WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2023 – 06:37 PM EDT

PDB ID	:	2GC4
Title	:	Structural comparison of the oxidized ternary electron transfer complex of methylamine dehydrogenase, amicyanin and cytochrome c551i from Paracoccus denitrificans with the substrate-reduced, copper free complex at 1.9 A resolution.
Authors	:	Chen, Z.; Durley, R.; Davidson, V.L.; Mathews, F.S.
Deposited on	:	2006-03-13
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

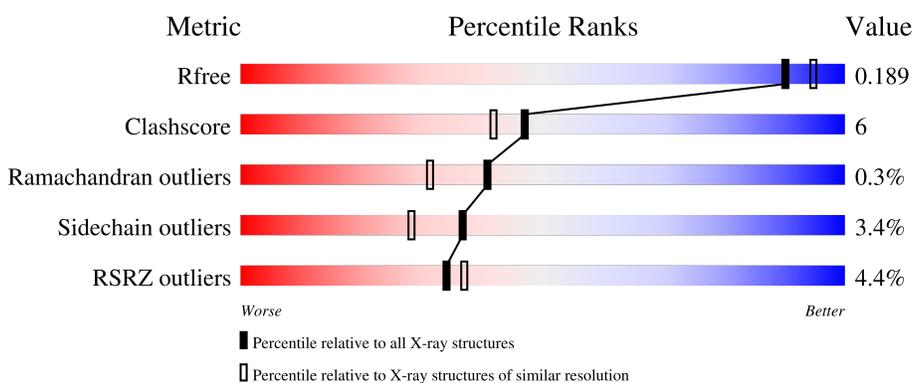|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.90 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.189
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		3.4%
RSRZ outliers		4.4%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	386	3% / 83% · 16% ·
1	E	386	3% / 86% · 13% ·
1	I	386	3% / 82% · 17% ·
1	M	386	3% / 85% · 13% ··
2	B	131	2% / 88% · 6% · 5%

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Mol	Chain	Length	Quality of chain
2	F	131	2% 88% 6% · 5%
2	J	131	2% 88% 6% · 5%
2	N	131	4% 87% 7% · 5%
3	C	105	10% 86% 13% ·
3	G	105	5% 90% 10%
3	K	105	6% 92% 8%
3	O	105	16% 75% 21% ·
4	D	147	5% 82% 16% ·
4	H	147	7% 77% 22% ·
4	L	147	5% 80% 18% ·
4	P	147	6% 73% 25% ·

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 24820 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 Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	E	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	I	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	M	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	F	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	J	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	N	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	TRQ	TRP	modified residue	UNP P22619
F	57	TRQ	TRP	modified residue	UNP P22619
J	57	TRQ	TRP	modified residue	UNP P22619
N	57	TRQ	TRP	modified residue	UNP P22619

- Molecule 3 is a protein called Amicyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total 807	C 516	N 133	O 152	S 6	0	0	0
3	G	105	Total 807	C 516	N 133	O 152	S 6	0	0	0
3	K	105	Total 807	C 516	N 133	O 152	S 6	0	0	0
3	O	105	Total 807	C 516	N 133	O 152	S 6	0	0	0

- Molecule 4 is a protein called Cytochrome c-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total 1145	C 724	N 182	O 231	S 8	0	0	0
4	H	147	Total 1145	C 724	N 182	O 231	S 8	0	0	0
4	L	147	Total 1145	C 724	N 182	O 231	S 8	0	0	0
4	P	147	Total 1145	C 724	N 182	O 231	S 8	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Cu 1	0	0
5	G	1	Total 1	Cu 1	0	0
5	K	1	Total 1	Cu 1	0	0
5	O	1	Total 1	Cu 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Na 1	0	0
6	H	1	Total 1	Na 1	0	0
6	L	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total Na		0	0
			1 1			

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

HEC
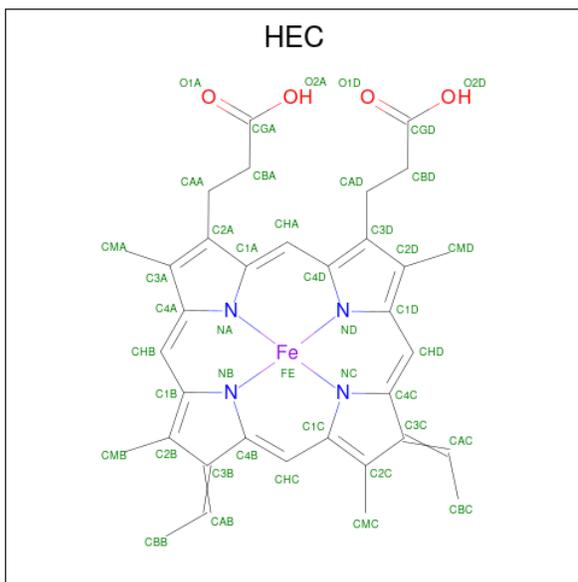
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	170	Total	O	0	0
			170	170		
8	B	54	Total	O	0	0
			54	54		
8	C	19	Total	O	0	0
			19	19		
8	D	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	160	Total 160	O 160	0	0
8	F	60	Total 60	O 60	0	0
8	G	22	Total 22	O 22	0	0
8	H	40	Total 40	O 40	0	0
8	I	155	Total 155	O 155	0	0
8	J	64	Total 64	O 64	0	0
8	K	27	Total 27	O 27	0	0
8	L	48	Total 48	O 48	0	0
8	M	173	Total 173	O 173	0	0
8	N	55	Total 55	O 55	0	0
8	O	14	Total 14	O 14	0	0
8	P	43	Total 43	O 43	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Methylamine dehydrogenase heavy chain

Chain A:

- Molecule 1: Methylamine dehydrogenase heavy chain

Chain E:

- Molecule 1: Methylamine dehydrogenase heavy chain

Chain I:

L345 L346 Y347 A348 K354 I358 A361 R368 L373 G386

• Molecule 1: Methylamine dehydrogenase heavy chain

Chain M:

