



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:20 AM UTC

PDB ID : 2FBW / pdb\_00002fbw  
Title : Avian respiratory complex II with carboxin bound  
Authors : Huang, L.S.; Sun, G.; Cobessi, D.; Wang, A.C.; Shen, J.T.; Tung, E.Y.; Anderson, V.E.; Berry, E.A.  
Deposited on : 2005-12-10  
Resolution : 2.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

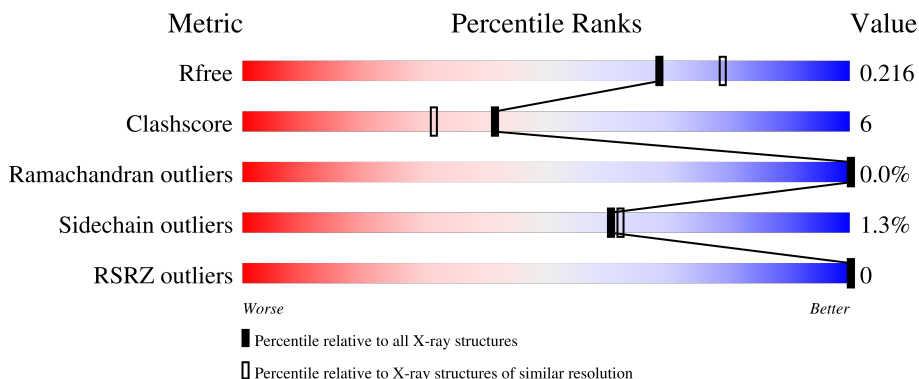
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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  $\geq 3$ , 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	86% 12% .
1	N	621	86% 13% .
2	B	252	87% 8% 5%
2	O	252	86% 10% .
3	C	140	84% 15% .

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Mol	Chain	Length	Quality of chain
3	P	140	 81% 18%
4	D	103	 83% 16%
4	Q	103	 80% 18%

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
6	Y3P	A	1002	-	X	X	-
8	AZI	A	1004	-	X	-	-
8	AZI	B	1005	-	X	-	-
8	AZI	N	1004	-	X	-	-
9	UNL	A	1368	-	-	X	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 19296 atoms, of which 4 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 [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	612	4737	2963	850	895	29	1	4	0
1	N	612	4733	2962	847	895	29	2	4	0

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1944	1228	331	363	22	1	2	0
2	O	241	1953	1234	333	364	22	0	2	0

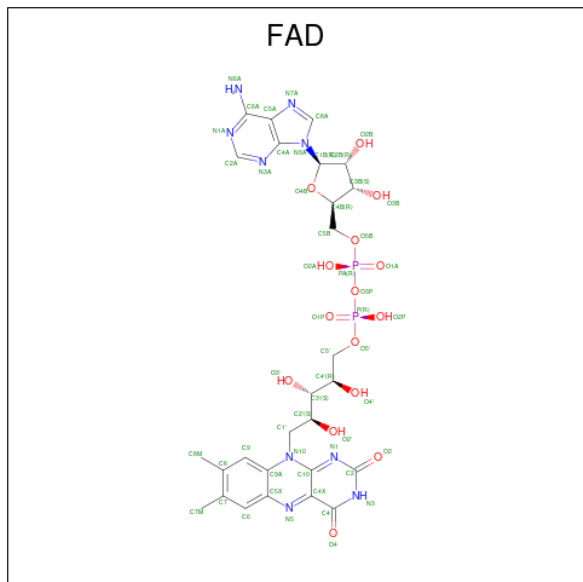
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	139	1083	712	179	187	5	0	1	0
3	P	139	1083	712	179	187	5	0	1	0

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

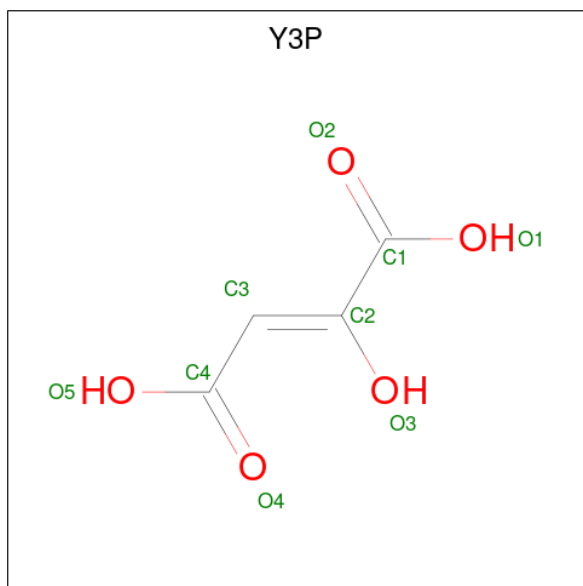
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	101	767	505	122	137	3	0	1	0
4	Q	101	766	505	121	137	3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is ( {Z} )-2-oxidanylbut-2-enedioic acid (CCD ID: Y3P) (formula:  $C_4H_4O_5$ ) (labeled as "Ligand of Interest" by depositor).

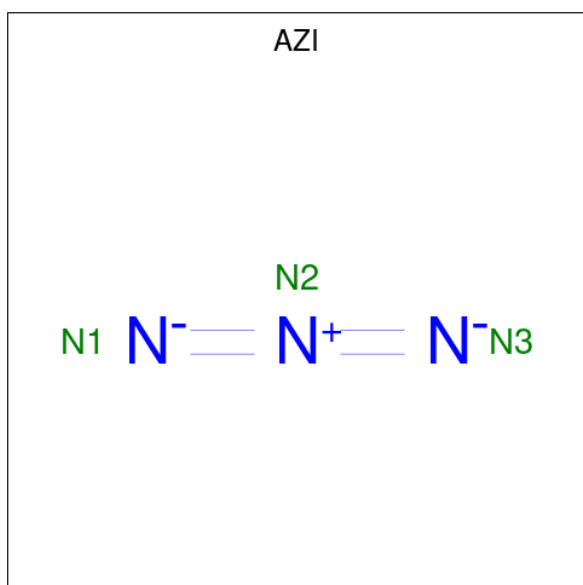


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			11	4	2	5		
6	N	1	Total	C	H	O	0	0
			11	4	2	5		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 8 is AZIDE ION (CCD ID: AZI) (formula: N<sub>3</sub>).

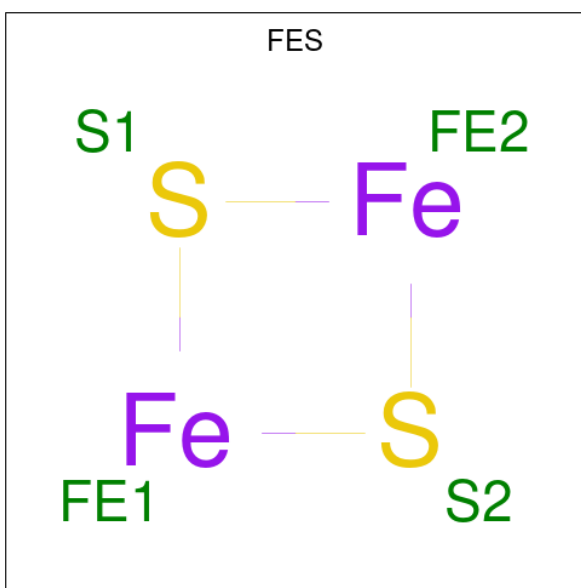


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	N	0	0
			3	3		
8	B	1	Total	N	0	0
			3	3		
8	N	1	Total	N	0	0
			3	3		

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

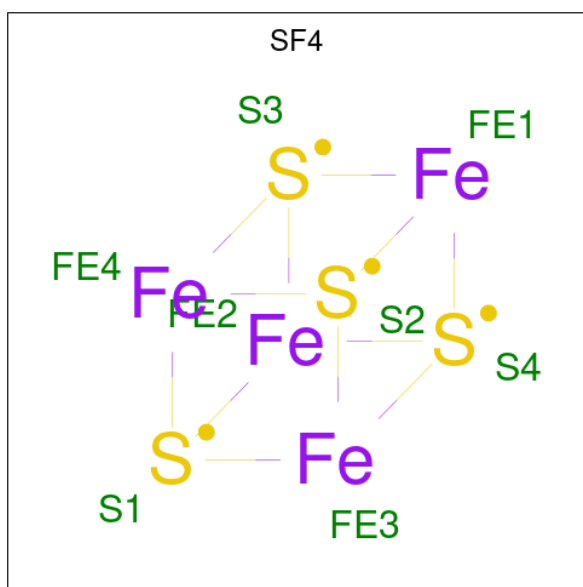
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	66	Total C N O S 129 30 15 83 1	0	8
9	B	43	Total C N O 77 11 15 51	0	5
9	C	19	Total C O 38 10 28	0	6
9	D	10	Total C O 52 29 23	0	1
9	N	64	Total C N O 142 31 21 90	0	11
9	O	36	Total C N O 84 20 12 52	0	9
9	P	9	Total C N O 43 26 3 14	0	0
9	Q	9	Total C O 74 45 29	0	1

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



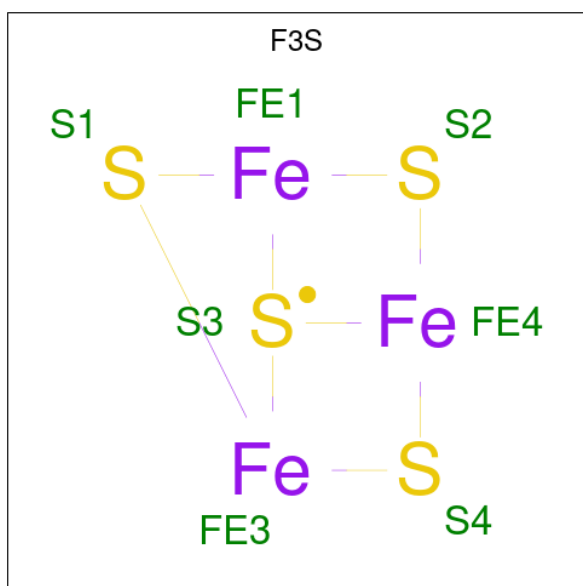
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 4 2 2	0	0
10	O	1	Total Fe S 4 2 2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: 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 (CCD ID: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

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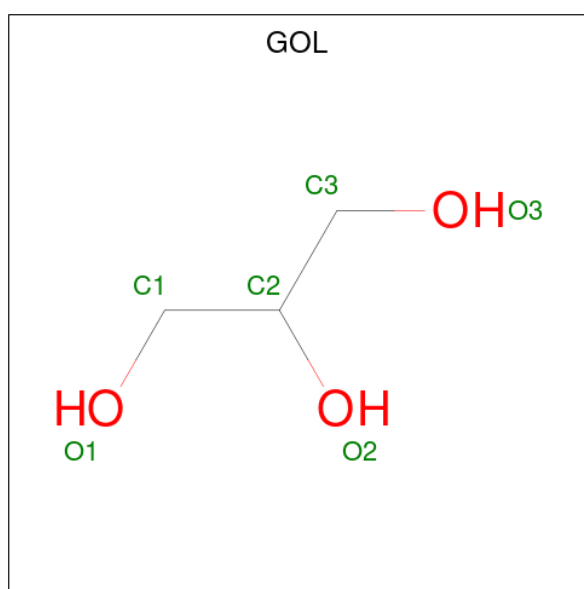
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	O	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is SODIUM ION (CCD ID: NA) (formula: Na).

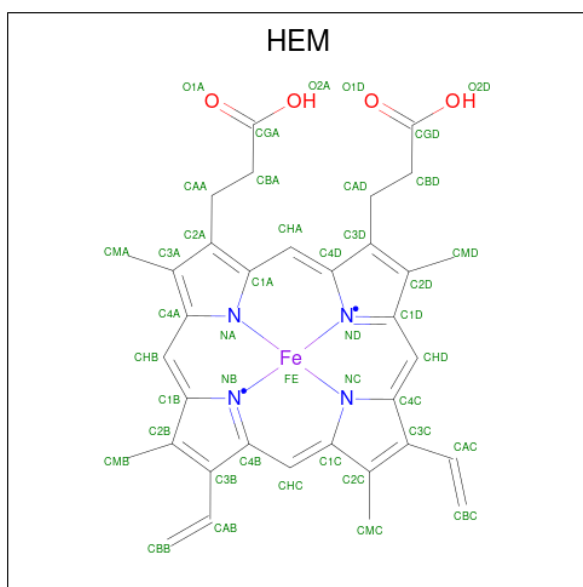
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Na	0	0
			1	1		

- Molecule 14 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



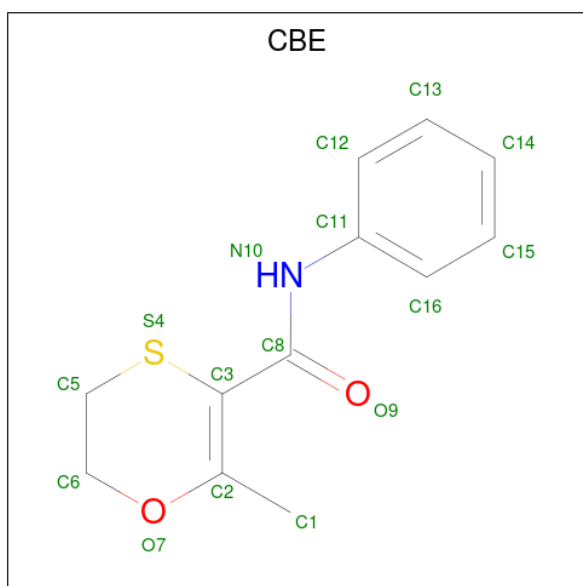
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	O	0	0
			6	3	3		
14	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 16 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (CCD ID: CBE) (formula:  $C_{12}H_{13}NO_2S$ ) (labeled as "Ligand of Interest" by depositor).



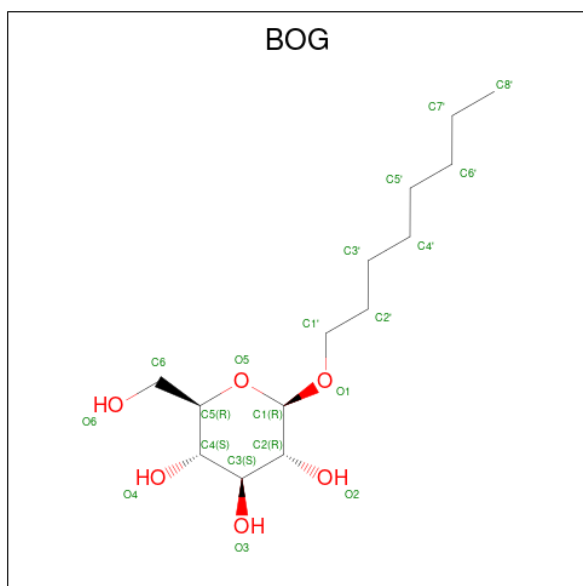
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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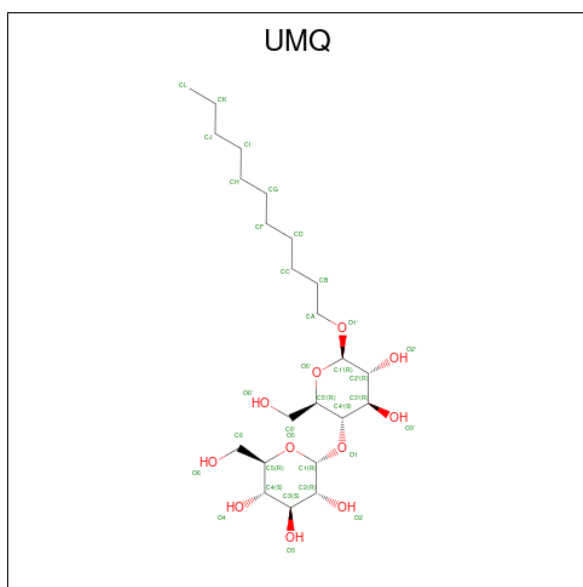
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
16	P	1	16	12	1	2	1	0	0

- Molecule 17 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
17	C	1	18	12	6	0	0
17	D	1	17	11	6	0	0
17	P	1	20	14	6	0	0

- Molecule 18 is UNDECYL-MALTOSE (CCD ID: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	P	1	Total	C O	0	0
			26	16 10		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	361	Total	O	0	1
			362	362		
19	B	164	Total	O	0	1
			165	165		
19	C	39	Total	O	0	0
			39	39		
19	D	18	Total	O	0	0
			18	18		
19	N	377	Total	O	0	1
			378	378		
19	O	188	Total	O	0	0
			188	188		
19	P	44	Total	O	0	0
			44	44		
19	Q	12	Total	O	0	0
			12	12		

### 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.

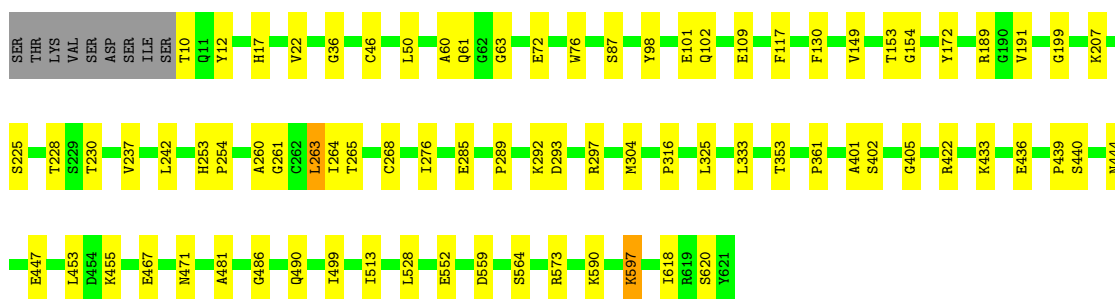
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A: 




- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain N: 



- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B: 



- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain O: 



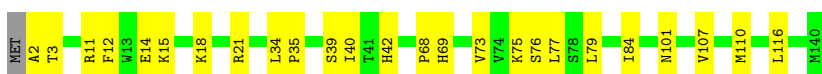
- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

Chain C: 84% 15%



- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

Chain P: 81% 18%



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D: 83% 16%



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain Q: 80% 18%



## 4 Data and refinement statistics i

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 – 2.06 64.09 – 2.06	Depositor EDS
% Data completeness (in resolution range)	85.2 (64.09-2.06) 85.6 (64.09-2.06)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.62 (at 2.05Å)	Xtrriage
Refinement program	PHENIX dev_3150	Depositor
R, $R_{free}$	0.171 , 0.215 0.171 , 0.216	Depositor DCC
$R_{free}$ test set	8237 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtrriage
Anisotropy	0.525	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.287 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	19296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage'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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, Y3P, F3S, GOL, NA, BOG, HEM, UNL, FAD, FES, CBE, K, AZI, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/4845	0.53	0/6559
1	N	0.34	0/4848	0.54	0/6564
2	B	0.34	0/1987	0.49	0/2678
2	O	0.32	0/1996	0.49	0/2689
3	C	0.21	0/1112	0.38	0/1511
3	P	0.21	0/1112	0.37	0/1511
4	D	0.18	0/798	0.29	0/1093
4	Q	0.17	0/789	0.28	0/1082
All	All	0.31	0/17487	0.49	0/23687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4737	0	4614	58	0
1	N	4733	0	4616	56	0
2	B	1944	0	1937	28	0
2	O	1953	0	1950	26	0
3	C	1083	0	1125	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1083	0	1125	22	0
4	D	767	0	752	10	0
4	Q	766	0	761	15	0
5	A	53	0	29	3	0
5	N	53	0	29	4	0
6	A	9	2	0	4	0
6	N	9	2	0	2	0
7	A	1	0	0	0	0
7	N	1	0	0	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	N	3	0	0	0	0
9	A	129	0	0	9	0
9	B	77	0	0	4	0
9	C	38	0	0	3	0
9	D	52	0	0	1	0
9	N	142	0	0	7	0
9	O	84	0	0	3	0
9	P	43	0	0	0	0
9	Q	74	0	0	2	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	1	0	0	0	0
14	B	6	0	8	0	0
14	N	6	0	8	3	0
15	C	41	0	24	1	0
15	P	41	0	24	2	0
16	C	16	0	13	1	0
16	P	16	0	13	2	0
17	C	18	0	21	0	0
17	D	17	0	19	2	0
17	P	20	0	28	4	0
18	P	26	0	25	7	0
19	A	362	0	0	7	0
19	B	165	0	0	0	0
19	C	39	0	0	0	0
19	D	18	0	0	0	0
19	N	378	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	188	0	0	3	0
19	P	44	0	0	0	0
19	Q	12	0	0	0	0
All	All	19292	4	17121	226	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 6.

