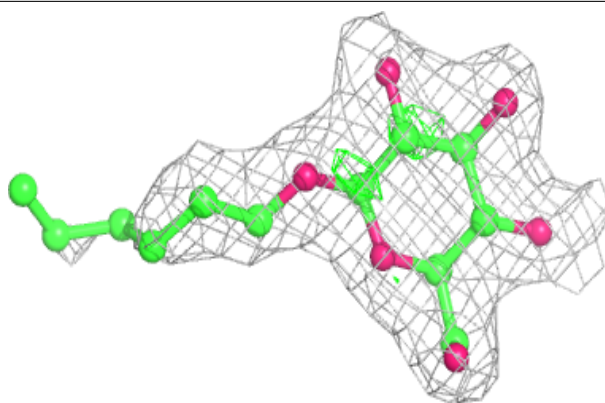
**Electron density around BHG C 142:**

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

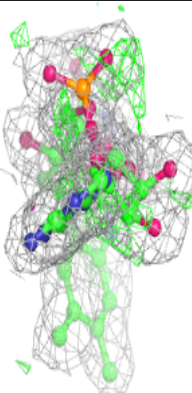
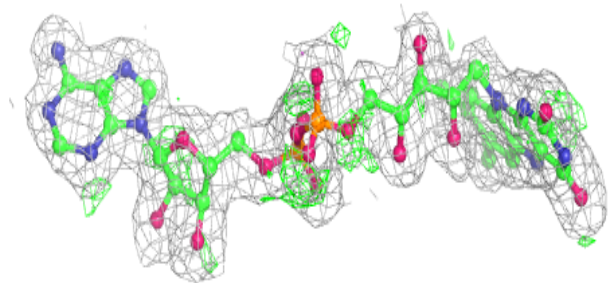
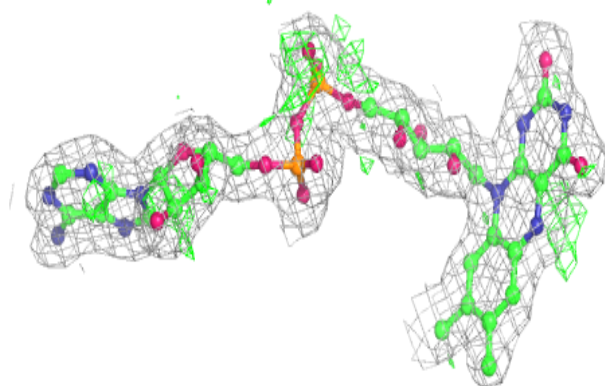


**Electron density around BHG P 204:**

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

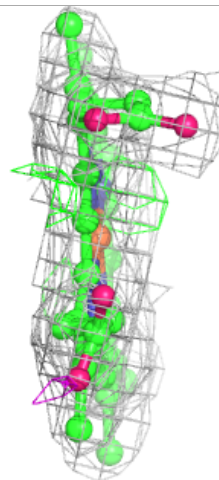
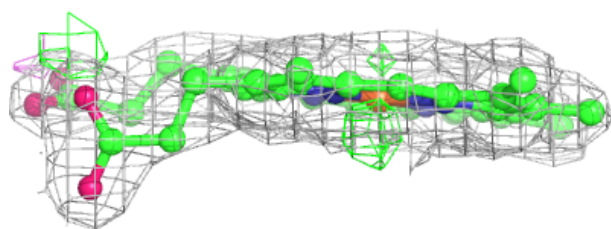
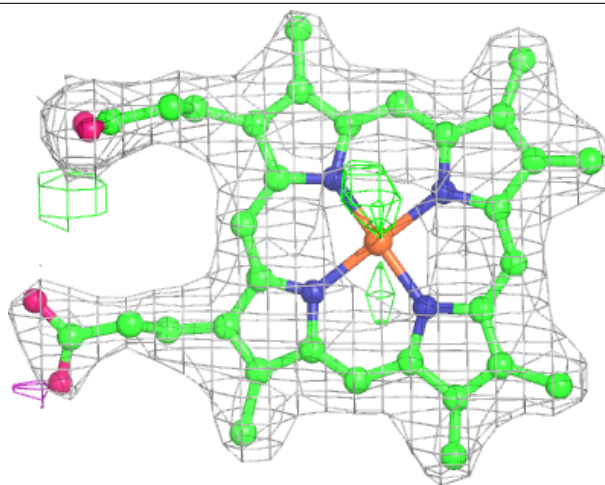
**Electron density around FAD N 1001:**