3%
85%
13%

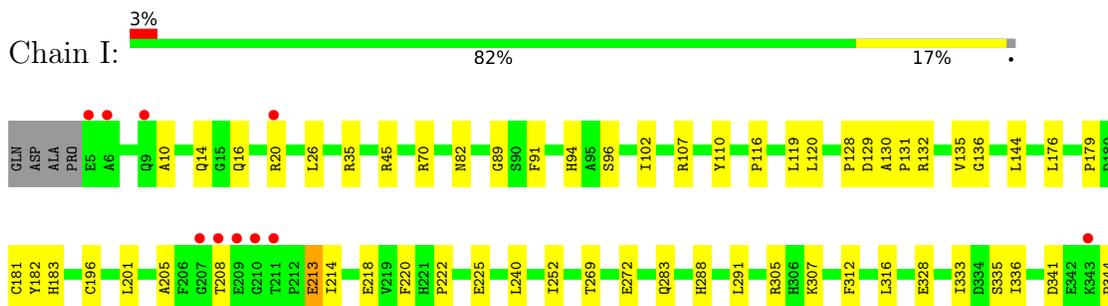GLN ASP ALA PRO E5 A6 Q9 A10 Q11 E12 T13 Q14 L26 R35 R45 E67 M74 I75 N82 G89 H94 A95 S96 I102 R107 Y110 T118 L119 L120 P128 D129 A130 P131 R132 V135 G136 L144 K173 P179 D180 C181 Y182

H183 C196 G207 T208 E209 G210 T211 I214 L227 L240 V241 W242 I252 D253 L254 Q283 H288 L291 L297 K307 S310 L316 D317 A318 K319 S335 E342 K343 P344 L345 A361 L367 G386

• Molecule 2: Methylamine dehydrogenase light chain

Chain B:

2%
88%
6% • 5%

ALA ASP ALA PRO ALA GLY T7 D8 Q16 D17 N18 Y25 H28 N45 W57 P96 V97 Y98 N104 W108 S131

• Molecule 2: Methylamine dehydrogenase light chain

Chain F:

2%
88%
6% • 5%

ALA ASP ALA PRO ALA GLY T7 D8 P9 W13 Q16 Q21 N45 A55 S56 W57 A103 N104 W108 A130 S131

• Molecule 2: Methylamine dehydrogenase light chain

Chain J:

2%
88%
6% • 5%

ALA ASP ALA PRO ALA GLY T7 D8 P9 Q16 Q21 N45 A55 S56 W57 P96 V97 Y98 N104 W108 S131

• Molecule 2: Methylamine dehydrogenase light chain

Chain N:

4%
87%
7% • 5%

ALA ASP ALA PRO ALA GLY T7 D8 Q16 D17 N18 Y25 H28 N45 P48 A55 S56 W57 Q68 A103 N104 W108 S131

• Molecule 3: Amicyanin

Chain C:

10%
86%
13% •

D1 I5 E8 V16 A17 D18 G19 I25 E31 L35 H36 V37 K38 V39 G40 D41 I46 N47 A59 G60 G63 E64 E84 T93 P94 E105

• Molecule 3: Amicyanin

Chain G:

5%

90%　　　　　　　　　　10%

D1 A12 E15 V16 A17 D18 G19 L35 K38 E64 A65 T93 P94 K101 E105

• Molecule 3: Amicyanin

Chain K:

6%

92%　　　　　　　　　　8%

D1 I5 E8 A17 D18 G19 E34 L35 K38 E64 T93 P94 E105

• Molecule 3: Amicyanin

Chain O:

16%

75%　　　　　　　　　　21%　　·

D1 K2 A3 T4 I5 E8 F11 A12 A13 A14 E15 V16 A17 D18 G19 A20 I21 K27 L35 H36 V37 K38 D41 R48 A59 G60 V61 L62 G63 E64 K73 Q76 E84 A85 G86 T87 T93 P94 K101 E105

• Molecule 4: Cytochrome c-L

Chain D:

5%

82%　　　　　　　　　　16%　　·

A1 F4 L13 E20 R23 D24 T25 V28 E41 D42 P43 E44 I45 L46 L52 C60 H61 K68 I69 L93 Q100 T109 L110 D111 E112 H122 D127 P128 K129 D130 W133 L134 T135 Q138 Q146 P147

• Molecule 4: Cytochrome c-L

Chain H:

7%

77%　　　　　　　　　　22%　　·

A1 P2 I7 I8 N14 F15 D16 D17 A18 M19 E20 R23 D24 T25 V28 K29 Y53 M56 C57 H61 G62 H63 Y64 K68 L93 Y94 Q100 P103 M104 W105 T109 L110 E112 D127 P128 K129 D130 W133 L134 Q138 Q146 P147

• Molecule 4: Cytochrome c-L

Chain L:

5%

80%　　　　　　　　　　18%　　·

A1 F4 F5 N6 I7 I8 L13 A18 M19 E20 E21 G22 R23 D24 K29 H30 T34 G35 E36 I45 E48 M56 H61 K68 I69 M101 T109 E112 D127 P128 K129 D130 W133 L134 T135 Q138 Q146 P147

• Molecule 4: Cytochrome c-L

Chain P:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.37Å 188.98Å 128.84Å 90.00° 99.74° 90.00°	Depositor
Resolution (Å)	29.95 – 1.90 29.95 – 1.84	Depositor EDS
% Data completeness (in resolution range)	84.3 (29.95-1.90) 79.8 (29.95-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.173 , 0.197 0.166 , 0.189	Depositor DCC
R_{free} test set	21026 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.7	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	24820	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3668e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEC, NA, TRQ