All (226) 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:N:189:ARG:HD3	1:N:439:PRO:HB2	1.34	1.07
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.37	1.07
1:A:223:CYS:O	2:B:66[B]:ARG:NH2	2.02	0.93
1:A:218[A]:ARG:HH22	2:B:66[A]:ARG:HH21	1.19	0.90
1:A:297:ARG:HH22	6:A:1002:Y3P:C3	1.86	0.88
2:O:65[A]:CYS:O	2:O:66[A]:ARG:HB3	1.75	0.83
1:N:422:ARG:NE	14:N:1005:GOL:O1	2.15	0.78
4:Q:69:ASN:ND2	9:Q:214[A]:UNL:O6	2.19	0.75
1:N:261:GLY:HA2	9:N:1386:UNL:C	2.16	0.75
4:D:73:TYR:CE2	17:D:201:BOG:H62	2.21	0.75
1:N:36:GLY:O	14:N:1005:GOL:H32	1.86	0.75
1:N:297:ARG:HH22	6:N:1002:Y3P:C3	2.00	0.75
19:O:1150:HOH:O	15:P:201:HEM:O2D	2.05	0.74
1:N:260:ALA:O	2:O:66[B]:ARG:NH2	2.19	0.74
1:A:262:CYS:HA	2:B:66[B]:ARG:HE	1.54	0.73
3:P:84:ILE:HD13	4:Q:103:ILE:HG22	1.71	0.71
1:N:467:GLU:OE1	19:N:1119:HOH:O	2.08	0.71
1:A:401:ALA:N	1:A:402:SER:HA	2.06	0.71
9:A:1386:UNL:O	9:A:1396[B]:UNL:O	2.10	0.70
1:N:401:ALA:N	1:N:402:SER:HA	2.07	0.70
2:O:223:ARG:HA	3:P:116:LEU:HD11	1.72	0.70
2:B:65[A]:CYS:HB3	2:B:70:CYS:HB3	1.74	0.69
3:P:11:ARG:NH1	3:P:15:LYS:HB2	2.09	0.67
2:O:137:GLN:NE2	9:O:1211[B]:UNL:O	2.26	0.67
1:N:564:SER:HB2	1:N:618:ILE:HD11	1.76	0.66
1:N:552:GLU:OE2	9:N:1432:UNL:O	2.14	0.66
1:A:564:SER:HB2	1:A:618:ILE:HD11	1.77	0.66
1:A:224:THR:HA	2:B:66[B]:ARG:NH2	2.11	0.65
1:N:76:TRP:CE2	1:N:101:GLU:HG3	2.31	0.65
2:O:246:LYS:O	2:O:247:GLU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:VAL:HA	3:C:110:MET:HE2	1.79	0.65
1:A:10:THR:N	19:A:1345:HOH:O	2.30	0.64
2:B:223:ARG:HA	3:C:116:LEU:HD11	1.79	0.64
1:A:36:GLY:O	1:A:39:GLU:HG2	1.98	0.64
3:P:107:VAL:HA	3:P:110:MET:HE2	1.78	0.64
9:A:1368:UNL:C1	2:B:88:LYS:HE3	2.28	0.63
9:N:1388:UNL:C11	3:P:2:ALA:HB3	2.29	0.63
9:B:1179:UNL:O2	9:B:1199:UNL:O	2.16	0.62
5:N:1001:FAD:H2B	19:N:1182:HOH:O	1.99	0.62
2:B:65[A]:CYS:O	2:B:66[A]:ARG:HG2	1.99	0.62
1:A:87:SER:HB2	1:A:405:GLY:HA3	1.82	0.61
1:A:297:ARG:HH22	6:A:1002:Y3P:C2	2.13	0.61
3:C:14:GLU:O	3:C:18:LYS:HG2	2.00	0.61
2:O:223:ARG:HH12	18:P:203:UMQ:C5	2.14	0.61
1:N:87:SER:HB2	1:N:405:GLY:HA3	1.81	0.61
2:O:198:TYR:O	2:O:202:ARG:HG3	2.01	0.60
1:A:422:ARG:NE	19:A:1146:HOH:O	2.32	0.60
1:A:184:GLU:OE2	1:A:442:LYS:NZ	2.27	0.60
2:O:66[A]:ARG:NH2	9:O:1220:UNL:O	2.33	0.60
19:N:1219:HOH:O	2:O:66[A]:ARG:HB2	2.00	0.60
3:C:15:LYS:NZ	9:C:247:UNL:O	2.25	0.59
1:A:76:TRP:CE2	1:A:101:GLU:HG3	2.37	0.59
1:A:174:VAL:HG12	1:A:175:GLU:HG3	1.84	0.59
1:N:481:ALA:HB1	9:N:1420[B]:UNL:O	2.01	0.59
1:A:573:ARG:HD3	19:A:1302:HOH:O	2.03	0.58
2:O:65[A]:CYS:HB3	2:O:70:CYS:HB3	1.85	0.58
1:N:444:ASN:ND2	1:N:447:GLU:OE2	2.37	0.58
1:N:422:ARG:HE	14:N:1005:GOL:HO1	1.52	0.57
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.86	0.57
2:B:65[A]:CYS:O	2:B:66[A]:ARG:CB	2.52	0.56
19:N:1248:HOH:O	2:O:66[B]:ARG:NH2	2.38	0.56
3:C:139:ALA:O	18:P:203:UMQ:O2	2.24	0.56
1:N:10:THR:HG22	1:N:12:TYR:H	1.70	0.56
3:P:40:ILE:HD11	16:P:202:CBE:C16	2.36	0.56
1:A:564:SER:CB	1:A:618:ILE:HD11	2.35	0.56
3:C:8:GLU:OE2	9:C:254:UNL:O	2.23	0.55
2:O:98:LYS:HE2	19:O:1159:HOH:O	2.06	0.55
3:P:14:GLU:OE2	3:P:18:LYS:NZ	2.31	0.55
1:N:50:LEU:HD21	1:N:228:THR:HG21	1.89	0.55
2:O:248:LYS:HZ1	4:Q:3:SER:N	2.05	0.54
1:A:486:GLY:O	1:A:490:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:590:LYS:NZ	19:N:1290:HOH:O	2.38	0.54
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.90	0.54
1:N:564:SER:CB	1:N:618:ILE:HD11	2.36	0.54
3:C:15:LYS:HE3	3:C:21:ARG:HH12	1.72	0.54
1:N:297:ARG:HH22	6:N:1002:Y3P:C2	2.21	0.53
3:P:77:LEU:HB2	3:P:79:LEU:CD1	2.37	0.53
1:A:98:TYR:O	1:A:102:GLN:HG2	2.08	0.53
2:O:237:GLU:OE1	19:O:1080:HOH:O	2.18	0.53
1:N:98:TYR:O	1:N:102:GLN:HG2	2.09	0.53
1:N:237:VAL:HG13	1:N:242:LEU:HB2	1.90	0.53
2:O:155:LEU:CD1	2:O:192:ILE:HD11	2.39	0.53
3:C:84:ILE:HD13	4:D:103:ILE:HG22	1.91	0.52
2:O:248:LYS:O	4:Q:3:SER:HB3	2.09	0.52
2:B:198:TYR:O	2:B:202:ARG:HG3	2.09	0.52
2:B:66[B]:ARG:O	2:B:66[B]:ARG:HG2	2.08	0.52
3:C:77:LEU:HB2	3:C:79:LEU:CD1	2.39	0.52
2:O:123:LYS:NZ	3:P:3:THR:O	2.42	0.52
1:N:199:GLY:HA2	1:N:513:ILE:HG13	1.91	0.52
1:N:17:HIS:HA	9:N:1395:UNL:C3	2.40	0.52
1:N:10:THR:HA	9:N:1391:UNL:N3	2.25	0.52
2:O:141:GLN:HG3	9:O:1207[A]:UNL:O	2.10	0.51
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.40	0.51
1:A:237:VAL:HG13	1:A:242:LEU:HB2	1.93	0.51
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.41	0.51
3:P:75:LYS:HE2	4:Q:102:SER:O	2.10	0.51
18:P:203:UMQ:C6'	17:P:204:BOG:H61	2.40	0.51
18:P:203:UMQ:H6'2	17:P:204:BOG:H61	1.93	0.51
1:A:453:LEU:C	1:A:453:LEU:HD23	2.36	0.51
1:N:60:ALA:HA	5:N:1001:FAD:C6	2.40	0.51
2:B:246:LYS:O	2:B:247:GLU:HG2	2.11	0.51
1:A:207:LYS:HE3	1:A:436:GLU:OE1	2.11	0.50
9:A:1389:UNL:O	9:A:1390:UNL:O	2.30	0.50
1:N:46:CYS:HB3	1:N:172:TYR:CD2	2.46	0.50
1:N:63:GLY:HA2	1:N:153:THR:HG21	1.92	0.50
1:A:253:HIS:O	1:A:361:PRO:HA	2.12	0.49
3:C:15:LYS:HE3	3:C:21:ARG:NH1	2.27	0.49
1:N:207:LYS:HE3	1:N:436:GLU:OE1	2.12	0.49
1:A:63:GLY:HA2	1:A:153:THR:HG21	1.93	0.49
4:D:27:ALA:HB1	9:D:221:UNL:C7	2.43	0.49
4:Q:63:THR:HB	4:Q:64:PRO:HD3	1.95	0.49
2:B:65[A]:CYS:O	2:B:66[A]:ARG:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1412:UNL:O	9:A:1413:UNL:O	2.32	0.48
1:N:60:ALA:HB3	1:N:154:GLY:HA3	1.94	0.48
1:A:184:GLU:HG2	19:A:1221:HOH:O	2.11	0.48
4:D:63:THR:HB	4:D:64:PRO:HD3	1.95	0.48
2:O:248:LYS:HA	4:Q:4:LYS:HG3	1.96	0.48
3:P:15:LYS:HE3	3:P:21:ARG:HH12	1.79	0.48
1:A:559:ASP:O	1:A:573:ARG:NH1	2.46	0.48
1:A:184:GLU:CG	19:A:1221:HOH:O	2.61	0.48
1:A:263:LEU:HG	1:A:264:ILE:N	2.27	0.48
9:A:1391:UNL:O	9:A:1392:UNL:O	2.32	0.48
1:N:486:GLY:O	1:N:490:GLN:HG3	2.14	0.48
9:B:1195:UNL:O	9:B:1202:UNL:O	2.31	0.48
1:N:316:PRO:HG2	19:N:1318:HOH:O	2.13	0.48
1:A:261:GLY:C	2:B:66[B]:ARG:HH21	2.21	0.48
1:A:297:ARG:HH22	6:A:1002:Y3P:C4	2.27	0.47
19:A:1244:HOH:O	2:B:66[A]:ARG:HA	2.14	0.47
2:B:123:LYS:NZ	3:C:3:THR:O	2.44	0.47
1:A:218[A]:ARG:HH22	2:B:66[A]:ARG:NH2	2.00	0.47
3:C:42:HIS:HB2	3:C:101:ASN:HD22	1.79	0.47
1:N:263:LEU:HG	1:N:264:ILE:N	2.29	0.47
2:O:245:TYR:CE1	4:Q:4:LYS:HE3	2.49	0.47
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.96	0.47
2:B:65[A]:CYS:O	2:B:66[A]:ARG:CG	2.62	0.47
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.96	0.47
1:A:254:PRO:O	1:A:304:MET:HE1	2.14	0.47
3:P:34:LEU:HB3	3:P:35:PRO:HD3	1.96	0.47
18:P:203:UMQ:H6'1	17:P:204:BOG:O4	2.14	0.47
1:N:253:HIS:O	1:N:361:PRO:HA	2.15	0.47
1:N:453:LEU:C	1:N:453:LEU:HD23	2.39	0.47
1:A:199:GLY:HA2	1:A:513:ILE:HG13	1.96	0.46
2:B:141:GLN:HG3	9:B:1201[A]:UNL:O	2.15	0.46
1:N:285:GLU:HG2	1:N:292:LYS:HE3	1.96	0.46
18:P:203:UMQ:O3'	18:P:203:UMQ:H11	2.15	0.46
3:C:42:HIS:HB2	3:C:101:ASN:ND2	2.30	0.46
4:D:28:TYR:HD1	4:D:29:LEU:HD23	1.80	0.46
1:N:61:GLN:OE1	1:N:265:THR:HB	2.16	0.46
3:P:42:HIS:HB2	3:P:101:ASN:ND2	2.31	0.46
3:P:42:HIS:HB2	3:P:101:ASN:HD22	1.80	0.46
4:Q:93:ILE:O	4:Q:97:VAL:HG23	2.15	0.46
3:P:15:LYS:HE3	3:P:21:ARG:NH1	2.31	0.45
3:P:77:LEU:HB2	3:P:79:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:60:HIS:HE1	9:Q:215:UNL:C2	2.29	0.45
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.96	0.45
2:O:155:LEU:HD12	2:O:192:ILE:HD11	1.97	0.45
3:P:77:LEU:HB2	3:P:79:LEU:HD12	1.98	0.45
1:A:109:GLU:OE2	9:A:1401[B]:UNL:O	2.34	0.45
1:A:253:HIS:NE2	1:A:263:LEU:HD11	2.31	0.45
3:P:39:SER:OG	16:P:202:CBE:H51	2.16	0.45
2:B:200:GLU:OE1	2:B:247:GLU:HG3	2.17	0.45
3:C:77:LEU:HB2	3:C:79:LEU:HD12	1.98	0.45
2:O:246:LYS:HD2	2:O:246:LYS:HA	1.63	0.45
3:P:69:HIS:O	3:P:73:VAL:HG23	2.17	0.45
1:A:285:GLU:HG2	1:A:292:LYS:HE3	1.98	0.44
9:A:1368:UNL:C2	2:B:42:PRO:HG3	2.47	0.44
3:C:43:ARG:CZ	16:C:202:CBE:H62	2.48	0.44
1:N:597:LYS:HB3	1:N:597:LYS:HE2	1.78	0.44
3:C:69:HIS:O	3:C:73:VAL:HG23	2.16	0.44
1:N:230:THR:HA	1:N:528:LEU:HD21	1.99	0.44
1:A:253:HIS:CD2	1:A:263:LEU:HD11	2.51	0.44
1:A:455:LYS:HD2	19:A:1280:HOH:O	2.17	0.44
1:N:60:ALA:HA	5:N:1001:FAD:C5X	2.48	0.44
1:N:109:GLU:OE1	9:N:1414[B]:UNL:O	2.36	0.44
3:P:68:PRO:HB3	4:Q:99:MET:HE1	2.00	0.44
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.48	0.44
4:Q:28:TYR:HD1	4:Q:29:LEU:HD23	1.83	0.43
1:N:471[A]:ASN:ND2	1:N:499:ILE:HG12	2.33	0.43
4:Q:44:THR:HG21	4:Q:80:PHE:HB2	2.00	0.43
3:C:77:LEU:HB2	3:C:79:LEU:HD11	2.00	0.43
1:N:440:SER:HB3	19:N:1262:HOH:O	2.19	0.43
1:N:455:LYS:HD2	19:N:1292:HOH:O	2.19	0.43
3:P:73:VAL:O	3:P:76:SER:OG	2.33	0.43
1:A:61:GLN:OE1	1:A:265:THR:HB	2.19	0.43
1:A:333:LEU:HD12	1:A:353:THR:HG22	1.99	0.43
1:A:58:VAL:HB	1:A:158:LEU:HD23	2.01	0.43
1:N:333:LEU:HD12	1:N:353:THR:HG22	2.00	0.43
4:D:48:HIS:CD2	17:D:201:BOG:H3'2	2.54	0.42
2:O:116:SER:HG	3:P:12:PHE:HD1	1.67	0.42
4:Q:21:LEU:O	4:Q:25:PRO:HD2	2.19	0.42
1:A:16:ASP:OD1	1:A:203:ARG:HB2	2.20	0.42
1:A:230:THR:HA	1:A:528:LEU:HD21	2.02	0.42
1:N:254:PRO:O	1:N:304:MET:HE1	2.19	0.42
1:A:597:LYS:HB3	1:A:597:LYS:HE2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:ILE:O	4:D:97:VAL:HG23	2.19	0.42
1:A:297:ARG:NH2	6:A:1002:Y3P:C3	2.69	0.42
15:P:201:HEM:NB	4:Q:46:HIS:CD2	2.88	0.42
1:N:60:ALA:HA	5:N:1001:FAD:N5	2.35	0.42
1:A:60:ALA:HB1	5:A:1001:FAD:C4X	2.50	0.42
1:N:276:ILE:HD12	19:N:1301:HOH:O	2.20	0.42
1:N:433:LYS:HG3	1:N:436:GLU:OE2	2.20	0.42
1:N:268:CYS:HB3	1:N:325:LEU:HD21	2.02	0.41
1:A:262:CYS:SG	2:B:66[B]:ARG:HG2	2.60	0.41
2:B:43:MET:O	2:B:46:ASP:HB2	2.21	0.41
2:B:155:LEU:HD12	2:B:192:ILE:HD11	2.01	0.41
2:B:66[A]:ARG:NH2	9:B:1180:UNL:N3	2.68	0.41
3:C:68:PRO:HB3	4:D:99:MET:HE1	2.02	0.41
1:N:253:HIS:CD2	1:N:263:LEU:HD11	2.56	0.41
1:A:205:ARG:HG2	1:A:441:ILE:HD13	2.03	0.41
1:A:224:THR:HA	2:B:66[B]:ARG:HH21	1.81	0.41
1:A:11:GLN:OE1	9:A:1408:UNL:O	2.39	0.41
1:A:197:GLU:O	1:A:197:GLU:HG2	2.21	0.41
15:C:201:HEM:O2D	9:C:249[B]:UNL:O	2.39	0.41
1:N:289:PRO:HD2	19:N:1382:HOH:O	2.19	0.41
1:N:559:ASP:O	1:N:573:ARG:NH1	2.51	0.41
2:O:43:MET:O	2:O:46:ASP:HB2	2.20	0.41
1:A:305:THR:O	1:A:309:ARG:HG3	2.21	0.41
4:D:21:LEU:O	4:D:25:PRO:HD2	2.21	0.41
9:A:1373:UNL:N3	9:A:1388:UNL:O	2.54	0.40
1:N:117:PHE:HA	1:N:149:VAL:HG22	2.03	0.40
2:O:102:LEU:HA	2:O:103:PRO:HD3	1.90	0.40
1:N:199:GLY:CA	1:N:513:ILE:HG13	2.51	0.40
1:N:590:LYS:N	1:N:590:LYS:HD3	2.37	0.40
18:P:203:UMQ:H6'1	17:P:204:BOG:H61	2.04	0.40