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



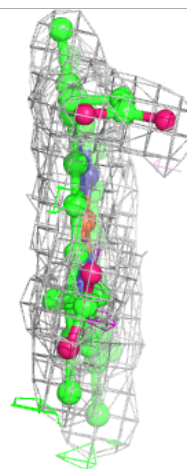
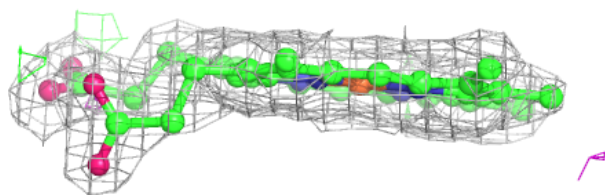
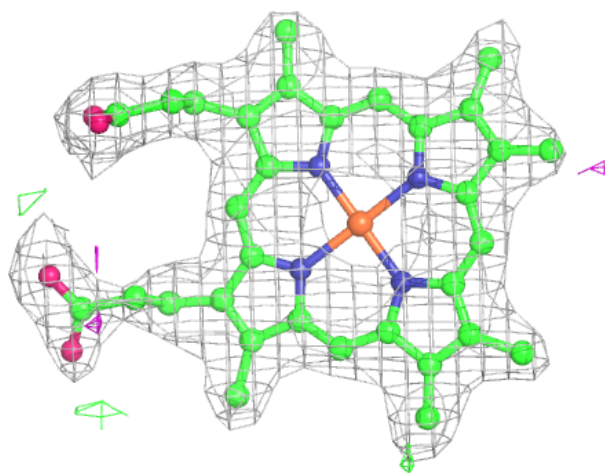
**Electron density around HEM P 201:**

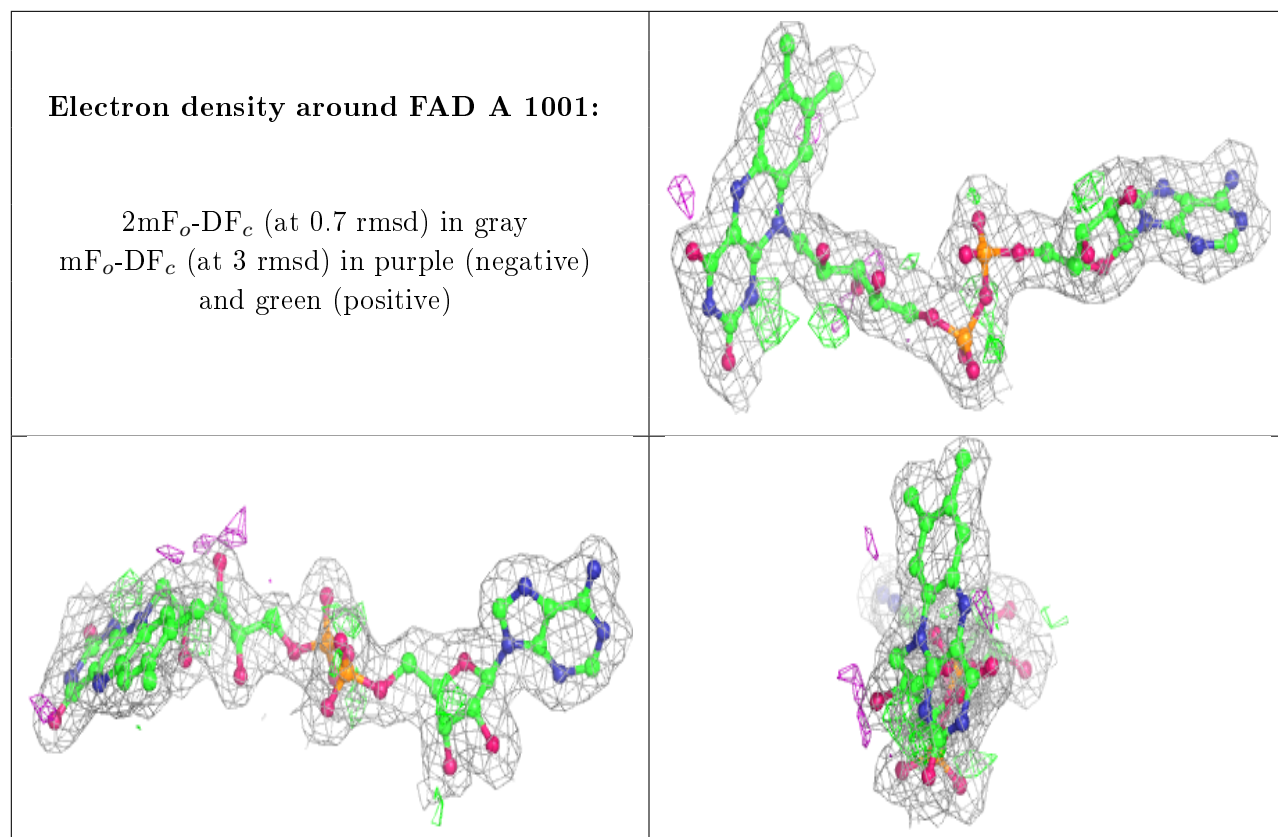
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 143:**

$2mF_o-DF_c$  (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.