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	0.32	0/3044	0.64	0/4148
1	E	0.31	0/3044	0.63	0/4148
1	I	0.32	0/3044	0.64	0/4148
1	M	0.32	0/3044	0.64	0/4148
2	B	0.32	0/964	0.61	0/1315
2	F	0.32	0/964	0.61	0/1315
2	J	0.33	0/964	0.61	0/1315
2	N	0.31	0/964	0.61	0/1315
3	C	0.32	0/828	0.55	0/1124
3	G	0.32	0/828	0.58	0/1124
3	K	0.33	0/828	0.60	0/1124
3	O	0.30	0/828	0.57	0/1124
4	D	0.33	0/1180	0.63	1/1605 (0.1%)
4	H	0.37	1/1180 (0.1%)	0.65	1/1605 (0.1%)
4	L	0.35	1/1180 (0.1%)	0.63	1/1605 (0.1%)
4	P	0.34	1/1180 (0.1%)	0.61	1/1605 (0.1%)
All	All	0.32	3/24064 (0.0%)	0.62	4/32768 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	61	HIS	CE1-NE2	5.26	1.44	1.32
4	H	61	HIS	CE1-NE2	5.25	1.44	1.32
4	P	61	HIS	CE1-NE2	5.05	1.44	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	61	HIS	ND1-CG-CD2	8.05	120.07	108.80
4	H	61	HIS	ND1-CG-CD2	8.04	120.06	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	61	HIS	ND1-CG-CD2	7.98	119.97	108.80
4	D	61	HIS	ND1-CG-CD2	7.97	119.95	108.80

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	2967	0	2845	39	0
1	E	2967	0	2845	31	0
1	I	2967	0	2845	39	0
1	M	2967	0	2845	41	0
2	B	956	0	857	11	0
2	F	956	0	857	10	0
2	J	956	0	857	12	0
2	N	956	0	857	12	0
3	C	807	0	794	9	0
3	G	807	0	794	4	0
3	K	807	0	794	6	0
3	O	807	0	794	19	0
4	D	1145	0	1038	19	0
4	H	1145	0	1038	21	0
4	L	1145	0	1038	18	0
4	P	1145	0	1038	23	0
5	C	1	0	0	0	0
5	G	1	0	0	0	0
5	K	1	0	0	0	0
5	O	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	L	1	0	0	0	0
6	P	1	0	0	0	0
7	D	43	0	30	2	0
7	H	43	0	30	2	0
7	L	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	43	0	30	2	0
8	A	170	0	0	4	0
8	B	54	0	0	0	0
8	C	19	0	0	1	0
8	D	36	0	0	0	0
8	E	160	0	0	1	0
8	F	60	0	0	1	0
8	G	22	0	0	0	0
8	H	40	0	0	0	0
8	I	155	0	0	1	0
8	J	64	0	0	1	0
8	K	27	0	0	0	0
8	L	48	0	0	0	0
8	M	173	0	0	2	0
8	N	55	0	0	0	0
8	O	14	0	0	1	0
8	P	43	0	0	0	0
All	All	24820	0	22256	285	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.

The worst 5 of 285 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)
2:J:21:GLN:HE22	1:M:11:GLN:HG3	1.28	0.92
2:J:57:TRQ:HB2	2:J:108:TRP:NE1	1.89	0.88
2:B:57:TRQ:HB2	2:B:108:TRP:NE1	1.87	0.88
2:J:21:GLN:NE2	1:M:11:GLN:HG3	1.89	0.88
2:N:57:TRQ:HB2	2:N:108:TRP:NE1	1.88	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	380/386 (98%)	367 (97%)	12 (3%)	1 (0%)	41	31
1	E	380/386 (98%)	367 (97%)	13 (3%)	0	100	100
1	I	380/386 (98%)	364 (96%)	15 (4%)	1 (0%)	41	31
1	M	380/386 (98%)	366 (96%)	13 (3%)	1 (0%)	41	31
2	B	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	F	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	J	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	N	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
3	C	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	G	103/105 (98%)	98 (95%)	4 (4%)	1 (1%)	15	6
3	K	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	O	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	8	1
4	D	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
4	H	145/147 (99%)	140 (97%)	4 (3%)	1 (1%)	22	12
4	L	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
4	P	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
All	All	3000/3076 (98%)	2897 (97%)	93 (3%)	10 (0%)	41	31

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	17	ALA
3	O	18	ASP
4	H	68	LYS
3	O	19	GLY
4	P	68	LYS

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	308/311 (99%)	296 (96%)	12 (4%)	32	23
1	E	308/311 (99%)	299 (97%)	9 (3%)	42	35
1	I	308/311 (99%)	296 (96%)	12 (4%)	32	23
1	M	308/311 (99%)	298 (97%)	10 (3%)	39	30
2	B	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	F	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	J	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	N	104/106 (98%)	102 (98%)	2 (2%)	57	53
3	C	85/85 (100%)	83 (98%)	2 (2%)	49	43
3	G	85/85 (100%)	81 (95%)	4 (5%)	26	16
3	K	85/85 (100%)	84 (99%)	1 (1%)	71	70
3	O	85/85 (100%)	79 (93%)	6 (7%)	14	6
4	D	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	H	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	L	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	P	118/118 (100%)	110 (93%)	8 (7%)	16	7
All	All	2460/2480 (99%)	2376 (97%)	84 (3%)	37	28

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	134	LEU
3	O	4	THR
1	M	94	HIS
1	M	319	LYS
3	O	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	14	ASN
4	P	30	HIS
1	I	82	ASN
3	O	76	GLN
1	M	288	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
2	TRQ	J	57	2	13,17,18	4.72	3 (23%)	14,24,26	2.67	5 (35%)
2	TRQ	B	57	2	13,17,18	4.71	3 (23%)	14,24,26	3.04	5 (35%)
2	TRQ	N	57	2	13,17,18	4.71	3 (23%)	14,24,26	2.98	5 (35%)
2	TRQ	F	57	2	13,17,18	4.68	3 (23%)	14,24,26	2.99	5 (35%)