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	614/621 (99%)	594 (97%)	20 (3%)	0	100	100
1	N	614/621 (99%)	596 (97%)	18 (3%)	0	100	100
2	B	240/252 (95%)	234 (98%)	6 (2%)	0	100	100
2	O	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	30	23
3	C	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
3	P	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
4	D	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
4	Q	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
All	All	2184/2232 (98%)	2128 (97%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	247	GLU

### 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	496/506 (98%)	491 (99%)	5 (1%)	68	71
1	N	497/506 (98%)	488 (98%)	9 (2%)	51	51
2	B	218/219 (100%)	213 (98%)	5 (2%)	44	41
2	O	219/219 (100%)	216 (99%)	3 (1%)	59	60
3	C	118/118 (100%)	118 (100%)	0	100	100
3	P	118/118 (100%)	118 (100%)	0	100	100
4	D	79/79 (100%)	78 (99%)	1 (1%)	61	62
4	Q	78/79 (99%)	77 (99%)	1 (1%)	61	62
All	All	1823/1844 (99%)	1799 (99%)	24 (1%)	61	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	130	PHE
1	A	191	VAL
1	A	597	LYS
1	A	620	SER
2	B	66[A]	ARG
2	B	66[B]	ARG
2	B	67	GLU
2	B	125	ILE
2	B	224	THR
4	D	8	LEU
1	N	22	VAL
1	N	72	GLU
1	N	130	PHE
1	N	191	VAL
1	N	225	SER
1	N	263	LEU
1	N	293	ASP
1	N	597	LYS
1	N	620	SER
2	O	67	GLU
2	O	125	ILE
2	O	224	THR
4	Q	8	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	320	HIS
1	A	324	GLN
4	D	69	ASN
1	N	324	GLN
4	Q	60	HIS
4	Q	69	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 323 ligands modelled in this entry, 3 are monoatomic and 297 are unknown - 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
8	AZI	B	1005	-	2,2,2	3.20	2 (100%)	0,1,1	-	-
14	GOL	B	1006	-	5,5,5	0.08	0	5,5,5	0.32	0
6	Y3P	N	1002	-	8,8,8	2.68	6 (75%)	9,10,10	1.08	0
15	HEM	C	201	3,4	48,48,50	1.36	7 (14%)	66,80,82	1.14	5 (7%)
17	BOG	D	201	-	17,17,20	0.69	1 (5%)	22,22,25	0.73	1 (4%)
11	SF4	B	1002	2	0,12,12	-	-	-	-	-
16	CBE	C	202	-	16,17,17	1.52	3 (18%)	17,22,22	2.02	4 (23%)
14	GOL	N	1005	-	5,5,5	0.06	0	5,5,5	0.27	0
12	F3S	O	1003	2	0,9,9	-	-	-	-	-
6	Y3P	A	1002	-	8,8,8	2.62	5 (62%)	9,10,10	1.53	3 (33%)
17	BOG	C	203	-	18,18,20	0.55	0	23,23,25	0.66	0
5	FAD	A	1001	1	58,58,58	0.88	2 (3%)	85,89,89	0.93	2 (2%)
8	AZI	A	1004	-	2,2,2	3.19	2 (100%)	0,1,1	-	-
18	UMQ	P	203	-	27,27,35	0.24	0	37,37,46	0.45	0
10	FES	O	1001	2	0,4,4	-	-	-	-	-
8	AZI	N	1004	-	2,2,2	3.18	2 (100%)	0,1,1	-	-
16	CBE	P	202	-	16,17,17	1.48	2 (12%)	17,22,22	2.02	3 (17%)
15	HEM	P	201	3,4	48,48,50	1.36	7 (14%)	66,80,82	1.11	5 (7%)
5	FAD	N	1001	1	58,58,58	0.95	3 (5%)	85,89,89	1.01	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BOG	P	204	-	20,20,20	0.50	0	25,25,25	0.69	1 (4%)
10	FES	B	1001	2	0,4,4	-	-	-		
11	SF4	O	1002	2	0,12,12	-	-	-		
12	F3S	B	1003	2	0,9,9	-	-	-		

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	GOL	B	1006	-	-	0/4/4/4	-
6	Y3P	N	1002	-	-	4/8/8/8	-
15	HEM	C	201	3,4	-	1/10/50/54	-
17	BOG	D	201	-	-	1/8/28/31	0/1/1/1
11	SF4	B	1002	2	-	-	0/6/5/5
16	CBE	C	202	-	-	2/6/19/19	0/2/2/2
14	GOL	N	1005	-	-	0/4/4/4	-
12	F3S	O	1003	2	-	-	0/3/3/3
6	Y3P	A	1002	-	-	4/8/8/8	-
17	BOG	C	203	-	-	4/9/29/31	0/1/1/1
5	FAD	A	1001	1	-	6/34/50/50	0/6/6/6
18	UMQ	P	203	-	-	3/12/49/60	0/2/2/2
10	FES	O	1001	2	-	-	0/1/1/1
16	CBE	P	202	-	-	2/6/19/19	0/2/2/2
15	HEM	P	201	3,4	-	1/10/50/54	-
5	FAD	N	1001	1	-	5/34/50/50	0/6/6/6
17	BOG	P	204	-	-	1/11/31/31	0/1/1/1
10	FES	B	1001	2	-	-	0/1/1/1
11	SF4	O	1002	2	-	-	0/6/5/5
12	F3S	B	1003	2	-	-	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1002	Y3P	C2-C1	4.78	1.55	1.48
6	A	1002	Y3P	C2-C1	4.72	1.55	1.48
16	P	202	CBE	C3-S4	-3.80	1.67	1.74
6	A	1002	Y3P	O2-C1	3.68	1.31	1.22
16	C	202	CBE	C11-N10	-3.62	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	201	HEM	FE-ND	3.62	2.06	1.94
16	C	202	CBE	C3-S4	-3.60	1.67	1.74
5	A	1001	FAD	P-O3P	3.58	1.63	1.59
15	P	201	HEM	FE-NB	3.40	2.05	1.94
15	P	201	HEM	FE-NC	3.35	2.06	1.95
15	C	201	HEM	FE-NB	3.34	2.05	1.94
8	N	1004	AZI	N3-N2	-3.24	1.16	1.23
8	B	1005	AZI	N3-N2	-3.24	1.16	1.23
8	A	1004	AZI	N3-N2	-3.19	1.16	1.23
8	A	1004	AZI	N1-N2	-3.19	1.16	1.23
16	P	202	CBE	C11-N10	-3.18	1.35	1.41
8	B	1005	AZI	N1-N2	-3.17	1.16	1.23
15	P	201	HEM	FE-ND	3.13	2.04	1.94
8	N	1004	AZI	N1-N2	-3.12	1.16	1.23
6	N	1002	Y3P	O2-C1	3.04	1.30	1.22
5	N	1001	FAD	C5X-N5	-2.85	1.34	1.39
15	C	201	HEM	FE-NA	2.84	2.04	1.95
6	N	1002	Y3P	O4-C4	2.74	1.29	1.23
5	N	1001	FAD	C6-C7	-2.52	1.36	1.39
6	N	1002	Y3P	O3-C2	2.25	1.39	1.33
15	P	201	HEM	CMB-C2B	2.18	1.55	1.50
15	C	201	HEM	CAC-C3C	2.18	1.55	1.50
17	D	201	BOG	O1-C1	2.17	1.43	1.40
15	P	201	HEM	CMD-C2D	2.17	1.55	1.50
6	A	1002	Y3P	O1-C1	-2.15	1.24	1.30
6	A	1002	Y3P	C3-C2	-2.14	1.32	1.36
15	P	201	HEM	CMC-C2C	2.12	1.55	1.50
6	N	1002	Y3P	O1-C1	-2.11	1.24	1.30
5	N	1001	FAD	C9A-N10	-2.10	1.37	1.41
15	C	201	HEM	CMC-C2C	2.10	1.55	1.50
6	A	1002	Y3P	O3-C2	2.09	1.39	1.33
15	P	201	HEM	CAC-C3C	2.08	1.55	1.50
15	C	201	HEM	CAB-C3B	2.08	1.55	1.50
6	N	1002	Y3P	C3-C2	-2.05	1.32	1.36
15	C	201	HEM	CMB-C2B	2.04	1.55	1.50
5	A	1001	FAD	C5X-N5	-2.03	1.35	1.39
16	C	202	CBE	C8-C3	-2.03	1.45	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	202	CBE	O7-C2-C1	6.92	117.48	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	202	CBE	O7-C2-C1	6.80	117.34	109.30
5	N	1001	FAD	O3P-PA-O1A	-2.87	102.06	110.70
16	C	202	CBE	C6-O7-C2	2.78	123.39	115.85
5	N	1001	FAD	O2A-PA-O3P	2.61	114.32	107.27
6	A	1002	Y3P	O4-C4-C3	-2.58	116.13	124.02
5	A	1001	FAD	C4'-C3'-C2'	-2.57	109.29	113.57
17	D	201	BOG	O5-C5-C6	2.49	112.61	106.44
15	C	201	HEM	C1B-NB-C4B	2.48	108.15	105.21
16	P	202	CBE	C6-O7-C2	2.46	122.52	115.85
6	A	1002	Y3P	O2-C1-C2	-2.46	117.31	120.12
16	P	202	CBE	C5-S4-C3	2.36	106.96	100.70
17	P	204	BOG	O5-C5-C6	2.33	112.22	106.44
15	C	201	HEM	C3D-C4D-ND	-2.32	107.62	110.17
5	A	1001	FAD	O4B-C1B-N9A	2.30	112.50	108.09
15	P	201	HEM	CHD-C4C-NC	2.27	126.92	124.45
15	P	201	HEM	C1B-NB-C4B	2.25	107.87	105.21
16	C	202	CBE	C11-N10-C8	-2.15	123.64	127.45
15	P	201	HEM	C2A-C1A-NA	-2.15	107.77	110.15
15	C	201	HEM	C3B-C4B-NB	-2.13	107.44	109.90
15	C	201	HEM	C4D-ND-C1D	2.13	107.73	105.21
6	A	1002	Y3P	O5-C4-C3	2.12	119.70	113.40
5	N	1001	FAD	O2'-C2'-C3'	-2.12	104.29	109.25
5	N	1001	FAD	O2A-PA-O1A	2.10	122.20	112.44
5	N	1001	FAD	C1'-C2'-C3'	2.07	115.27	109.66
15	P	201	HEM	C3D-C4D-ND	-2.05	107.92	110.17
16	C	202	CBE	C5-S4-C3	2.04	106.11	100.70
15	P	201	HEM	C3B-C4B-NB	-2.03	107.56	109.90
15	C	201	HEM	CHD-C4C-NC	2.00	126.63	124.45

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
5	N	1001	FAD	N10-C1'-C2'-O2'
5	N	1001	FAD	N10-C1'-C2'-C3'
6	A	1002	Y3P	O1-C1-C2-O3
6	A	1002	Y3P	O2-C1-C2-O3
6	N	1002	Y3P	O1-C1-C2-O3
6	N	1002	Y3P	O2-C1-C2-O3
17	C	203	BOG	O5-C1-O1-C1'

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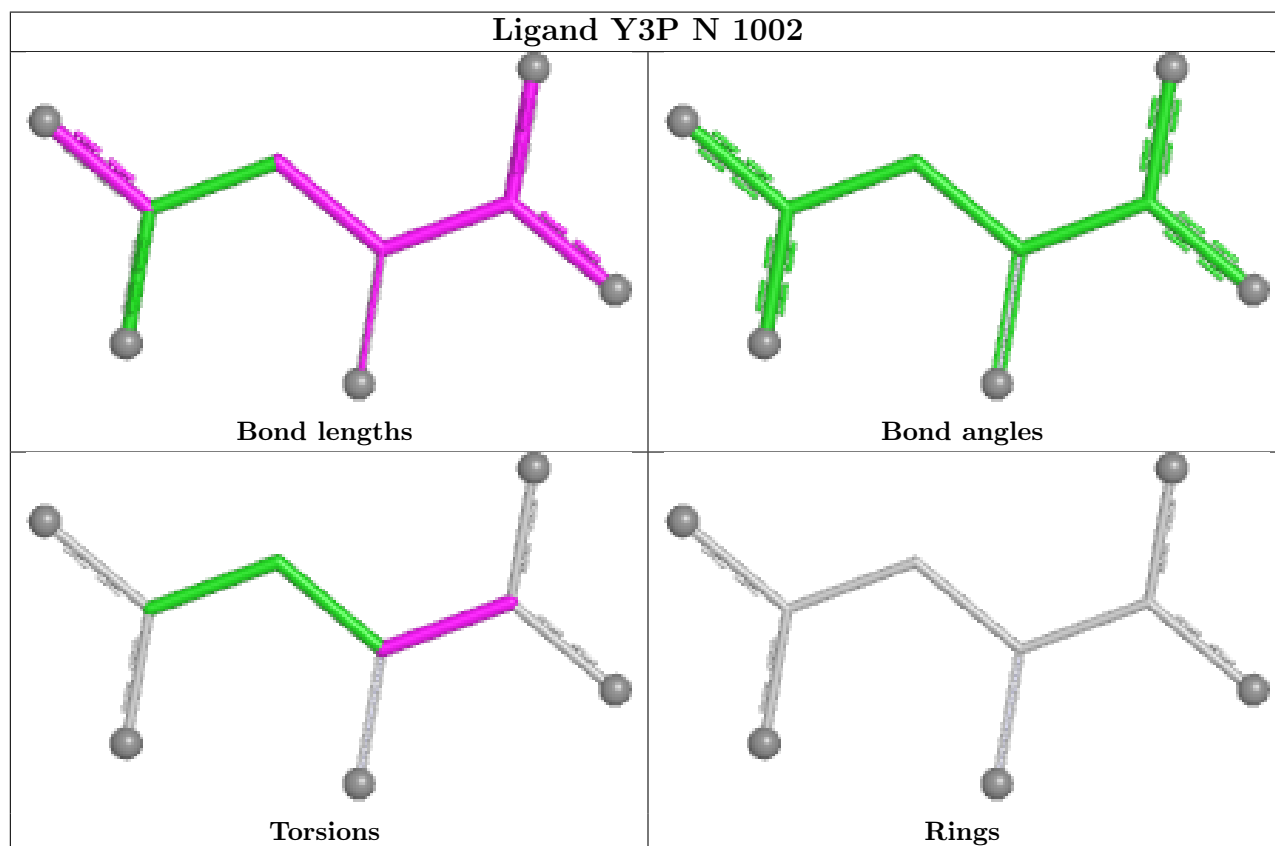
Mol	Chain	Res	Type	Atoms
17	C	203	BOG	C1'-C2'-C3'-C4'
17	C	203	BOG	O1-C1'-C2'-C3'
17	C	203	BOG	C2'-C3'-C4'-C5'
15	C	201	HEM	C2A-CAA-CBA-CGA
15	P	201	HEM	C2A-CAA-CBA-CGA
5	A	1001	FAD	PA-O3P-P-O5'
5	N	1001	FAD	PA-O3P-P-O5'
18	P	203	UMQ	C3'-C4'-O1-C1
17	D	201	BOG	O1-C1'-C2'-C3'
18	P	203	UMQ	C5'-C4'-O1-C1
6	A	1002	Y3P	O1-C1-C2-C3
6	A	1002	Y3P	O2-C1-C2-C3
6	N	1002	Y3P	O1-C1-C2-C3
6	N	1002	Y3P	O2-C1-C2-C3
5	A	1001	FAD	C5B-O5B-PA-O1A
5	N	1001	FAD	P-O3P-PA-O2A
16	C	202	CBE	C2-C3-C8-O9
16	C	202	CBE	C2-C3-C8-N10
16	P	202	CBE	C2-C3-C8-O9
16	P	202	CBE	C2-C3-C8-N10
17	P	204	BOG	C4-C5-C6-O6
5	A	1001	FAD	P-O3P-PA-O2A
5	N	1001	FAD	P-O3P-PA-O1A
18	P	203	UMQ	O5-C1-O1-C4'
5	A	1001	FAD	P-O3P-PA-O1A

