Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 09:50 pm GMT

PDB ID	:	5L91
Title	:	The 2.2 A crystal structure of CYP109E1 from Bacillus megaterium bound with four corticosterone molecules
Authors	:	Jozwik, I.K.; Thunnissen, A.M.W.H.
Deposited on	:	2016-06-09
Resolution	:	2.20 Å(reported)

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

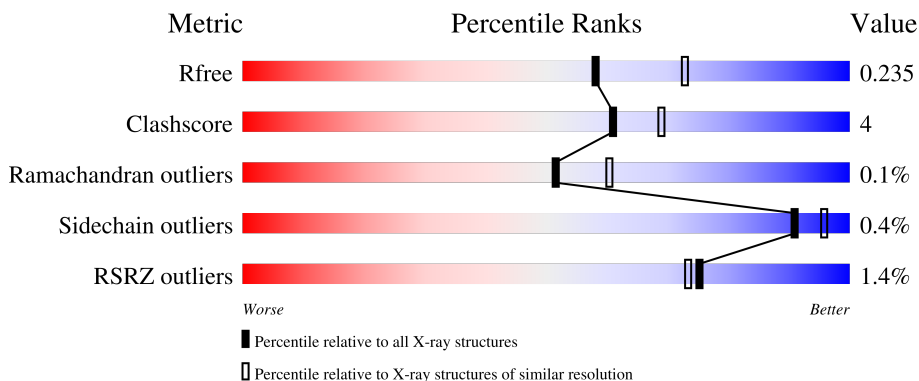|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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		0.235
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0.4%
RSRZ outliers		1.4%

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	410	88% 8% 5%
1	B	410	2% 87% 8% 5%

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
3	C0R	A	503	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6882 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 Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			3209	2043	554	600	12			
1	B	389	Total	C	N	O	S	0	1	0
			3190	2032	549	597	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	HIS	-	expression tag	UNP D5DKI8
A	406	HIS	-	expression tag	UNP D5DKI8
A	407	HIS	-	expression tag	UNP D5DKI8
A	408	HIS	-	expression tag	UNP D5DKI8
A	409	HIS	-	expression tag	UNP D5DKI8
A	410	HIS	-	expression tag	UNP D5DKI8
B	405	HIS	-	expression tag	UNP D5DKI8
B	406	HIS	-	expression tag	UNP D5DKI8
B	407	HIS	-	expression tag	UNP D5DKI8
B	408	HIS	-	expression tag	UNP D5DKI8
B	409	HIS	-	expression tag	UNP D5DKI8
B	410	HIS	-	expression tag	UNP D5DKI8