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
2	TRQ	J	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	B	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	N	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	F	57	2	-	0/4/19/21	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	TRQ	CH2-CZ2	-14.80	1.37	1.54
2	J	57	TRQ	CH2-CZ2	-14.76	1.37	1.54
2	N	57	TRQ	CH2-CZ2	-14.59	1.37	1.54
2	F	57	TRQ	CH2-CZ2	-14.57	1.37	1.54
2	N	57	TRQ	CE2-CZ2	-7.59	1.40	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	57	TRQ	O7-CZ2-CH2	6.47	126.61	119.00
2	N	57	TRQ	O7-CZ2-CH2	6.39	126.52	119.00
2	F	57	TRQ	O7-CZ2-CH2	6.32	126.44	119.00
2	B	57	TRQ	O7-CZ2-CE2	-5.93	115.56	121.84
2	N	57	TRQ	O7-CZ2-CE2	-5.83	115.67	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	57	TRQ	2	0
2	B	57	TRQ	2	0
2	N	57	TRQ	2	0
2	F	57	TRQ	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	#$|Z| > 2$
7	HEC	L	200	4	32,50,50	1.98	12 (37%)	24,82,82	1.76	4 (16%)
7	HEC	H	200	4	32,50,50	2.05	11 (34%)	24,82,82	1.80	4 (16%)
7	HEC	D	200	4	32,50,50	2.21	13 (40%)	24,82,82	1.77	5 (20%)
7	HEC	P	200	4	32,50,50	2.01	12 (37%)	24,82,82	1.70	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	L	200	4	-	1/10/54/54	-
7	HEC	H	200	4	-	0/10/54/54	-
7	HEC	D	200	4	-	2/10/54/54	-
7	HEC	P	200	4	-	1/10/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	200	HEC	C3C-C2C	-5.58	1.34	1.40
7	P	200	HEC	C3C-C2C	-4.46	1.36	1.40
7	L	200	HEC	C3C-C2C	-4.25	1.36	1.40
7	P	200	HEC	C2B-C3B	-4.19	1.36	1.40
7	H	200	HEC	C3C-C2C	-4.16	1.36	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	200	HEC	CBD-CAD-C3D	-5.48	103.27	112.62
7	H	200	HEC	CBD-CAD-C3D	-4.96	104.16	112.62
7	D	200	HEC	CBD-CAD-C3D	-4.75	104.52	112.62
7	P	200	HEC	CBD-CAD-C3D	-4.70	104.60	112.62
7	H	200	HEC	CMC-C2C-C3C	3.33	129.74	125.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	200	HEC	CAD-CBD-CGD-O2D
7	D	200	HEC	CAD-CBD-CGD-O1D
7	D	200	HEC	CAD-CBD-CGD-O2D
7	L	200	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.
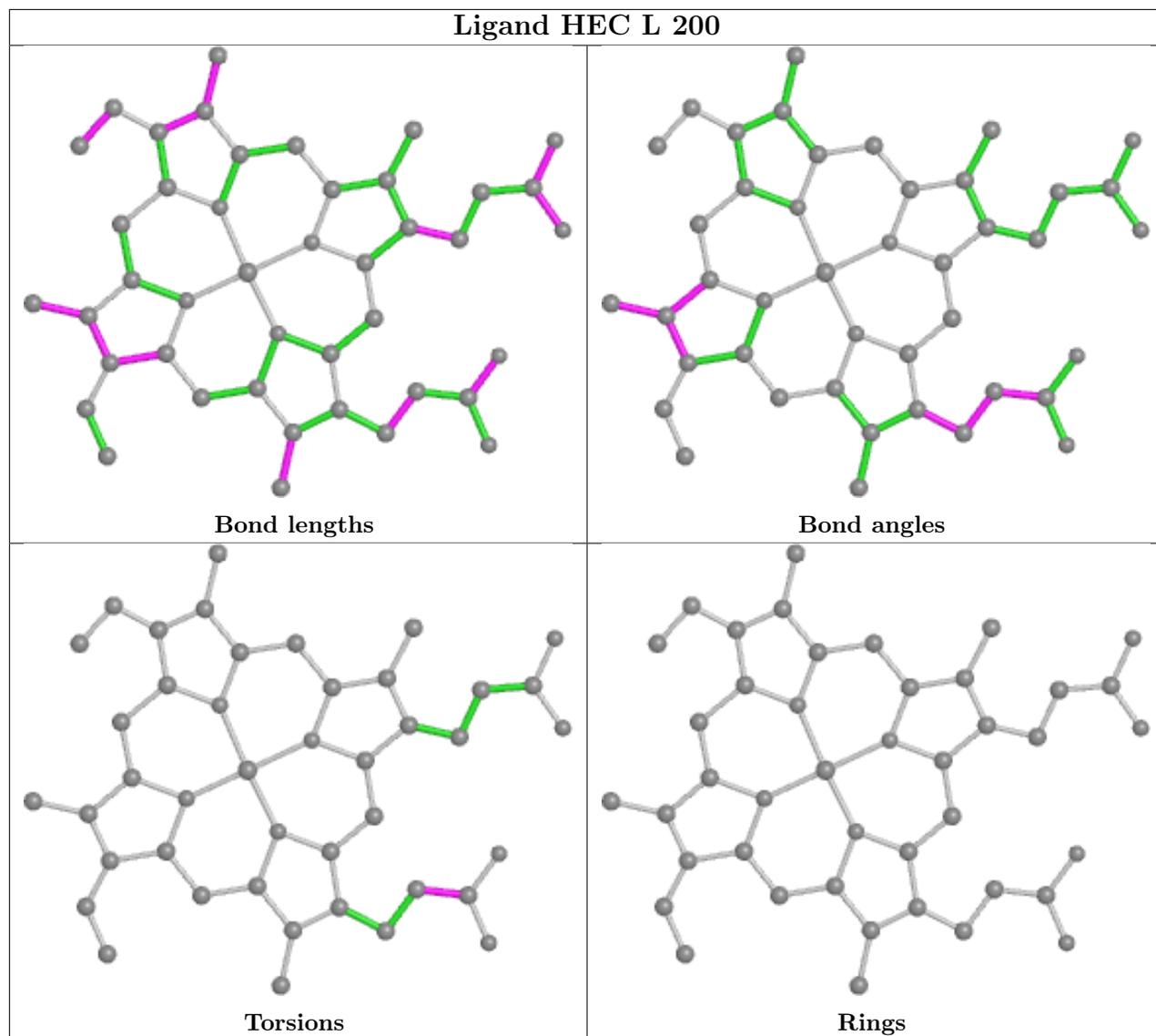
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	200	HEC	1	0
7	H	200	HEC	2	0

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Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	200	HEC	2	0
7	P	200	HEC	2	0

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

Ligand HEC L 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC H 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC D 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC P 200