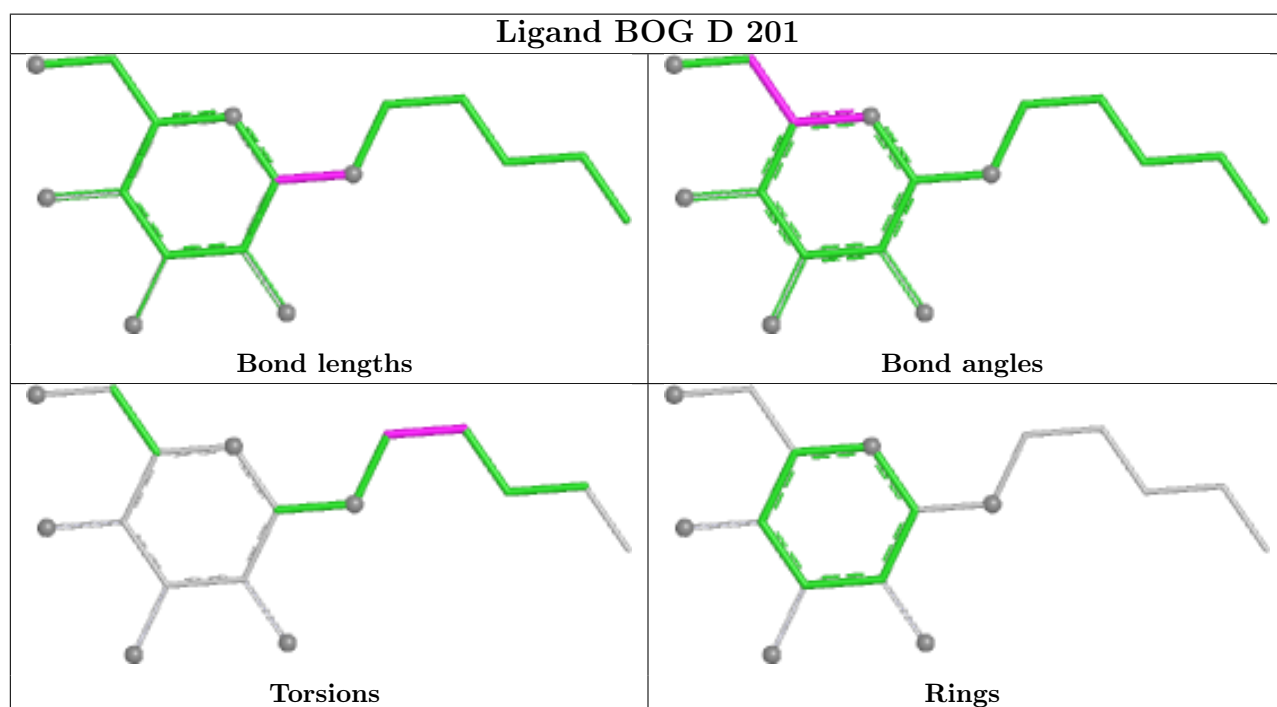
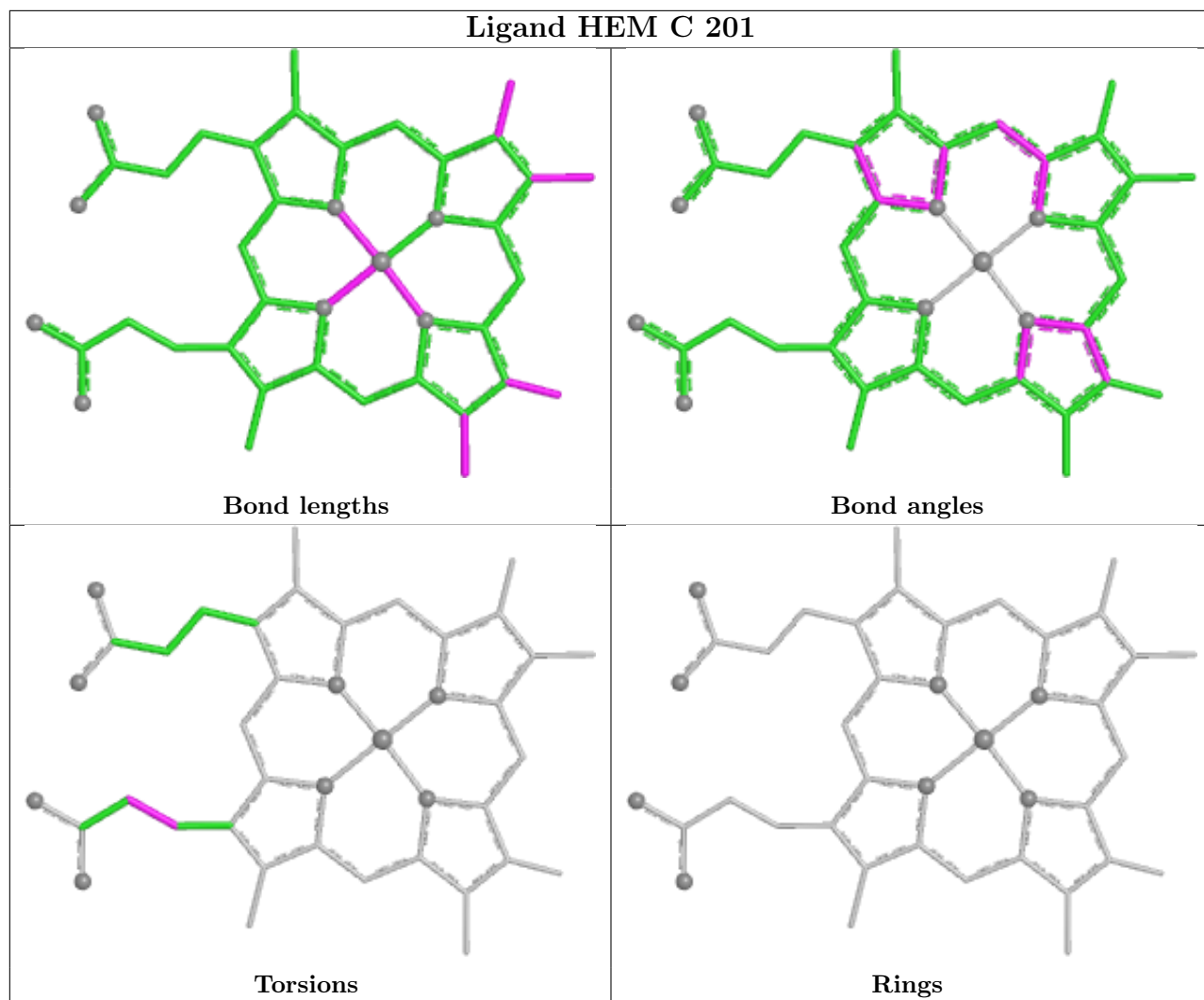
There are no ring outliers.

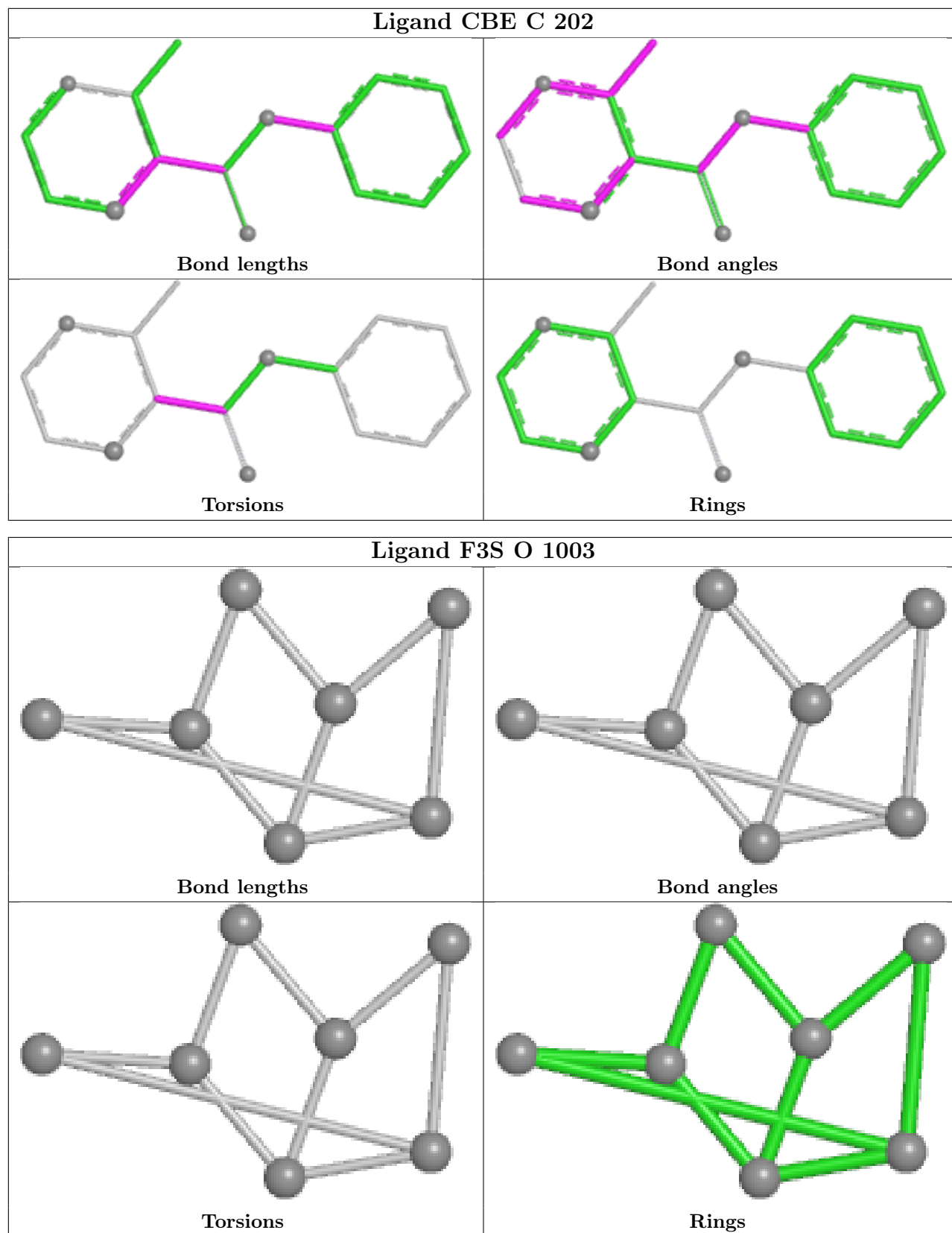
12 monomers are involved in 31 short contacts:

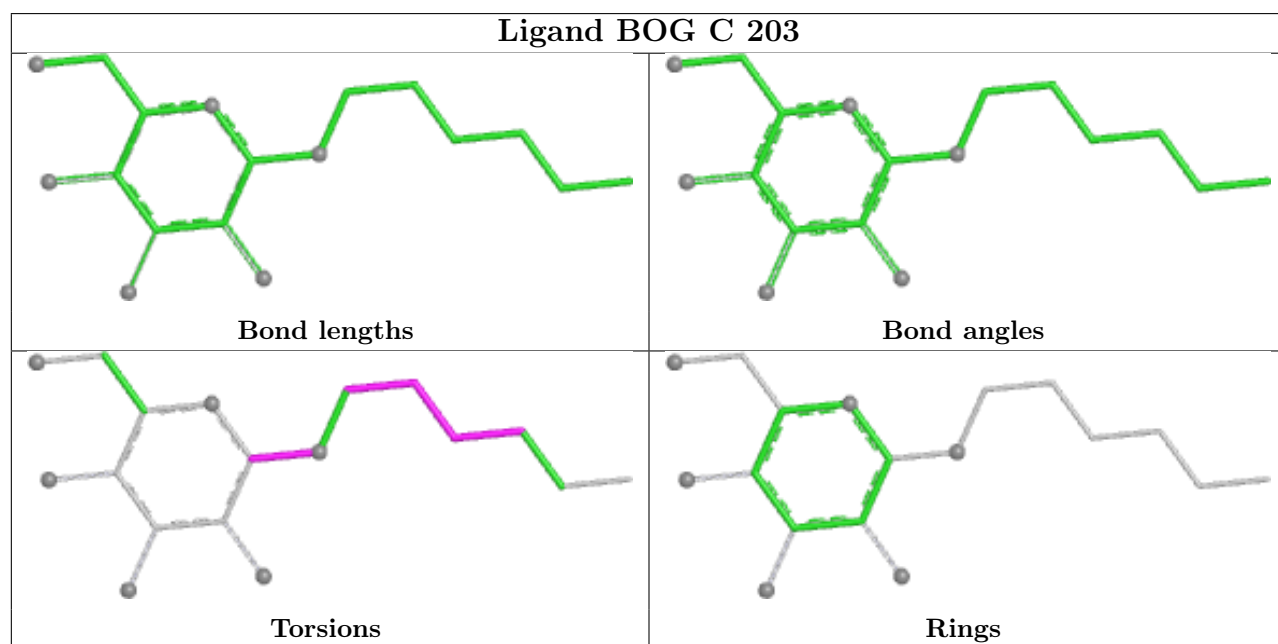
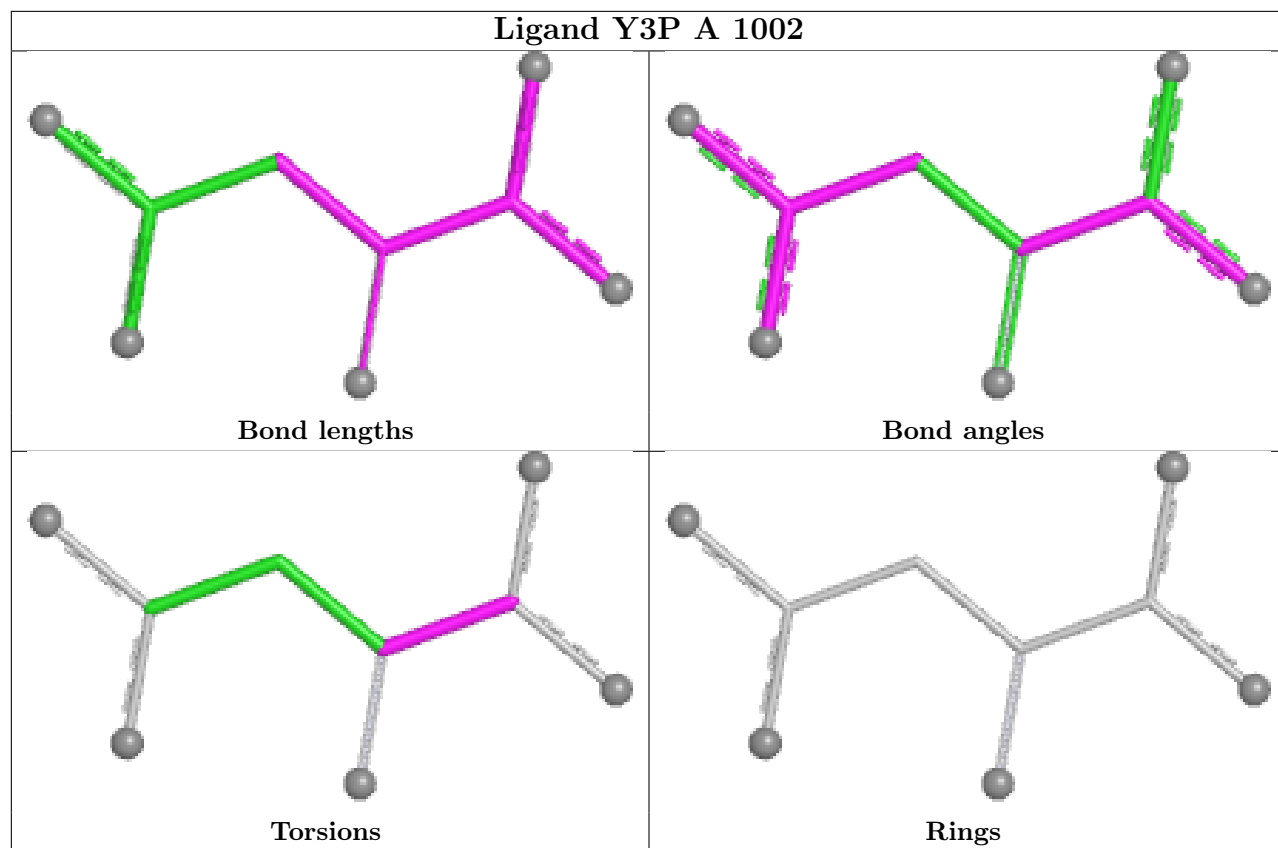
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	1002	Y3P	2	0
15	C	201	HEM	1	0
17	D	201	BOG	2	0
16	C	202	CBE	1	0
14	N	1005	GOL	3	0
6	A	1002	Y3P	4	0
5	A	1001	FAD	3	0
18	P	203	UMQ	7	0
16	P	202	CBE	2	0
15	P	201	HEM	2	0
5	N	1001	FAD	4	0
17	P	204	BOG	4	0