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
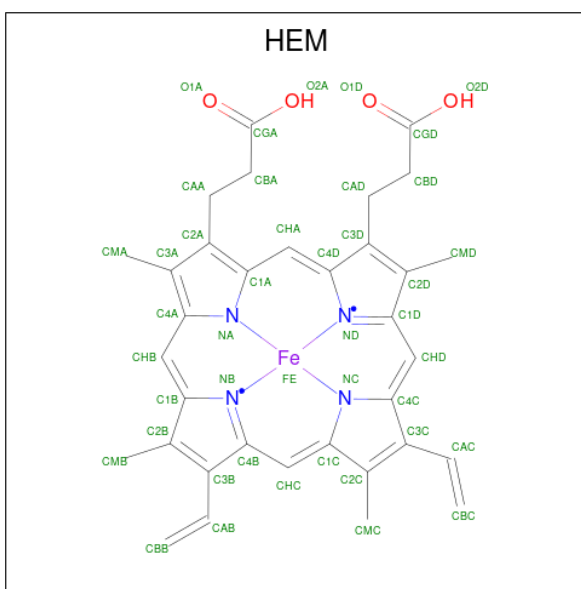
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CORTICOSTERONE (three-letter code: C0R) (formula: $C_{21}H_{30}O_4$).
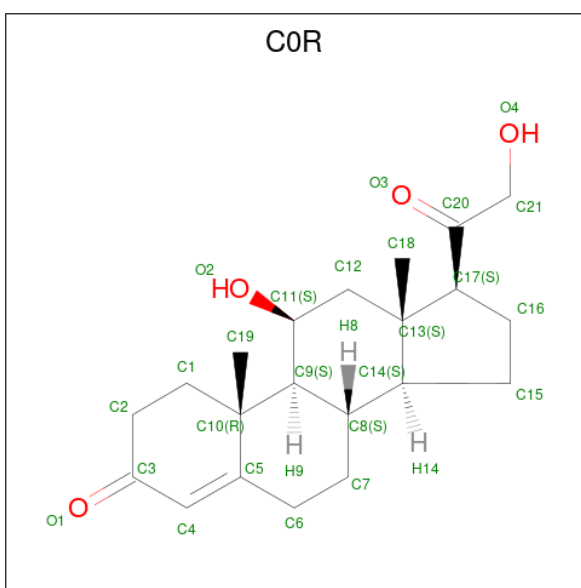
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 25	C 21	O 4	0	0
3	A	1	Total 25	C 21	O 4	0	0
3	B	1	Total 25	C 21	O 4	0	0
3	B	1	Total 25	C 21	O 4	0	0
3	B	1	Total 25	C 21	O 4	0	0
3	B	1	Total 25	C 21	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total 123	O 123	0	0
4	B	74	Total 74	O 74	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.
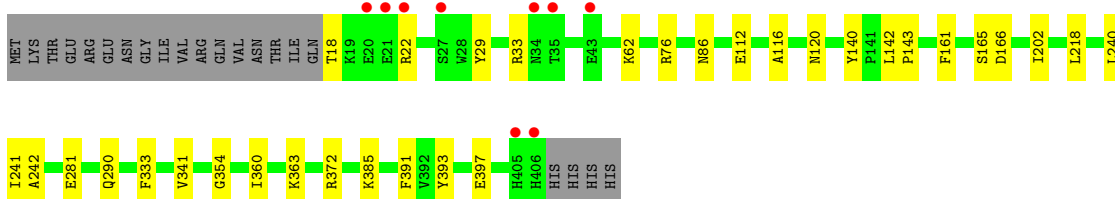
• Molecule 1: Cytochrome P450

Chain A:
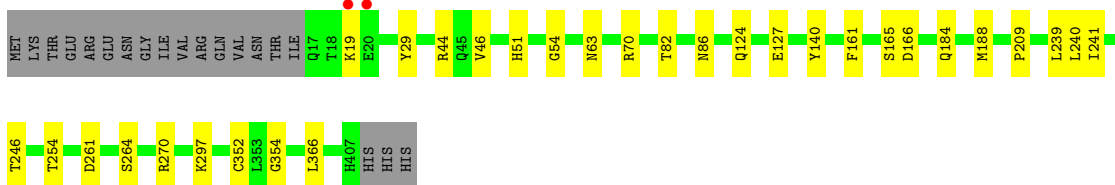
• Molecule 1: Cytochrome P450

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.42Å　　120.42Å　　140.80Å 90.00°　　　90.00°　　　120.00°	Depositor
Resolution (Å)	46.93　–　2.20 48.90　–　2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.93-2.20) 99.7 (48.90-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.185　,　0.232 0.191　,　0.235	Depositor DCC
R_{free} test set	3027 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.8	EDS
L-test for twinning [2]	$<|L|>$ = 0.48, $<L^2>$ = 0.31	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: C0R, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.65	1/3284 (0.0%)	0.71	1/4442 (0.0%)
1	B	0.59	0/3264	0.67	0/4415
All	All	0.62	1/6548 (0.0%)	0.69	1/8857 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TYR	CD2-CE2	-5.08	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	3209	0	3196	21	0
1	B	3190	0	3181	23	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	100	0	116	14	0
3	B	100	0	116	13	0
4	A	123	0	0	0	0
4	B	74	0	0	1	0
All	All	6882	0	6669	60	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 4.