Bond lengths

Bond angles

Torsions

Rings
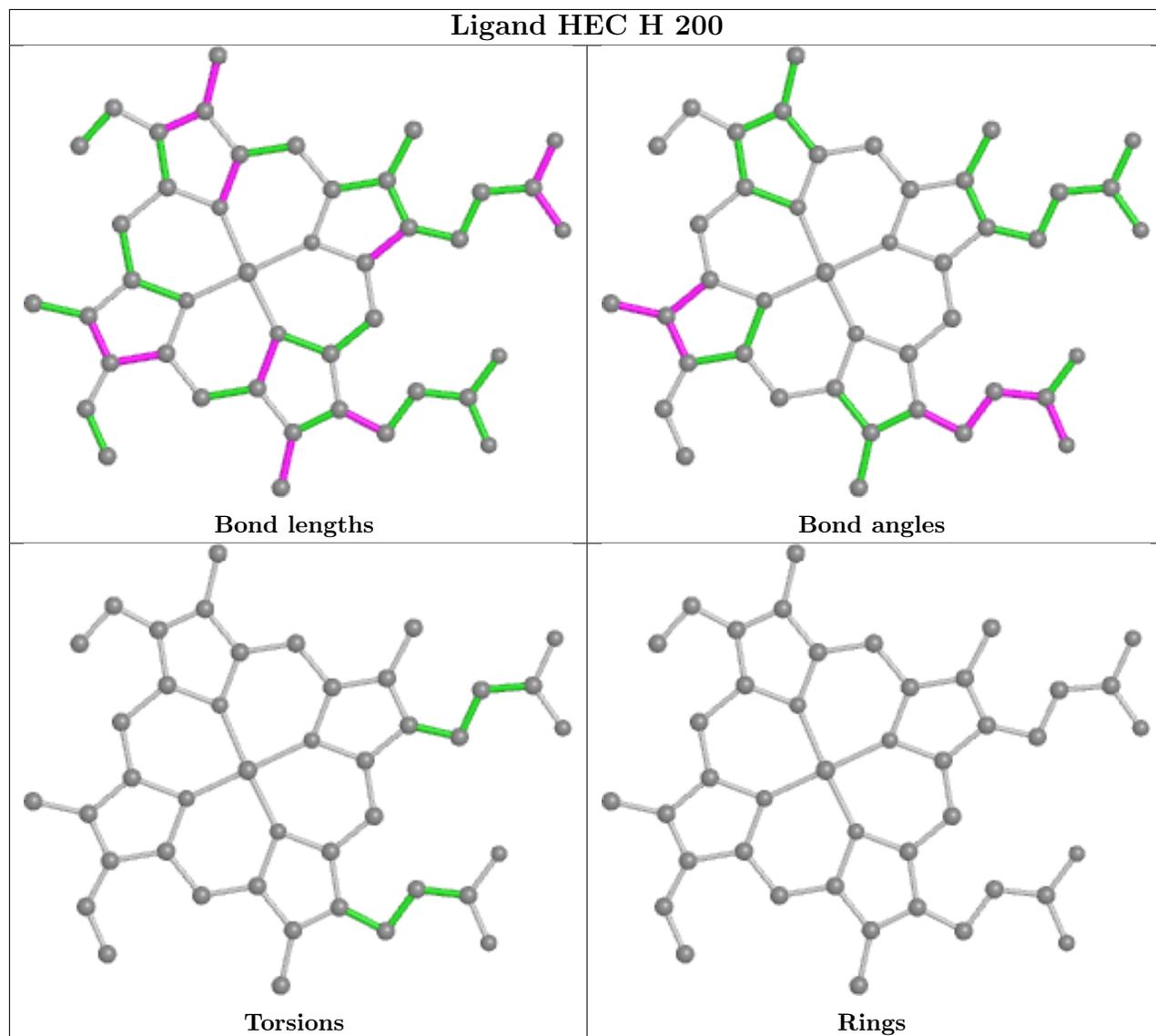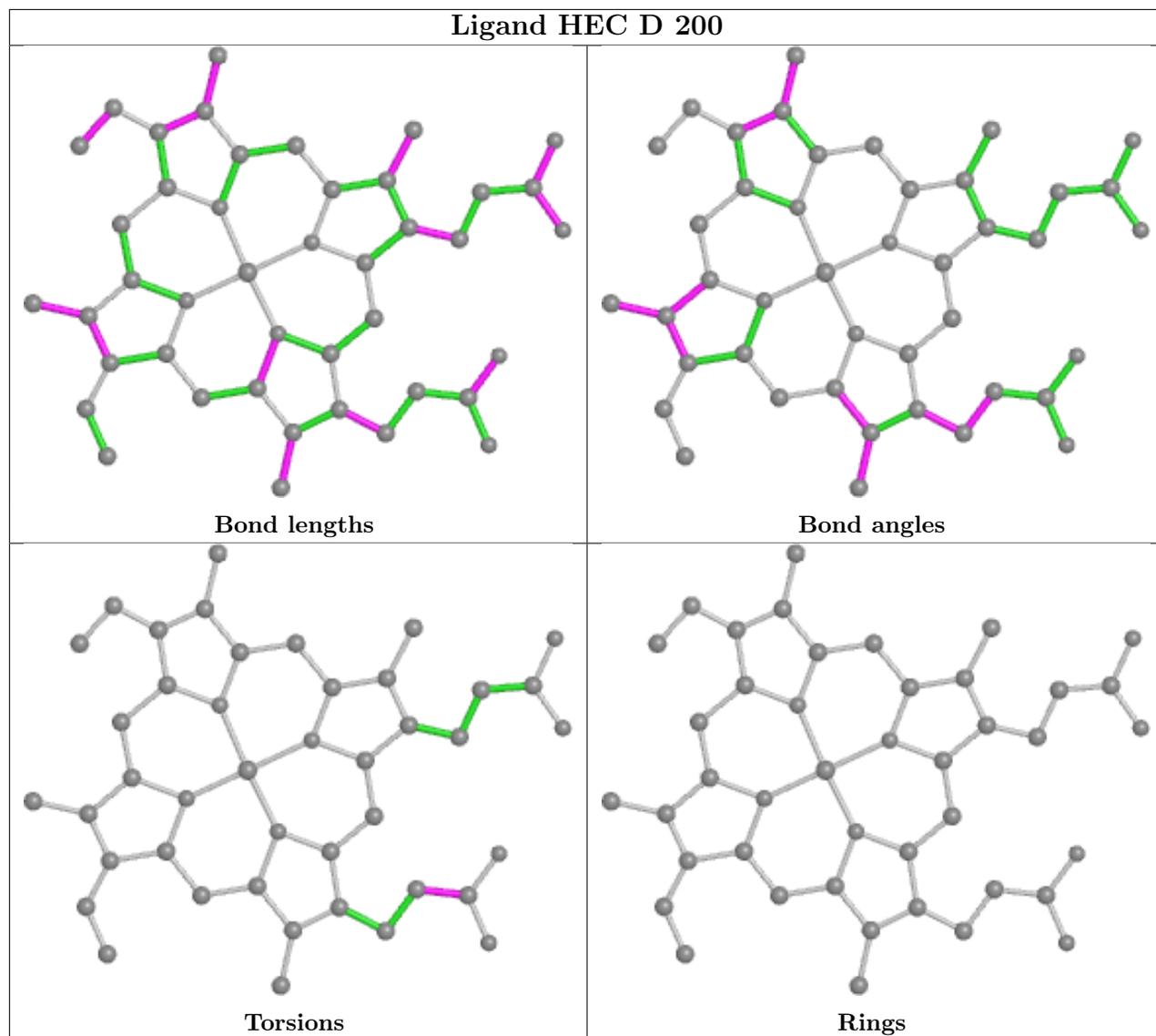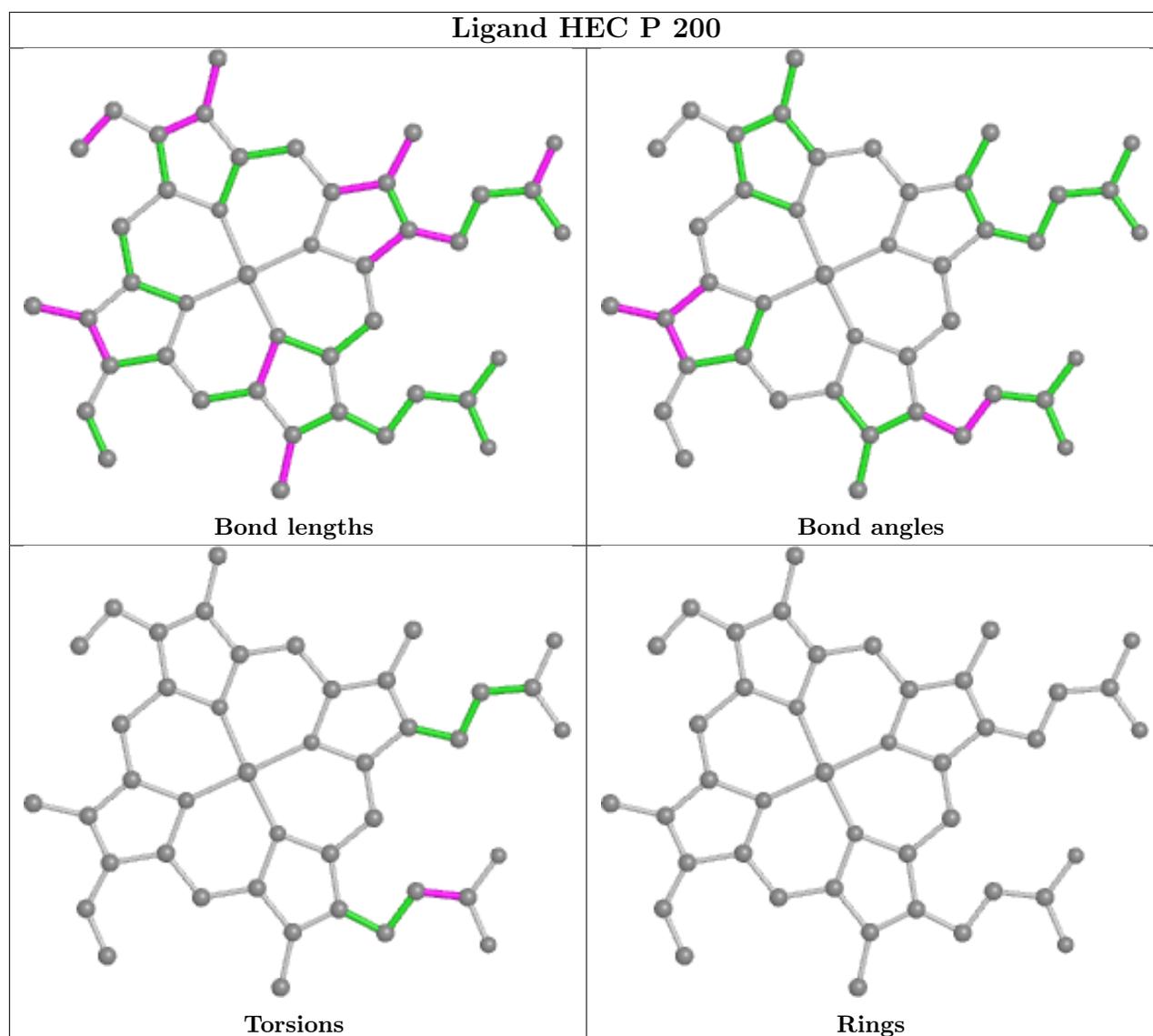
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	382/386 (98%)	-0.31	11 (2%)	51	54	21, 29, 49, 87	0
1	E	382/386 (98%)	-0.26	13 (3%)	45	48	21, 30, 51, 89	0
1	I	382/386 (98%)	-0.29	11 (2%)	51	54	21, 29, 53, 88	0
1	M	382/386 (98%)	-0.29	11 (2%)	51	54	20, 29, 50, 89	0
2	B	124/131 (94%)	-0.29	3 (2%)	59	62	22, 28, 48, 86	0
2	F	124/131 (94%)	-0.23	3 (2%)	59	62	20, 26, 46, 86	0
2	J	124/131 (94%)	-0.23	2 (1%)	72	74	19, 24, 45, 86	0
2	N	124/131 (94%)	-0.26	5 (4%)	38	41	22, 29, 49, 85	0
3	C	105/105 (100%)	0.35	10 (9%)	8	9	28, 42, 69, 81	0
3	G	105/105 (100%)	0.00	5 (4%)	30	33	25, 38, 60, 81	0
3	K	105/105 (100%)	-0.17	6 (5%)	23	26	24, 35, 57, 77	0