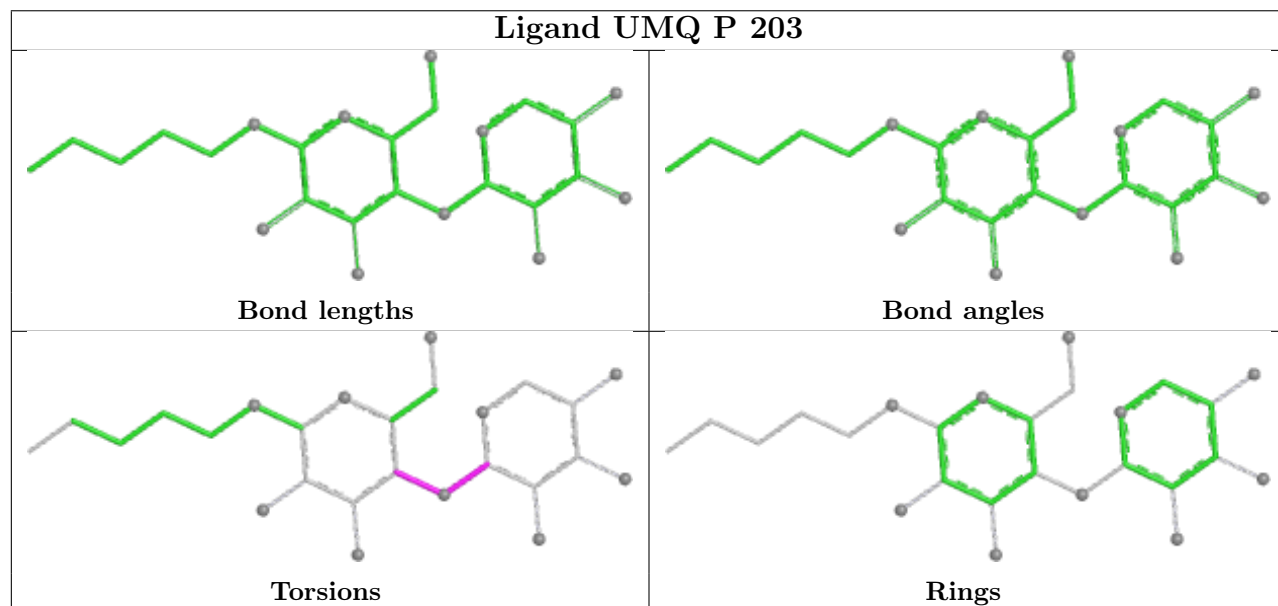
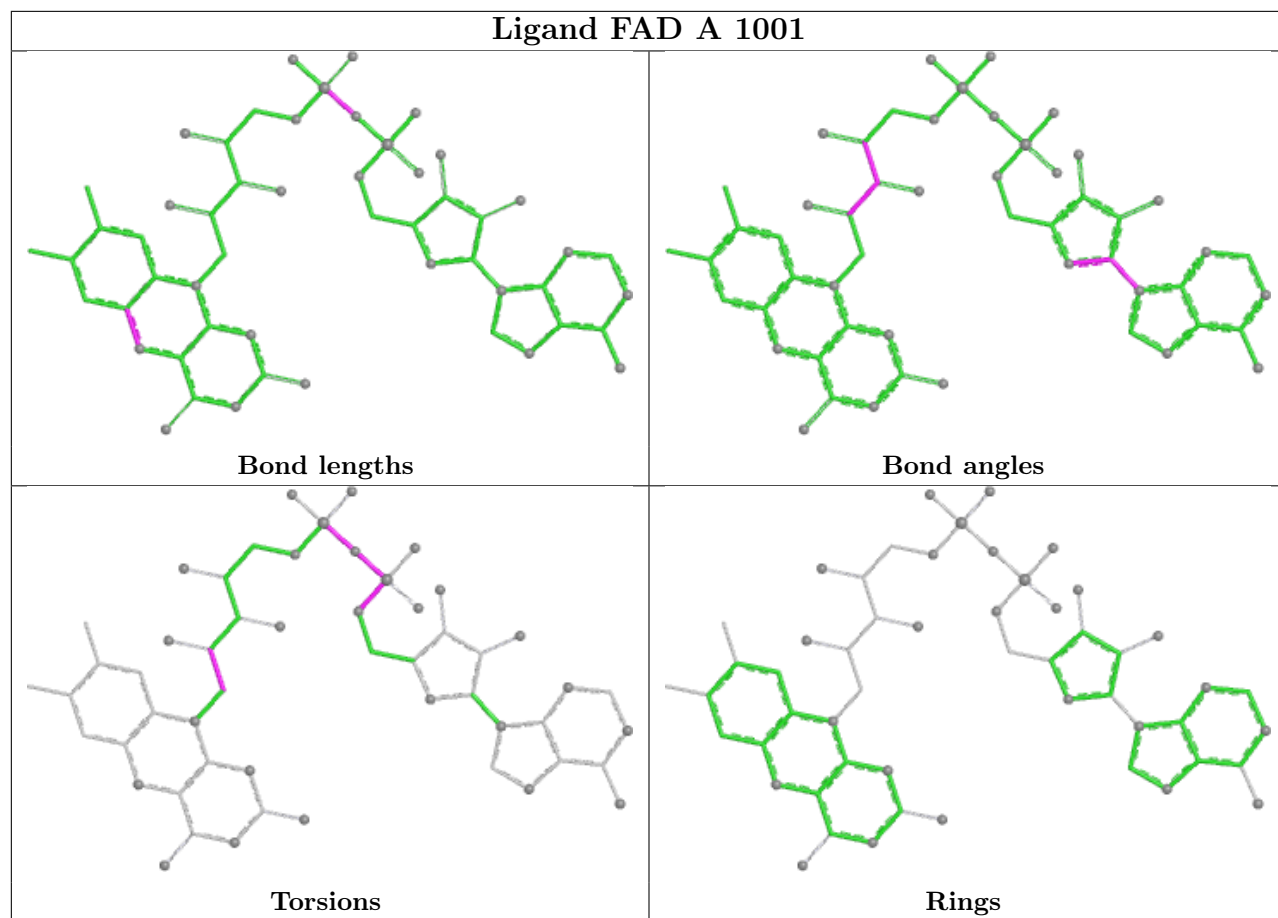
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

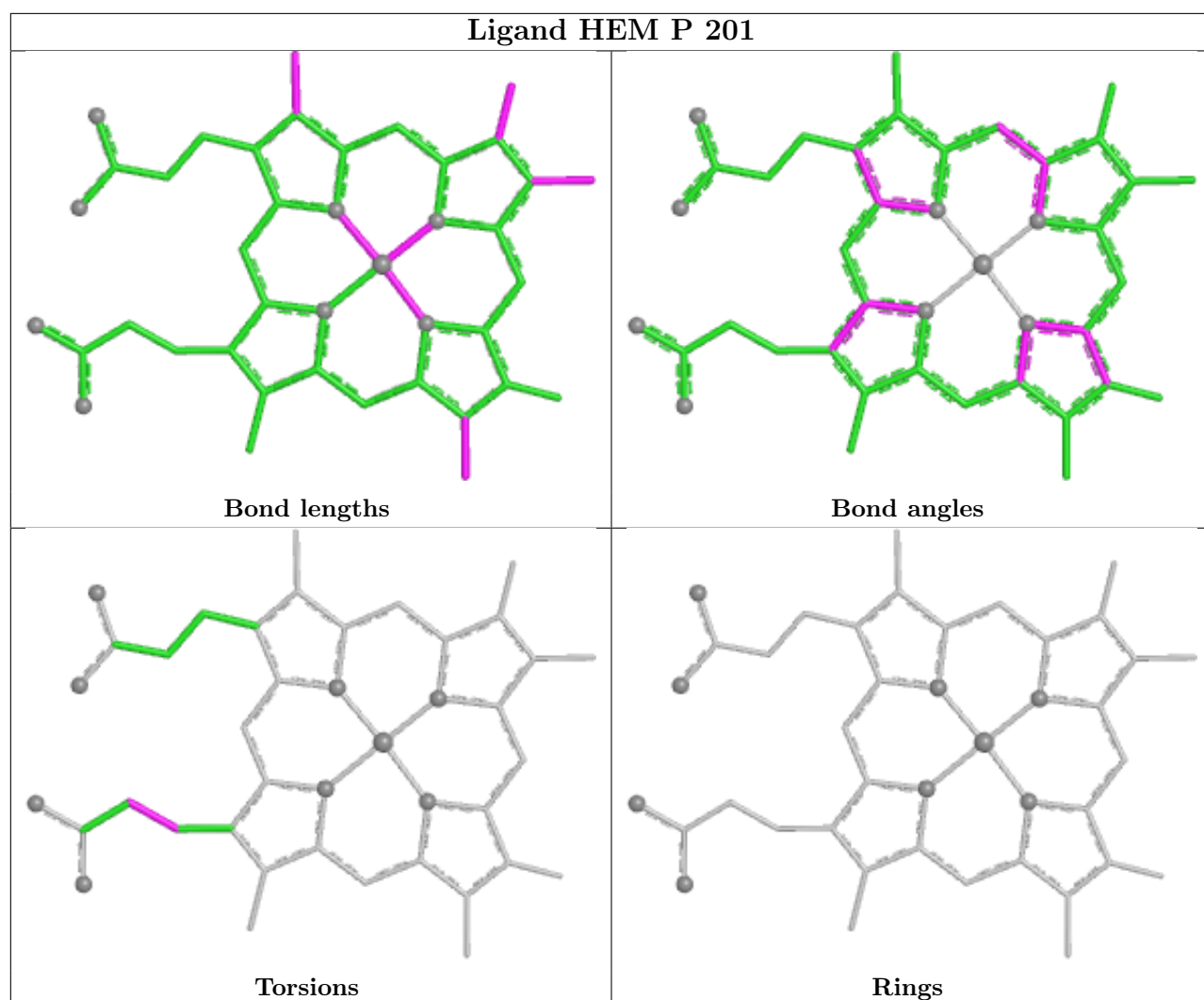
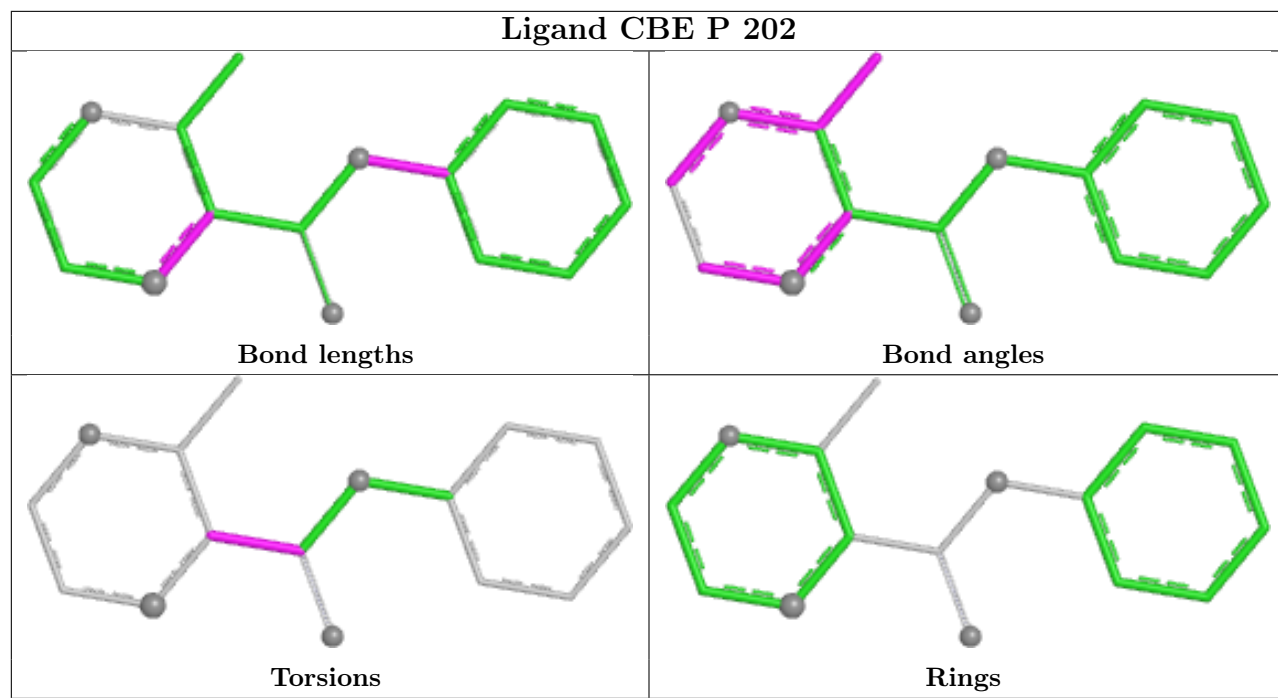