All (60) 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:A:140:TYR:OH	1:A:166:ASP:OD1	1.78	0.99
1:B:86:ASN:HD21	3:B:503:C0R:H191	1.31	0.94
1:B:86:ASN:ND2	3:B:503:C0R:H191	1.90	0.85
1:A:86:ASN:HD21	3:A:503:C0R:H191	1.47	0.78
1:B:18:THR:O	1:B:22:ARG:HG3	1.85	0.77
1:A:86:ASN:ND2	3:A:503:C0R:H191	2.03	0.73
3:A:503:C0R:C7	3:A:504:C0R:H61	2.20	0.71
1:B:86:ASN:OD1	3:B:503:C0R:H62	1.94	0.67
3:B:503:C0R:H71	3:B:504:C0R:H62	1.78	0.65
3:A:503:C0R:H71	3:A:504:C0R:H61	1.80	0.63
1:B:140:TYR:OH	1:B:166:ASP:OD1	2.13	0.61
3:A:503:C0R:H72	3:A:504:C0R:H61	1.81	0.61
1:A:161:PHE:CZ	1:A:240:LEU:HD21	2.36	0.60
3:A:502:C0R:H161	3:A:504:C0R:H22	1.86	0.58
3:B:503:C0R:C7	3:B:504:C0R:H62	2.36	0.55
1:A:124:GLN:NE2	1:A:127:GLU:OE1	2.41	0.53
1:A:254:THR:HG21	1:A:366:LEU:HD13	1.91	0.52
3:A:503:C0R:H71	3:A:504:C0R:C6	2.39	0.52
3:B:504:C0R:H72	3:B:504:C0R:H191	1.92	0.51
1:B:354:GLY:HA3	2:B:501:HEM:C3C	2.46	0.51
1:A:241:ILE:HG21	3:A:503:C0R:H21	1.92	0.51
1:B:76:ARG:NE	3:B:505:C0R:O4	2.39	0.49
1:A:86:ASN:OD1	3:A:503:C0R:H62	2.13	0.49
1:A:161:PHE:CE2	1:A:240:LEU:HD21	2.49	0.48
3:A:504:C0R:H193	3:A:504:C0R:O2	2.14	0.47
1:B:142:LEU:HB3	1:B:143:PRO:HD3	1.97	0.47
1:B:120[B]:ASN:OD1	1:B:372:ARG:NH2	2.47	0.47
3:A:503:C0R:H61	3:A:504:C0R:H4	1.97	0.47
3:A:503:C0R:H193	3:A:503:C0R:O2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:OD2	1:A:264:SER:OG	2.15	0.46
1:B:360:ILE:HD12	1:B:363:LYS:HE2	1.97	0.46
1:A:51:HIS:CE1	1:A:54:GLY:HA3	2.52	0.45
1:B:241:ILE:HG21	3:B:503:C0R:H21	1.96	0.45
1:A:44:ARG:NH2	1:A:46:VAL:HG21	2.32	0.44
1:B:242:ALA:HB1	4:B:610:HOH:O	2.17	0.44
1:A:354:GLY:HA3	2:A:501:HEM:C3C	2.53	0.44
1:A:246:THR:HB	2:A:501:HEM:C3B	2.53	0.44
1:B:202:ILE:HG23	1:B:218:LEU:HD21	1.99	0.44
1:B:391:PHE:CE1	3:B:504:C0R:H11	2.53	0.44
1:A:352:CYS:HB2	2:A:501:HEM:NA	2.32	0.43
3:A:502:C0R:H122	3:A:503:C0R:O1	2.19	0.43
1:B:112:GLU:HG2	1:B:360:ILE:HG12	2.00	0.43
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.93	0.43
1:A:63:ASN:O	1:A:297:LYS:HD2	2.19	0.42
1:B:29:TYR:O	1:B:33:ARG:HB2	2.20	0.42
1:B:86:ASN:HD21	3:B:503:C0R:H8	1.83	0.42
1:A:239:LEU:HD22	2:A:501:HEM:HAC	2.01	0.42
1:B:290:GLN:HG2	1:B:393:TYR:HB2	2.02	0.42
1:B:385:LYS:HD2	1:B:397:GLU:HG2	2.02	0.42
1:B:161:PHE:HZ	1:B:240:LEU:HD21	1.84	0.41
1:B:116:ALA:O	1:B:120[B]:ASN:ND2	2.53	0.41
3:B:502:C0R:H161	3:B:504:C0R:H22	2.01	0.41
1:A:70:ARG:HG2	1:A:82:THR:HG22	2.03	0.41
1:A:184:GLN:O	1:A:188:MET:HG3	2.20	0.41
3:A:502:C0R:O2	3:A:502:C0R:H182	2.21	0.41
3:B:502:C0R:H161	3:B:504:C0R:C2	2.51	0.41
1:B:281:GLU:HG3	1:B:333:PHE:CE1	2.55	0.40
1:B:341:VAL:O	1:B:341:VAL:HG23	2.21	0.40
3:B:505:C0R:H193	3:B:505:C0R:O2	2.22	0.40