3	O	105/105 (100%)	0.85	17 (16%)	1	1	32, 51, 76, 88	0
4	D	147/147 (100%)	-0.10	8 (5%)	25	29	24, 35, 62, 76	0
4	H	147/147 (100%)	0.03	10 (6%)	17	19	25, 38, 68, 78	0
4	L	147/147 (100%)	-0.15	8 (5%)	25	29	24, 33, 59, 74	0
4	P	147/147 (100%)	0.11	9 (6%)	21	24	25, 38, 68, 79	0
All	All	3032/3076 (98%)	-0.16	132 (4%)	34	37	19, 31, 61, 89	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	131	SER	14.5
2	F	131	SER	12.7
2	B	131	SER	12.1
1	E	5	GLU	11.0
1	I	208	THR	9.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	TRQ	F	57	16/17	0.96	0.10	20,23,26,27	0
2	TRQ	J	57	16/17	0.96	0.10	20,23,26,27	0
2	TRQ	N	57	16/17	0.96	0.08	21,26,29,29	0
2	TRQ	B	57	16/17	0.97	0.09	23,25,27,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	NA	P	602	1/1	0.98	0.11	28,28,28,28	0
7	HEC	D	200	43/43	0.98	0.11	21,25,29,34	0
7	HEC	H	200	43/43	0.98	0.09	25,29,34,36	0
7	HEC	L	200	43/43	0.98	0.10	20,24,29,33	0
7	HEC	P	200	43/43	0.98	0.11	23,28,31,34	0
5	CU	O	107	1/1	0.99	0.06	39,39,39,39	0
6	NA	D	604	1/1	0.99	0.04	32,32,32,32	0
6	NA	H	603	1/1	0.99	0.12	27,27,27,27	0
5	CU	C	107	1/1	0.99	0.05	33,33,33,33	0
6	NA	L	601	1/1	1.00	0.12	23,23,23,23	0
5	CU	K	107	1/1	1.00	0.09	29,29,29,29	0
5	CU	G	107	1/1	1.00	0.06	32,32,32,32	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.
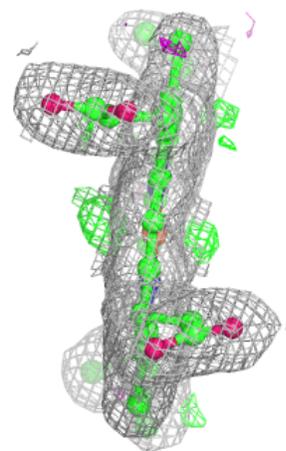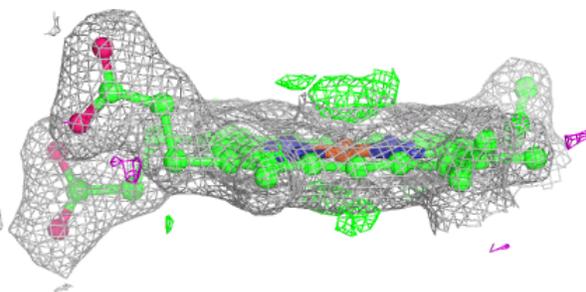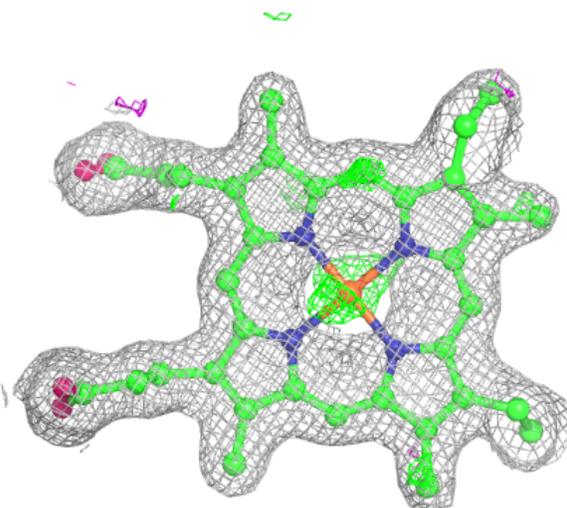
Electron density around HEC D 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
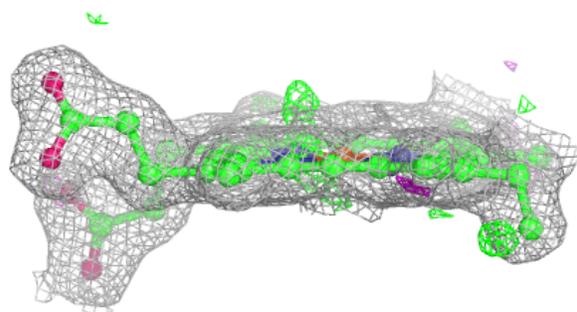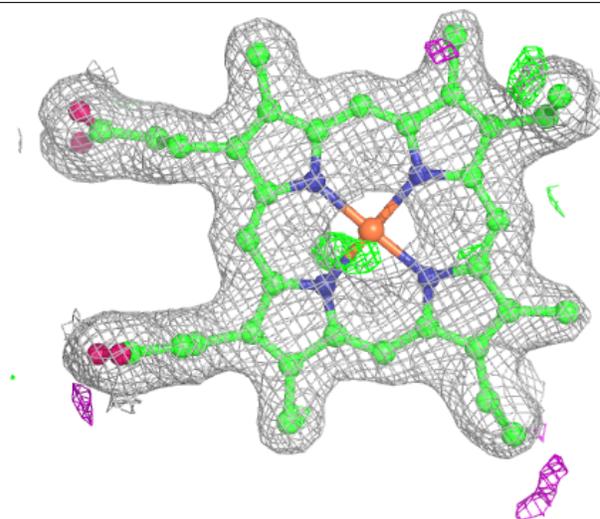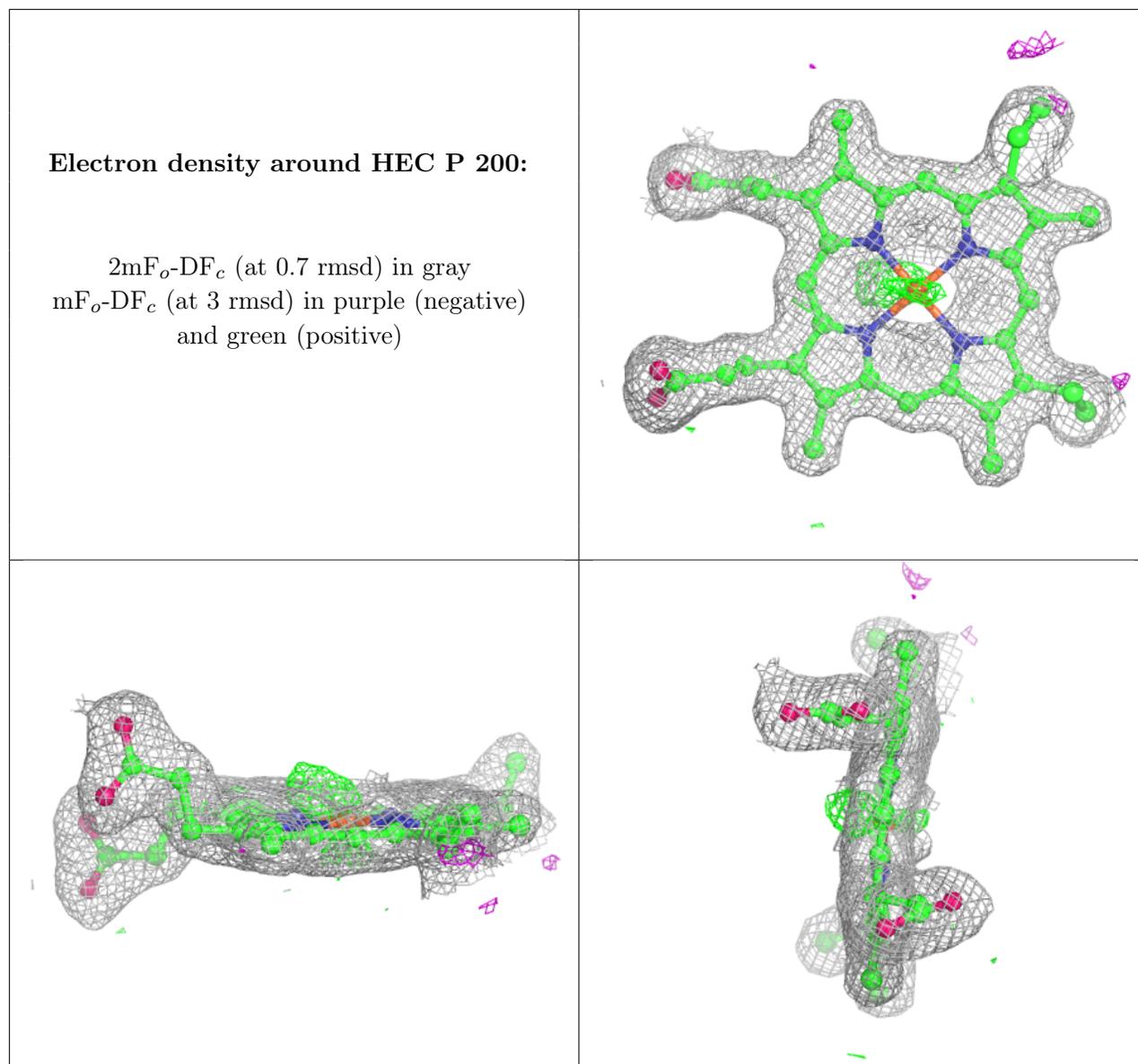
Electron density around HEC H 200:

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

Electron density around HEC L 200:

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

Electron density around HEC P 200:

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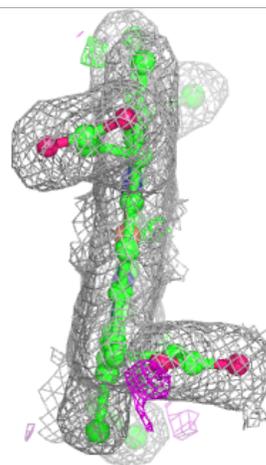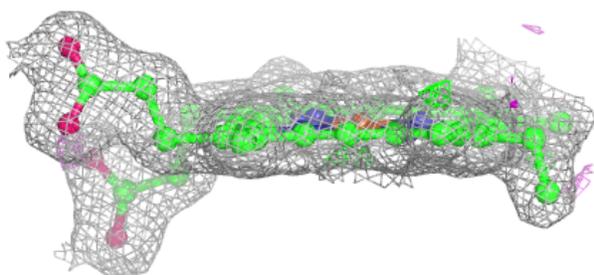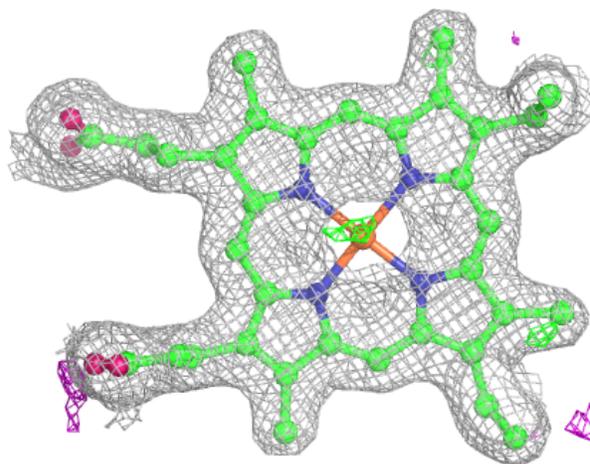
6.5 Other polymers (i)

There are no such residues in this entry.