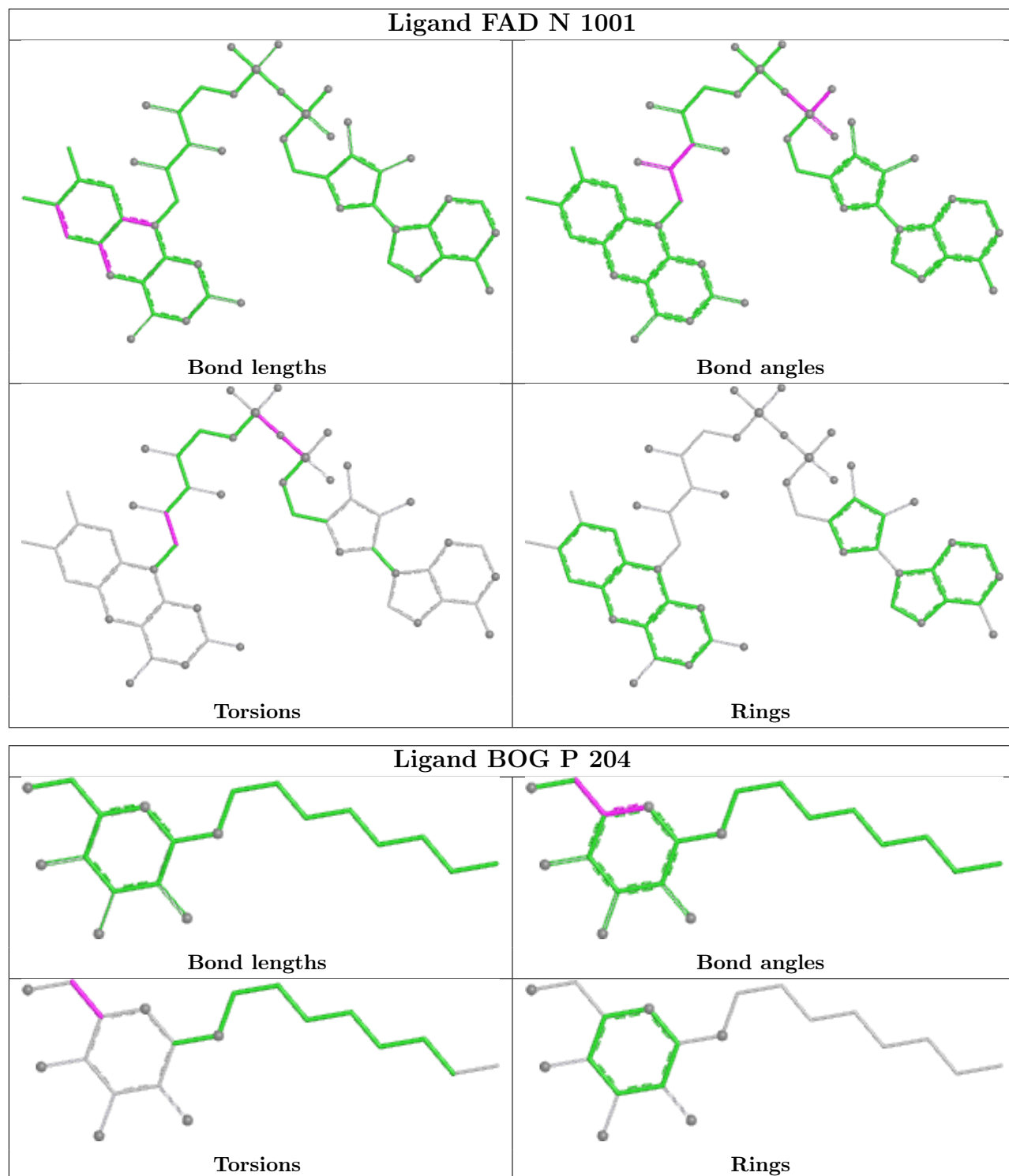


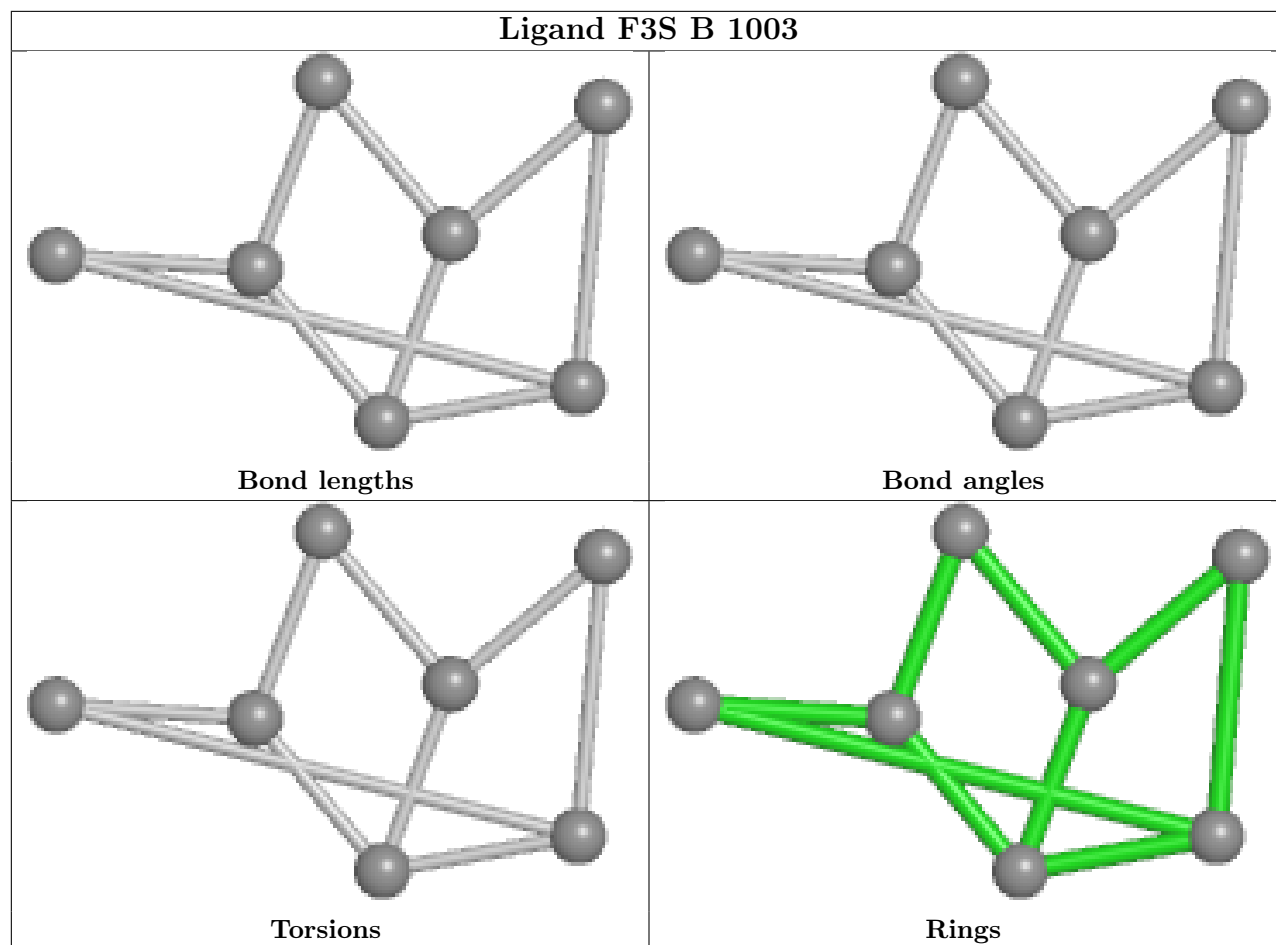












## 5.7 Other polymers [i](#)

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 [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, 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	612/621 (98%)	-1.41	0 100 100	16, 31, 54, 93	8 (1%)
1	N	612/621 (98%)	-1.44	0 100 100	18, 30, 54, 96	10 (1%)
2	B	240/252 (95%)	-1.41	0 100 100	11, 32, 50, 112	3 (1%)
2	O	241/252 (95%)	-1.45	0 100 100	10, 31, 51, 109	2 (0%)
3	C	139/140 (99%)	-1.03	0 100 100	27, 45, 80, 88	2 (1%)
3	P	139/140 (99%)	-0.93	0 100 100	27, 45, 87, 102	1 (0%)
4	D	101/103 (98%)	-0.93	0 100 100	34, 53, 78, 86	1 (0%)
4	Q	101/103 (98%)	-0.82	0 100 100	36, 55, 78, 93	0
All	All	2185/2232 (97%)	-1.32	0 100 100	10, 33, 66, 112	27 (1%)

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, 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( $\text{\AA}^2$ )	Q<0.9
9	UNL	D	227	1/-	0.92	0.07	75,75,75,75	0
9	UNL	A	1428	1/-	0.93	0.05	69,69,69,69	0
9	UNL	P	257	1/-	0.93	0.04	66,66,66,66	0
9	UNL	C	251[A]	1/-	0.95	0.08	11,11,11,11	1
9	UNL	C	251[B]	1/-	0.95	0.08	37,37,37,37	1
9	UNL	D	220	13/-	0.95	0.14	50,72,97,97	0
9	UNL	D	224	6/-	0.95	0.07	81,86,87,92	0
9	UNL	D	226[A]	1/-	0.95	0.09	47,47,47,47	1
9	UNL	D	226[B]	1/-	0.95	0.09	15,15,15,15	1
9	UNL	A	1416	1/-	0.95	0.05	66,66,66,66	0
9	UNL	A	1368	4/-	0.95	0.10	33,37,38,40	4
9	UNL	A	1418	1/-	0.96	0.05	65,65,65,65	0
9	UNL	A	1429	1/-	0.96	0.08	66,66,66,66	0
9	UNL	B	1181	3/-	0.96	0.16	54,54,59,61	0
9	UNL	B	1185	1/-	0.96	0.09	59,59,59,59	0
9	UNL	B	1193	1/-	0.96	0.07	53,53,53,53	0
9	UNL	B	1209	1/-	0.96	0.05	52,52,52,52	0
9	UNL	B	1211	1/-	0.96	0.10	61,61,61,61	0
9	UNL	N	1392	2/-	0.96	0.15	55,55,55,61	0
9	UNL	O	1195	3/-	0.96	0.12	48,48,63,78	0
9	UNL	C	244	3/-	0.96	0.12	45,45,59,60	0
9	UNL	C	261	1/-	0.97	0.07	55,55,55,55	0
9	UNL	B	1178	3/-	0.97	0.12	54,54,55,59	0
9	UNL	D	221	14/-	0.97	0.10	62,91,106,111	0
9	UNL	B	1213	1/-	0.97	0.06	42,42,42,42	0
9	UNL	B	1180	3/-	0.97	0.07	57,57,66,79	0
9	UNL	C	245	2/-	0.97	0.08	68,68,68,82	0
9	UNL	B	1202	1/-	0.97	0.05	50,50,50,50	0
9	UNL	N	1383	2/-	0.97	0.15	56,56,56,58	0
9	UNL	A	1431	1/-	0.97	0.05	47,47,47,47	0
9	UNL	N	1406	2/-	0.97	0.05	28,28,28,31	2
9	UNL	N	1408	4/-	0.97	0.11	57,59,60,67	0
9	UNL	N	1422[A]	1/-	0.97	0.07	25,25,25,25	1
9	UNL	N	1422[B]	1/-	0.97	0.07	28,28,28,28	1
9	UNL	N	1439	1/-	0.97	0.04	17,17,17,17	1
9	UNL	N	1444	1/-	0.97	0.06	59,59,59,59	0
9	UNL	C	255[A]	1/-	0.97	0.04	28,28,28,28	1
9	UNL	O	1196	3/-	0.97	0.05	63,63,73,83	0
9	UNL	O	1197	3/-	0.97	0.05	71,71,76,79	0
9	UNL	O	1200	3/-	0.97	0.05	81,81,90,92	0
9	UNL	O	1209[A]	1/-	0.97	0.14	45,45,45,45	1
9	UNL	O	1209[B]	1/-	0.97	0.14	24,24,24,24	1
9	UNL	O	1226	1/-	0.97	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	P	253	3/-	0.97	0.08	83,83,85,91	0
9	UNL	C	255[B]	1/-	0.97	0.04	29,29,29,29	1
9	UNL	Q	213	7/-	0.97	0.08	71,81,89,93	7
9	UNL	Q	215	3/-	0.97	0.10	38,38,61,64	0
9	UNL	Q	216	9/-	0.97	0.09	59,64,75,76	0
9	UNL	Q	218	12/-	0.97	0.10	58,80,96,103	0
17	BOG	P	204	20/20	0.97	0.09	64,83,102,104	0
9	UNL	C	246	3/-	0.98	0.08	52,52,58,66	0
9	UNL	A	1410	1/-	0.98	0.06	57,57,57,57	0
9	UNL	A	1415	1/-	0.98	0.05	60,60,60,60	0
9	UNL	A	1367	15/-	0.98	0.08	40,59,71,77	15
9	UNL	A	1417	1/-	0.98	0.05	60,60,60,60	0
9	UNL	C	257	1/-	0.98	0.03	58,58,58,58	0
9	UNL	C	258	1/-	0.98	0.03	49,49,49,49	0
9	UNL	C	259	1/-	0.98	0.14	60,60,60,60	0
9	UNL	C	260	1/-	0.98	0.09	55,55,55,55	0
9	UNL	A	1366	3/-	0.98	0.11	47,47,64,65	0
9	UNL	A	1424	1/-	0.98	0.05	58,58,58,58	0
9	UNL	A	1426	1/-	0.98	0.10	55,55,55,55	0
9	UNL	A	1370	4/-	0.98	0.07	40,45,55,91	0
9	UNL	A	1371	2/-	0.98	0.09	35,35,35,43	0
9	UNL	A	1376	3/-	0.98	0.04	61,61,66,73	0
9	UNL	B	1174	3/-	0.98	0.10	62,62,63,74	0
9	UNL	D	228	1/-	0.98	0.05	59,59,59,59	0
9	UNL	A	1377	4/-	0.98	0.06	75,76,79,81	0
9	UNL	N	1387	3/-	0.98	0.10	47,47,56,59	0
9	UNL	N	1388	14/-	0.98	0.07	36,54,70,72	14
9	UNL	N	1390	2/-	0.98	0.05	51,51,51,63	0
9	UNL	N	1391	3/-	0.98	0.04	46,46,59,59	0
9	UNL	A	1390	1/-	0.98	0.21	37,37,37,37	0
9	UNL	N	1398	2/-	0.98	0.15	53,53,53,57	0
9	UNL	N	1405	3/-	0.98	0.11	42,42,57,59	0
9	UNL	A	1397[A]	1/-	0.98	0.07	25,25,25,25	1
9	UNL	A	1397[B]	1/-	0.98	0.07	18,18,18,18	1
9	UNL	N	1412[A]	1/-	0.98	0.08	21,21,21,21	1
9	UNL	N	1412[B]	1/-	0.98	0.08	35,35,35,35	1
9	UNL	N	1414[A]	1/-	0.98	0.05	14,14,14,14	1
9	UNL	N	1414[B]	1/-	0.98	0.05	0,0,0,0	1
9	UNL	N	1415[A]	1/-	0.98	0.03	16,16,16,16	1
9	UNL	N	1415[B]	1/-	0.98	0.03	22,22,22,22	1
9	UNL	N	1417[A]	1/-	0.98	0.08	22,22,22,22	1
9	UNL	N	1417[B]	1/-	0.98	0.08	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	N	1419[A]	1/-	0.98	0.07	0,0,0,0	1
9	UNL	N	1419[B]	1/-	0.98	0.07	41,41,41,41	1
9	UNL	N	1421[A]	1/-	0.98	0.10	33,33,33,33	1
9	UNL	N	1421[B]	1/-	0.98	0.10	24,24,24,24	1
9	UNL	B	1188	1/-	0.98	0.04	48,48,48,48	0
9	UNL	B	1190	1/-	0.98	0.04	53,53,53,53	0
9	UNL	N	1427	1/-	0.98	0.12	45,45,45,45	0
9	UNL	N	1433	1/-	0.98	0.04	60,60,60,60	0
9	UNL	B	1191	1/-	0.98	0.08	51,51,51,51	0
9	UNL	N	1443	1/-	0.98	0.06	51,51,51,51	0
9	UNL	A	1398[A]	1/-	0.98	0.07	31,31,31,31	1
9	UNL	N	1446	1/-	0.98	0.09	59,59,59,59	0
9	UNL	O	1192	3/-	0.98	0.07	36,36,49,59	0
9	UNL	B	1200	1/-	0.98	0.04	56,56,56,56	0
9	UNL	B	1201[A]	1/-	0.98	0.10	17,17,17,17	1
9	UNL	B	1201[B]	1/-	0.98	0.10	42,42,42,42	1
9	UNL	O	1199	5/-	0.98	0.09	37,46,55,64	0
9	UNL	A	1398[B]	1/-	0.98	0.07	21,21,21,21	1
9	UNL	O	1202	5/-	0.98	0.08	53,65,68,69	0
9	UNL	B	1204	1/-	0.98	0.05	20,20,20,20	1
9	UNL	B	1205	1/-	0.98	0.06	44,44,44,44	0
9	UNL	O	1212[A]	1/-	0.98	0.06	41,41,41,41	1
9	UNL	O	1212[B]	1/-	0.98	0.06	33,33,33,33	1
9	UNL	O	1216[A]	1/-	0.98	0.08	44,44,44,44	1
9	UNL	O	1216[B]	1/-	0.98	0.08	35,35,35,35	1
9	UNL	O	1218	1/-	0.98	0.08	56,56,56,56	0
9	UNL	O	1220	1/-	0.98	0.06	56,56,56,56	0
9	UNL	O	1222	1/-	0.98	0.06	73,73,73,73	0
9	UNL	O	1223	1/-	0.98	0.14	54,54,54,54	0
9	UNL	O	1224	1/-	0.98	0.06	60,60,60,60	0
9	UNL	B	1206	1/-	0.98	0.06	63,63,63,63	0
9	UNL	O	1227	1/-	0.98	0.04	67,67,67,67	0
9	UNL	B	1208	1/-	0.98	0.06	51,51,51,51	0
9	UNL	P	254	1/-	0.98	0.05	56,56,56,56	0
9	UNL	A	1401[A]	1/-	0.98	0.08	29,29,29,29	1
9	UNL	B	1210	1/-	0.98	0.15	48,48,48,48	0
9	UNL	Q	214[A]	17/-	0.98	0.07	20,42,49,49	17
9	UNL	Q	214[B]	16/-	0.98	0.07	37,46,55,58	16
9	UNL	A	1401[B]	1/-	0.98	0.08	4,4,4,4	1
9	UNL	A	1402[A]	1/-	0.98	0.03	14,14,14,14	1
9	UNL	A	1402[B]	1/-	0.98	0.03	12,12,12,12	1
9	UNL	Q	221	1/-	0.98	0.03	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	BOG	C	203	18/20	0.98	0.06	56,77,95,104	0
9	UNL	A	1408	1/-	0.98	0.06	58,58,58,58	0
18	UMQ	P	203	26/34	0.98	0.06	42,58,107,113	0
9	UNL	C	250[B]	1/-	0.99	0.03	24,24,24,24	1
9	UNL	A	1407	1/-	0.99	0.04	35,35,35,35	0
9	UNL	A	1378	2/-	0.99	0.07	64,64,64,67	0
9	UNL	C	252[A]	1/-	0.99	0.08	32,32,32,32	1
9	UNL	C	252[B]	1/-	0.99	0.08	34,34,34,34	1
9	UNL	C	253	1/-	0.99	0.03	28,28,28,28	1
9	UNL	C	254	1/-	0.99	0.04	33,33,33,33	0
9	UNL	A	1409	1/-	0.99	0.10	44,44,44,44	0
9	UNL	A	1379	3/-	0.99	0.06	21,21,42,58	3
9	UNL	C	256	1/-	0.99	0.07	47,47,47,47	0
9	UNL	A	1411	1/-	0.99	0.04	52,52,52,52	0
9	UNL	A	1413	1/-	0.99	0.03	49,49,49,49	0
9	UNL	A	1414	1/-	0.99	0.04	47,47,47,47	0
9	UNL	A	1380	7/-	0.99	0.07	20,52,57,66	7
9	UNL	A	1381	3/-	0.99	0.07	31,31,55,67	0
9	UNL	A	1382	3/-	0.99	0.05	26,26,31,50	3
9	UNL	A	1383	5/-	0.99	0.05	65,66,72,73	0
9	UNL	D	222	9/-	0.99	0.04	52,61,65,66	0
9	UNL	D	223	4/-	0.99	0.05	60,60,67,74	0
9	UNL	A	1419	1/-	0.99	0.04	60,60,60,60	0
9	UNL	D	225	1/-	0.99	0.14	48,48,48,48	0
9	UNL	A	1420	1/-	0.99	0.05	50,50,50,50	0
9	UNL	A	1421	1/-	0.99	0.05	49,49,49,49	0
9	UNL	A	1422	1/-	0.99	0.05	54,54,54,54	0
9	UNL	A	1423	1/-	0.99	0.07	64,64,64,64	0
9	UNL	D	229	1/-	0.99	0.03	55,55,55,55	0
9	UNL	A	1384	2/-	0.99	0.04	55,55,55,63	0
9	UNL	N	1384	2/-	0.99	0.06	67,67,67,71	0
9	UNL	N	1385	4/-	0.99	0.04	72,75,76,82	0
9	UNL	N	1386	2/-	0.99	0.05	23,23,23,43	2
9	UNL	A	1425	1/-	0.99	0.03	53,53,53,53	0
9	UNL	A	1385[A]	1/-	0.99	0.09	45,45,45,45	1
9	UNL	N	1389	2/-	0.99	0.05	63,63,63,73	0
9	UNL	A	1427	1/-	0.99	0.09	59,59,59,59	0
9	UNL	A	1385[B]	1/-	0.99	0.09	21,21,21,21	1
9	UNL	A	1387	1/-	0.99	0.07	47,47,47,47	0
9	UNL	N	1393	3/-	0.99	0.04	64,64,69,73	0
9	UNL	N	1394	2/-	0.99	0.07	58,58,58,73	0
9	UNL	N	1395	6/-	0.99	0.04	51,57,61,70	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	N	1396	3/-	0.99	0.07	27,27,41,50	0
9	UNL	N	1397	3/-	0.99	0.03	50,50,56,74	0
9	UNL	A	1430	1/-	0.99	0.04	51,51,51,51	0
9	UNL	N	1400	2/-	0.99	0.04	66,66,66,75	0
9	UNL	N	1401	3/-	0.99	0.06	49,49,57,73	0
9	UNL	N	1402	3/-	0.99	0.03	24,24,31,41	3
9	UNL	N	1403	3/-	0.99	0.04	15,15,21,33	3
9	UNL	N	1404	7/-	0.99	0.05	37,62,71,71	0
9	UNL	A	1388	1/-	0.99	0.04	35,35,35,35	0
9	UNL	B	1171	7/-	0.99	0.06	54,72,78,79	0
9	UNL	N	1407	3/-	0.99	0.06	38,38,45,53	3
9	UNL	B	1172	4/-	0.99	0.04	68,71,74,77	0
9	UNL	N	1409	4/-	0.99	0.05	70,70,73,77	0
9	UNL	N	1410	4/-	0.99	0.04	17,25,27,37	4
9	UNL	N	1411	2/-	0.99	0.08	55,55,55,57	0
9	UNL	B	1173	3/-	0.99	0.03	42,42,47,64	0
9	UNL	A	1389	1/-	0.99	0.24	45,45,45,45	0
9	UNL	N	1413[A]	1/-	0.99	0.03	16,16,16,16	1
9	UNL	N	1413[B]	1/-	0.99	0.03	23,23,23,23	1
9	UNL	B	1175	3/-	0.99	0.05	53,53,65,66	0
9	UNL	B	1176	4/-	0.99	0.04	68,70,76,76	4
9	UNL	B	1177	3/-	0.99	0.06	55,55,64,65	0
9	UNL	A	1369	4/-	0.99	0.05	41,45,46,53	0
9	UNL	B	1179	4/-	0.99	0.06	63,70,73,73	0
9	UNL	A	1391	1/-	0.99	0.03	60,60,60,60	0
9	UNL	N	1418[A]	1/-	0.99	0.03	28,28,28,28	1
9	UNL	N	1418[B]	1/-	0.99	0.03	33,33,33,33	1
9	UNL	A	1392	1/-	0.99	0.04	62,62,62,62	0
9	UNL	B	1182[A]	1/-	0.99	0.03	21,21,21,21	1
9	UNL	N	1420[A]	1/-	0.99	0.07	26,26,26,26	1
9	UNL	N	1420[B]	1/-	0.99	0.07	8,8,8,8	1
9	UNL	B	1182[B]	1/-	0.99	0.03	4,4,4,4	1
9	UNL	B	1183[A]	1/-	0.99	0.04	24,24,24,24	1
9	UNL	B	1183[B]	1/-	0.99	0.04	6,6,6,6	1
9	UNL	B	1184[A]	1/-	0.99	0.08	22,22,22,22	1
9	UNL	N	1423	1/-	0.99	0.08	42,42,42,42	0
9	UNL	N	1424	1/-	0.99	0.07	47,47,47,47	0
9	UNL	N	1426	1/-	0.99	0.03	55,55,55,55	0
9	UNL	B	1184[B]	1/-	0.99	0.08	36,36,36,36	1
9	UNL	N	1428	1/-	0.99	0.12	47,47,47,47	0
9	UNL	N	1429	1/-	0.99	0.04	54,54,54,54	0
9	UNL	N	1430	1/-	0.99	0.04	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	N	1431	1/-	0.99	0.04	45,45,45,45	0
9	UNL	N	1432	1/-	0.99	0.11	51,51,51,51	0
9	UNL	A	1394	1/-	0.99	0.05	62,62,62,62	0
9	UNL	N	1434	1/-	0.99	0.13	58,58,58,58	0
9	UNL	N	1435	1/-	0.99	0.09	56,56,56,56	0
9	UNL	N	1437	1/-	0.99	0.05	52,52,52,52	0
9	UNL	N	1438	1/-	0.99	0.05	58,58,58,58	0
9	UNL	B	1186[A]	1/-	0.99	0.06	12,12,12,12	1
9	UNL	N	1440	1/-	0.99	0.06	57,57,57,57	0
9	UNL	N	1441	1/-	0.99	0.04	52,52,52,52	0
9	UNL	N	1442	1/-	0.99	0.03	51,51,51,51	0
9	UNL	B	1186[B]	1/-	0.99	0.06	4,4,4,4	1
9	UNL	B	1187	1/-	0.99	0.04	49,49,49,49	0
9	UNL	N	1445	1/-	0.99	0.05	50,50,50,50	0
9	UNL	A	1395	1/-	0.99	0.04	44,44,44,44	0
9	UNL	B	1189	1/-	0.99	0.05	47,47,47,47	0
9	UNL	O	1193	7/-	0.99	0.07	57,62,66,72	7
9	UNL	O	1194	6/-	0.99	0.04	35,43,53,56	0
9	UNL	A	1396[A]	1/-	0.99	0.08	20,20,20,20	1
9	UNL	A	1396[B]	1/-	0.99	0.08	36,36,36,36	1
9	UNL	B	1192	1/-	0.99	0.05	53,53,53,53	0
9	UNL	O	1198	4/-	0.99	0.04	52,60,61,70	0
8	AZI	N	1004	3/3	0.99	0.07	40,40,48,59	0
9	UNL	B	1194	1/-	0.99	0.06	52,52,52,52	0
9	UNL	O	1201	3/-	0.99	0.04	54,54,67,71	0
9	UNL	B	1195	1/-	0.99	0.02	45,45,45,45	0
9	UNL	O	1203	4/-	0.99	0.04	46,47,49,53	4
9	UNL	O	1204	3/-	0.99	0.06	54,54,55,66	0
9	UNL	O	1205	1/-	0.99	0.06	49,49,49,49	0
9	UNL	O	1206[A]	1/-	0.99	0.12	33,33,33,33	1
9	UNL	O	1206[B]	1/-	0.99	0.12	17,17,17,17	1
9	UNL	O	1208[A]	1/-	0.99	0.03	19,19,19,19	1
9	UNL	O	1208[B]	1/-	0.99	0.03	20,20,20,20	1
9	UNL	B	1196	1/-	0.99	0.08	46,46,46,46	0
9	UNL	B	1199	1/-	0.99	0.06	45,45,45,45	0
9	UNL	O	1210	1/-	0.99	0.10	50,50,50,50	0
9	UNL	O	1211[A]	1/-	0.99	0.05	33,33,33,33	1
9	UNL	O	1211[B]	1/-	0.99	0.05	8,8,8,8	1
6	Y3P	A	1002	9/9	0.99	0.03	22,31,41,50	0
9	UNL	A	1372	2/-	0.99	0.05	34,34,34,53	0
9	UNL	O	1213[A]	1/-	0.99	0.04	22,22,22,22	1
9	UNL	O	1213[B]	1/-	0.99	0.04	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	O	1214[A]	1/-	0.99	0.06	27,27,27,27	1
9	UNL	O	1214[B]	1/-	0.99	0.06	29,29,29,29	1
9	UNL	O	1215	1/-	0.99	0.04	47,47,47,47	0
9	UNL	A	1373	3/-	0.99	0.06	39,39,57,70	0
9	UNL	A	1399[A]	1/-	0.99	0.07	24,24,24,24	1
9	UNL	O	1217	1/-	0.99	0.15	42,42,42,42	0
9	UNL	B	1203	1/-	0.99	0.07	44,44,44,44	0
9	UNL	A	1399[B]	1/-	0.99	0.07	29,29,29,29	1
9	UNL	O	1221	1/-	0.99	0.08	36,36,36,36	0
9	UNL	A	1400[A]	1/-	0.99	0.03	26,26,26,26	1
9	UNL	A	1400[B]	1/-	0.99	0.03	24,24,24,24	1
9	UNL	A	1374	2/-	0.99	0.04	54,54,54,63	2
9	UNL	O	1225	1/-	0.99	0.08	42,42,42,42	0
9	UNL	A	1375	3/-	0.99	0.05	74,74,76,85	0
8	AZI	A	1004	3/3	0.99	0.03	41,41,47,59	0
9	UNL	P	249	9/-	0.99	0.07	58,72,86,93	0
9	UNL	P	250	6/-	0.99	0.04	69,74,80,82	0
9	UNL	P	251	2/-	0.99	0.13	59,59,59,70	0
9	UNL	P	252	19/-	0.99	0.07	42,61,85,88	19
8	AZI	B	1005	3/3	0.99	0.08	54,54,65,71	0
9	UNL	B	1212	1/-	0.99	0.05	51,51,51,51	0
9	UNL	P	255	1/-	0.99	0.07	54,54,54,54	0
9	UNL	P	256	1/-	0.99	0.11	57,57,57,57	0
9	UNL	A	1403	1/-	0.99	0.05	50,50,50,50	0
9	UNL	C	243	9/-	0.99	0.09	54,66,84,84	0
9	UNL	A	1404	1/-	0.99	0.03	57,57,57,57	0
9	UNL	A	1405	1/-	0.99	0.05	44,44,44,44	0
9	UNL	A	1406	1/-	0.99	0.05	47,47,47,47	0
9	UNL	C	247	1/-	0.99	0.04	48,48,48,48	0
9	UNL	Q	217	3/-	0.99	0.05	52,52,64,64	0
9	UNL	C	248[A]	1/-	0.99	0.04	28,28,28,28	1
9	UNL	Q	219	5/-	0.99	0.05	47,50,74,79	0
9	UNL	Q	220	1/-	0.99	0.10	60,60,60,60	0
9	UNL	C	248[B]	1/-	0.99	0.04	31,31,31,31	1
14	GOL	N	1005	6/6	0.99	0.05	35,36,38,49	6
9	UNL	C	249[A]	1/-	0.99	0.06	27,27,27,27	1
17	BOG	D	201	17/20	0.99	0.05	61,67,79,82	0
9	UNL	C	249[B]	1/-	0.99	0.06	19,19,19,19	1
9	UNL	C	250[A]	1/-	0.99	0.03	23,23,23,23	1
9	UNL	A	1393	1/-	1.00	0.06	55,55,55,55	0
9	UNL	N	1399	1/-	1.00	0.02	40,40,40,40	0
7	K	N	1003	1/1	1.00	0.01	28,28,28,28	0