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	390/410 (95%)	372 (95%)	17 (4%)	1 (0%)	41	46
1	B	388/410 (95%)	373 (96%)	15 (4%)	0	100	100
All	All	778/820 (95%)	745 (96%)	32 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO

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	352/369 (95%)	351 (100%)	1 (0%)	92	97
1	B	350/369 (95%)	348 (99%)	2 (1%)	86	93
All	All	702/738 (95%)	699 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	62	LYS
1	B	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands 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	#$|Z| > 2$
3	C0R	A	502	-	28,28,28	5.20	17 (60%)	44,45,45	2.03	17 (38%)
2	HEM	B	501	4,1	41,50,50	1.55	6 (14%)	45,82,82	1.21	3 (6%)
3	C0R	B	502	-	28,28,28	5.08	15 (53%)	44,45,45	2.10	16 (36%)
3	C0R	B	503	-	28,28,28	5.39	17 (60%)	44,45,45	2.39	18 (40%)
3	C0R	A	503	-	28,28,28	5.43	16 (57%)	44,45,45	2.20	16 (36%)
3	C0R	A	505	-	28,28,28	5.42	16 (57%)	44,45,45	2.15	16 (36%)
3	C0R	B	505	-	28,28,28	5.27	15 (53%)	44,45,45	1.98	16 (36%)
3	C0R	A	504	-	28,28,28	5.37	15 (53%)	44,45,45	2.16	15 (34%)
2	HEM	A	501	4,1	41,50,50	1.39	5 (12%)	45,82,82	1.31	6 (13%)
3	C0R	B	504	-	28,28,28	5.32	15 (53%)	44,45,45	2.35	19 (43%)

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
3	C0R	A	502	-	-	0/6/67/67	0/4/4/4
2	HEM	B	501	4,1	-	1/12/54/54	-
3	C0R	B	502	-	-	0/6/67/67	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C0R	B	503	-	-	1/6/67/67	0/4/4/4
3	C0R	A	503	-	-	1/6/67/67	0/4/4/4
3	C0R	A	505	-	-	0/6/67/67	0/4/4/4
3	C0R	B	505	-	-	0/6/67/67	0/4/4/4
3	C0R	A	504	-	-	1/6/67/67	0/4/4/4
2	HEM	A	501	4,1	-	0/12/54/54	-
3	C0R	B	504	-	-	2/6/67/67	0/4/4/4