*Continued on next page...*

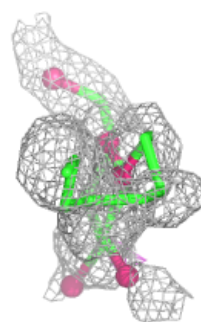
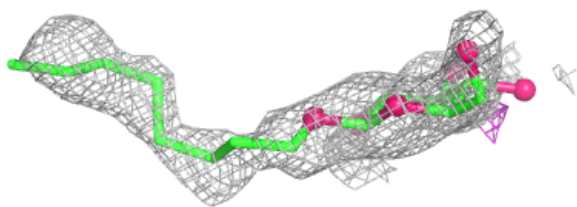
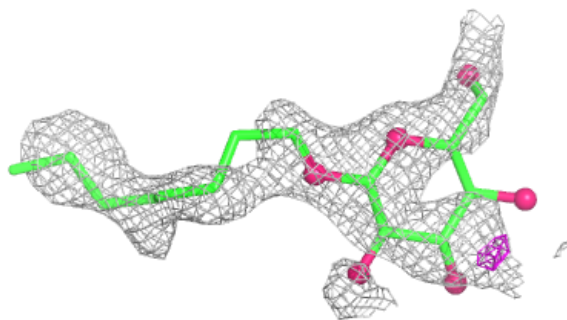
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	UNL	O	1207[A]	1/-	1.00	0.03	13,13,13,13	1
9	UNL	O	1207[B]	1/-	1.00	0.03	30,30,30,30	1
9	UNL	O	1219	1/-	1.00	0.02	26,26,26,26	1
5	FAD	N	1001	53/53	1.00	0.02	10,21,29,34	0
5	FAD	A	1001	53/53	1.00	0.02	9,22,32,37	0
6	Y3P	N	1002	9/9	1.00	0.02	24,29,41,41	0
9	UNL	A	1412	1/-	1.00	0.03	39,39,39,39	0
7	K	A	1003	1/1	1.00	0.01	33,33,33,33	0
9	UNL	N	1436	1/-	1.00	0.02	24,24,24,24	0
9	UNL	B	1197	1/-	1.00	0.02	46,46,46,46	0
9	UNL	B	1207	1/-	1.00	0.06	41,41,41,41	0
10	FES	B	1001	4/4	1.00	0.02	24,24,24,27	0
10	FES	O	1001	4/4	1.00	0.01	23,25,26,28	0
11	SF4	B	1002	8/8	1.00	0.01	24,26,28,30	0
11	SF4	O	1002	8/8	1.00	0.01	22,27,31,31	0
12	F3S	B	1003	7/7	1.00	0.02	27,28,30,34	0
12	F3S	O	1003	7/7	1.00	0.02	25,28,32,32	0
13	NA	B	1004	1/1	1.00	0.02	25,25,25,25	0
14	GOL	B	1006	6/6	1.00	0.03	32,40,43,45	0
9	UNL	N	1416[A]	1/-	1.00	0.05	24,24,24,24	1
15	HEM	C	201	41/43	1.00	0.03	20,40,55,69	0
15	HEM	P	201	41/43	1.00	0.04	28,41,57,63	0
16	CBE	C	202	16/16	1.00	0.02	29,36,43,47	0
16	CBE	P	202	16/16	1.00	0.02	27,35,47,48	0
9	UNL	N	1416[B]	1/-	1.00	0.05	34,34,34,34	1
9	UNL	N	1425	1/-	1.00	0.05	30,30,30,30	0
9	UNL	B	1198	1/-	1.00	0.06	50,50,50,50	0
9	UNL	A	1386	1/-	1.00	0.02	42,42,42,42	0

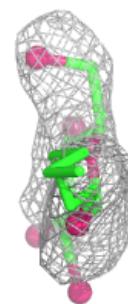
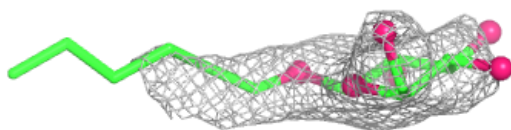
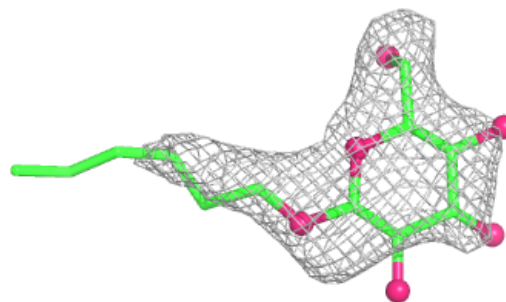
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BOG 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)

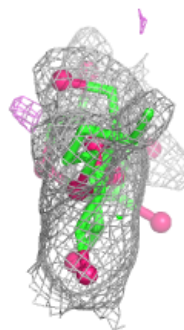
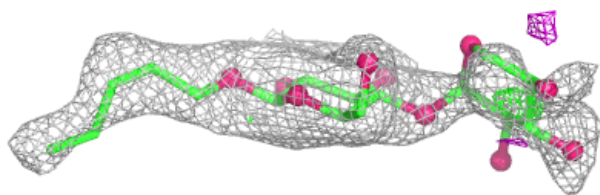
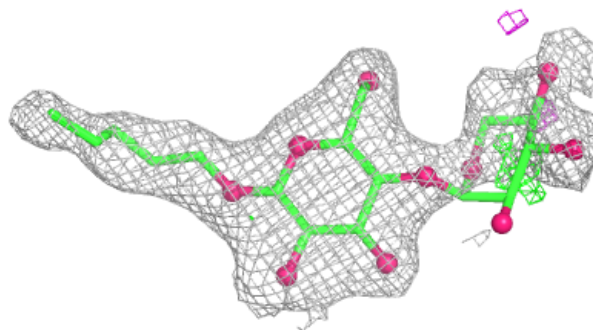
**Electron density around BOG C 203:**

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

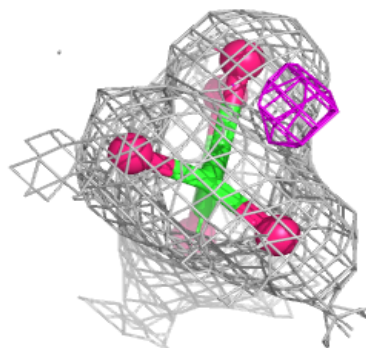
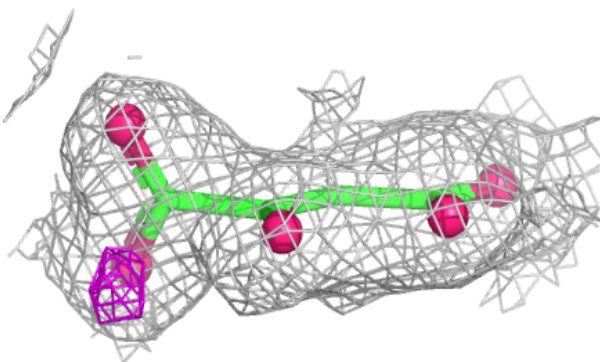
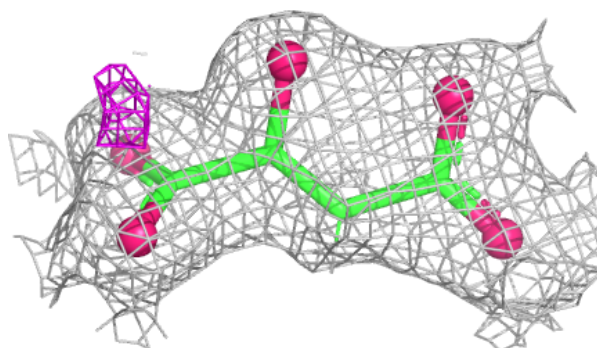


**Electron density around UMQ P 203:**

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

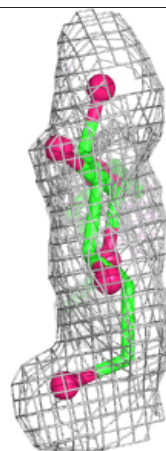
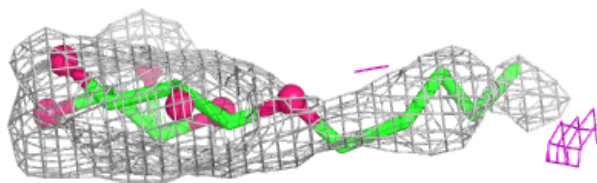
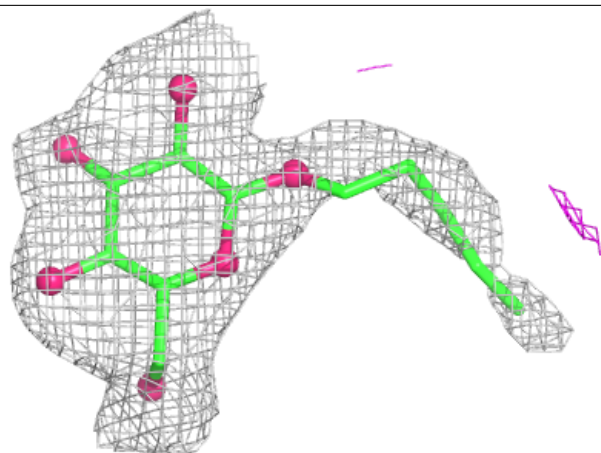
**Electron density around Y3P A 1002:**

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

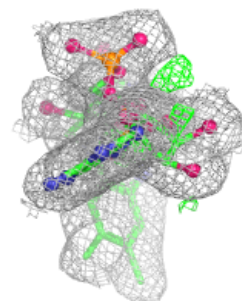
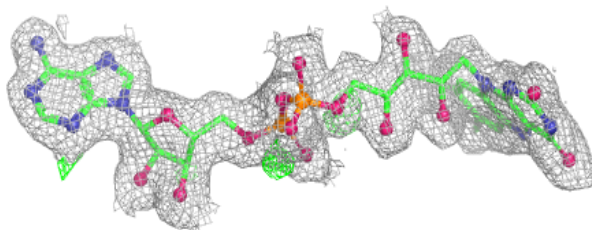
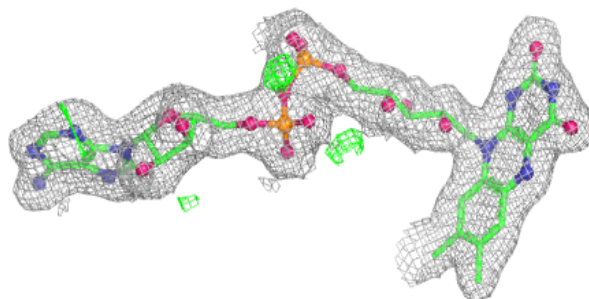


**Electron density around BOG D 201:**

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

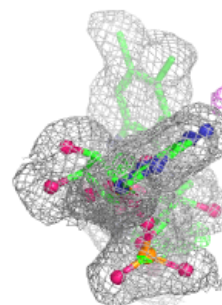
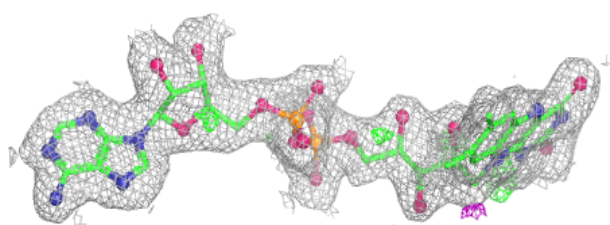
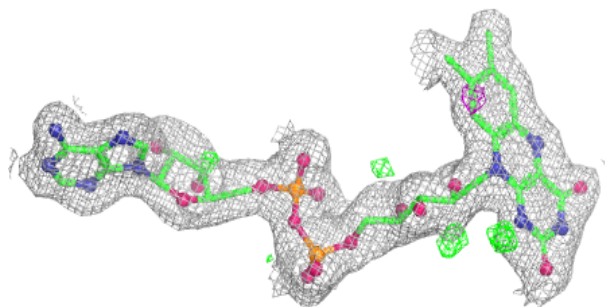
**Electron density around FAD N 1001:**

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

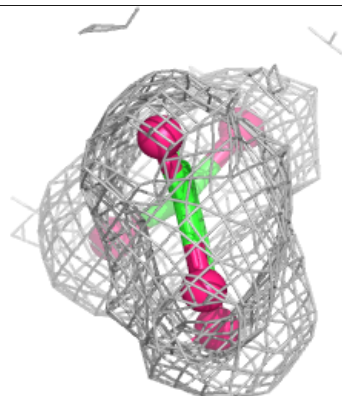
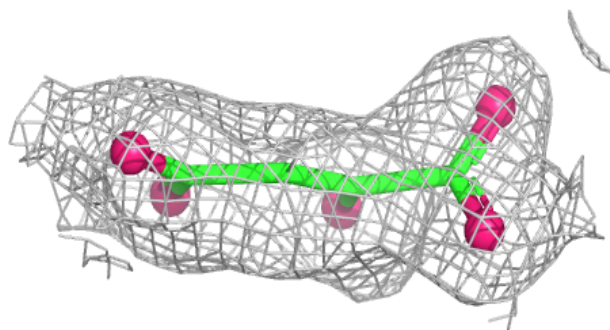
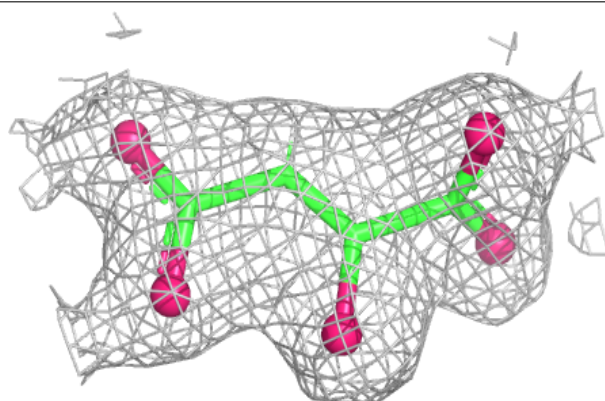


**Electron density around FAD A 1001:**

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

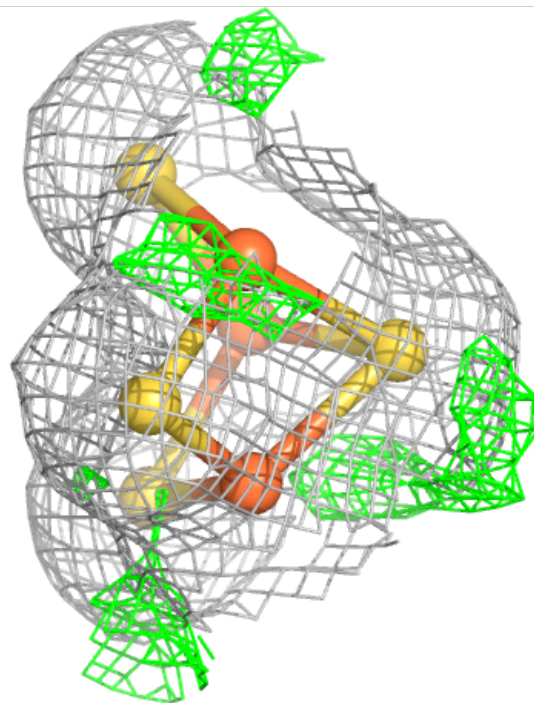
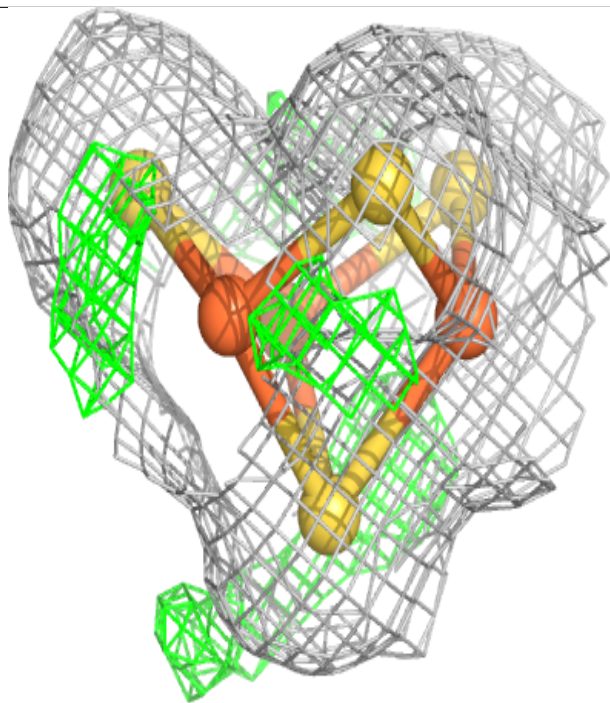
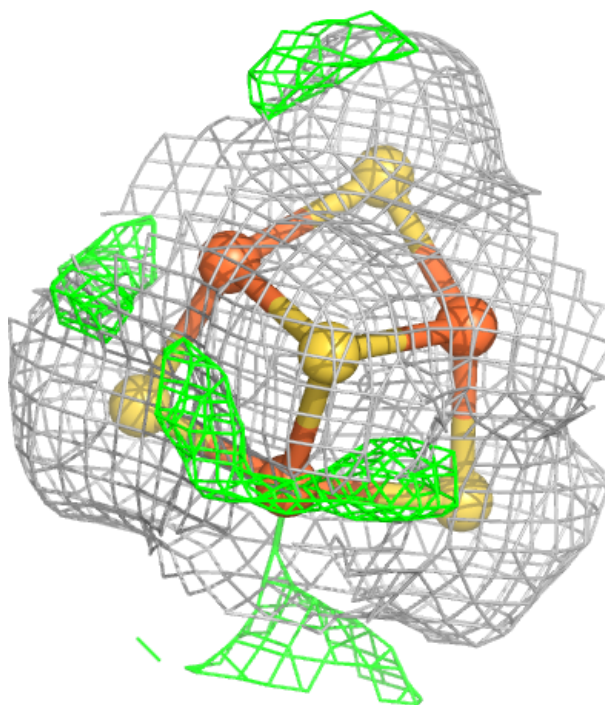
**Electron density around Y3P N 1002:**

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



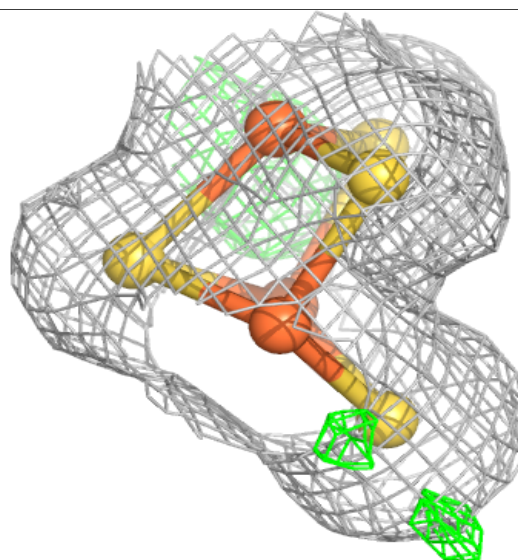
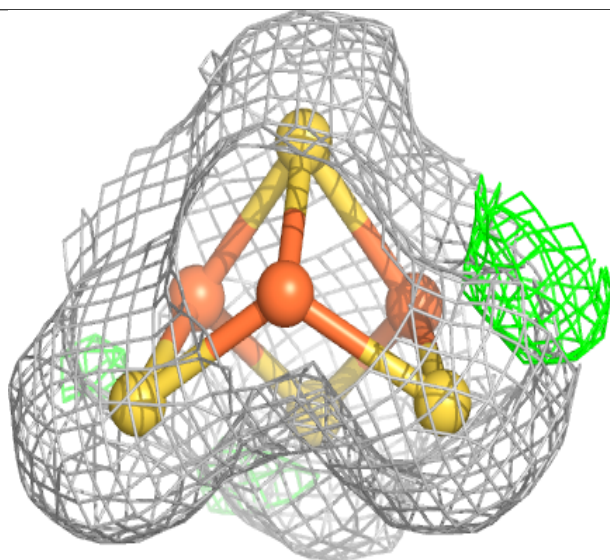
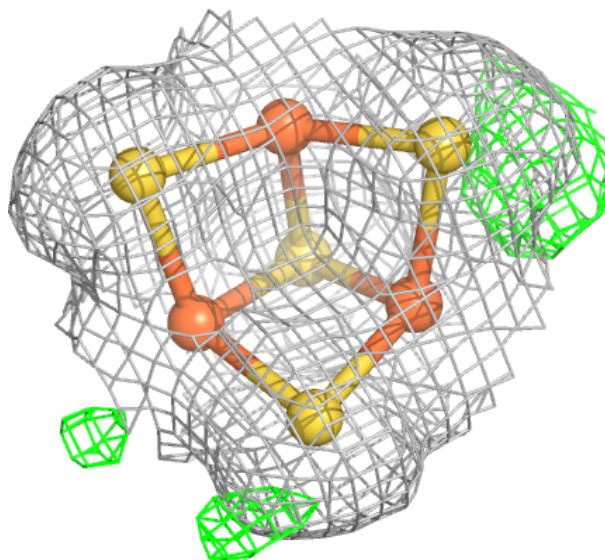
**Electron density around F3S B 1003:**

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



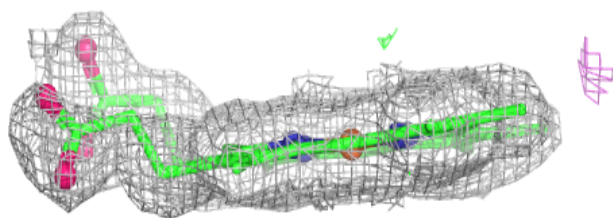
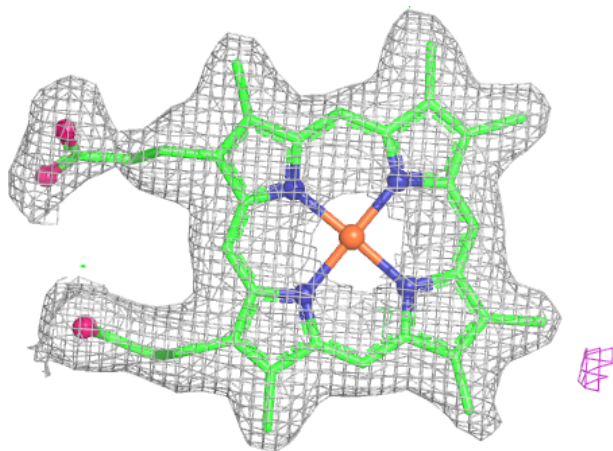
**Electron density around F3S O 1003:**

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



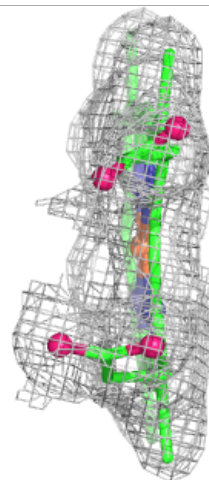
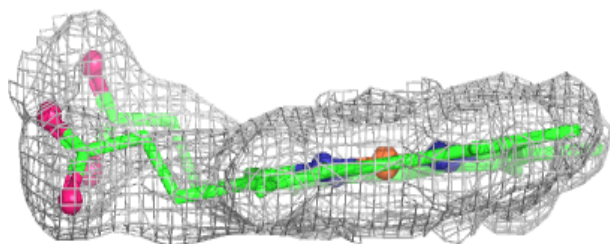
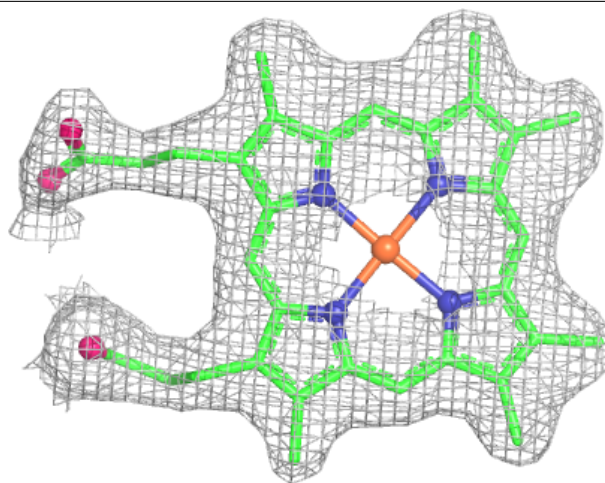
**Electron density around HEM C 201:**

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



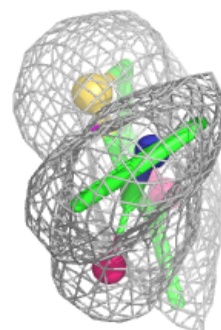
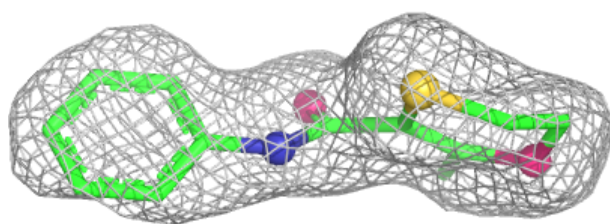
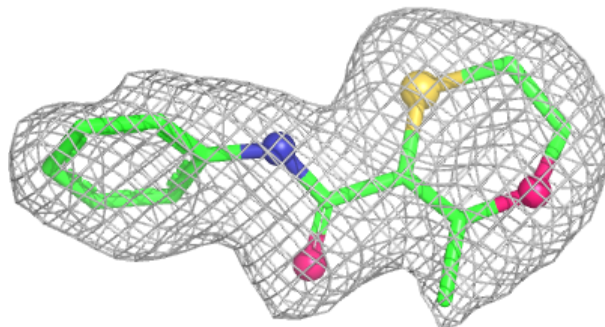
**Electron density around HEM P 201:**

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

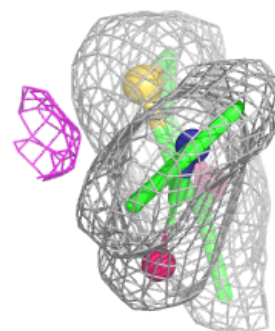
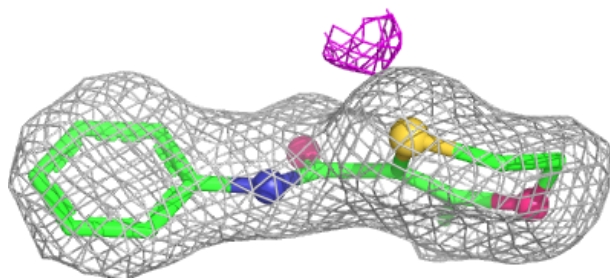
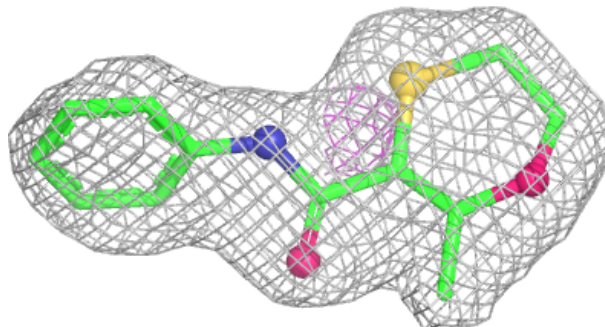


**Electron density around CBE C 202:**

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

**Electron density around CBE P 202:**

$2mF_o-DF_c$  (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.