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	C0R	C4-C5	14.68	1.56	1.34
3	A	505	C0R	C4-C5	14.59	1.55	1.34
3	B	505	C0R	C4-C5	14.27	1.55	1.34
3	A	503	C0R	C4-C5	14.22	1.55	1.34
3	B	504	C0R	C4-C5	14.10	1.55	1.34
3	B	503	C0R	C4-C5	13.94	1.55	1.34
3	A	502	C0R	C4-C5	13.90	1.54	1.34
3	B	502	C0R	C4-C5	13.02	1.53	1.34
3	A	503	C0R	C13-C17	-12.41	1.35	1.56
3	B	503	C0R	C13-C17	-12.23	1.35	1.56
3	B	504	C0R	C13-C17	-12.01	1.36	1.56
3	A	504	C0R	C13-C17	-11.86	1.36	1.56
3	A	505	C0R	C13-C17	-11.58	1.36	1.56
3	B	502	C0R	C13-C17	-11.57	1.36	1.56
3	B	505	C0R	C13-C17	-11.57	1.36	1.56
3	B	505	C0R	C15-C14	-11.18	1.31	1.54
3	A	502	C0R	C13-C17	-10.98	1.37	1.56
3	B	503	C0R	C15-C14	-10.65	1.32	1.54
3	B	504	C0R	C15-C14	-10.42	1.32	1.54
3	A	504	C0R	C15-C14	-10.41	1.32	1.54
3	A	503	C0R	C15-C14	-10.23	1.33	1.54
3	A	505	C0R	C15-C14	-10.05	1.33	1.54
3	B	502	C0R	C15-C14	-9.67	1.34	1.54
3	A	502	C0R	C15-C14	-9.28	1.35	1.54
3	A	503	C0R	C4-C3	8.54	1.64	1.45
3	A	504	C0R	C4-C3	8.49	1.63	1.45
3	A	502	C0R	C4-C3	8.47	1.63	1.45
3	B	503	C0R	C4-C3	8.31	1.63	1.45
3	A	505	C0R	C4-C3	8.26	1.63	1.45
3	B	502	C0R	C4-C3	8.09	1.63	1.45
3	A	504	C0R	C12-C11	7.95	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	505	C0R	C4-C3	7.87	1.62	1.45
3	B	504	C0R	C4-C3	7.68	1.62	1.45
3	B	503	C0R	C12-C11	7.51	1.64	1.53
3	A	505	C0R	C12-C11	7.45	1.64	1.53
3	B	505	C0R	C12-C11	7.16	1.63	1.53
3	B	504	C0R	C12-C11	7.02	1.63	1.53
3	B	504	C0R	C16-C17	6.89	1.72	1.54
3	A	503	C0R	C12-C11	6.88	1.63	1.53
3	A	503	C0R	C16-C17	6.72	1.71	1.54
3	A	502	C0R	C16-C17	6.68	1.71	1.54
3	A	505	C0R	C16-C17	6.67	1.71	1.54
3	A	502	C0R	C12-C11	6.56	1.63	1.53
3	B	503	C0R	C16-C17	6.41	1.70	1.54
3	B	502	C0R	C12-C11	6.41	1.62	1.53
3	A	504	C0R	C16-C17	6.29	1.70	1.54
3	B	502	C0R	C16-C17	6.17	1.70	1.54
3	B	505	C0R	C16-C17	5.82	1.69	1.54
3	B	504	C0R	C13-C14	5.75	1.66	1.55
3	A	505	C0R	C6-C5	5.72	1.60	1.50
3	A	502	C0R	C6-C5	5.56	1.60	1.50
3	A	505	C0R	C13-C14	5.54	1.65	1.55
3	A	503	C0R	C13-C14	5.38	1.65	1.55
3	A	504	C0R	O2-C11	-5.25	1.32	1.43
3	B	504	C0R	C7-C6	5.21	1.64	1.52
3	B	504	C0R	O2-C11	-5.18	1.32	1.43
3	B	505	C0R	C6-C5	5.18	1.59	1.50
3	B	503	C0R	C2-C3	5.16	1.61	1.49
3	A	505	C0R	O2-C11	-5.15	1.32	1.43
3	A	503	C0R	O2-C11	-5.13	1.32	1.43
3	A	503	C0R	C2-C3	5.09	1.61	1.49
3	A	504	C0R	C6-C5	5.08	1.59	1.50
3	B	502	C0R	C2-C3	5.08	1.61	1.49
3	A	502	C0R	C7-C6	5.04	1.64	1.52
3	A	502	C0R	C2-C3	5.04	1.60	1.49
3	B	503	C0R	O2-C11	-5.03	1.32	1.43
3	A	502	C0R	C13-C14	5.01	1.64	1.55
3	B	502	C0R	C6-C5	4.97	1.59	1.50
3	A	503	C0R	C9-C11	4.95	1.62	1.53
3	A	504	C0R	C2-C3	4.93	1.60	1.49
3	B	502	C0R	C13-C14	4.88	1.64	1.55
3	B	503	C0R	C7-C6	4.86	1.63	1.52
3	B	502	C0R	C9-C11	4.85	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	505	C0R	O2-C11	-4.80	1.33	1.43
3	B	504	C0R	C2-C3	4.79	1.60	1.49
3	B	503	C0R	C13-C14	4.78	1.64	1.55
3	A	502	C0R	C8-C9	4.78	1.61	1.54
3	B	505	C0R	C13-C14	4.77	1.64	1.55
3	A	505	C0R	C9-C11	4.77	1.62	1.53
3	A	504	C0R	C13-C14	4.77	1.64	1.55
3	B	504	C0R	C6-C5	4.76	1.58	1.50
2	B	501	HEM	C3C-C2C	-4.75	1.33	1.40
3	A	502	C0R	O2-C11	-4.68	1.33	1.43
3	A	505	C0R	C7-C6	4.67	1.63	1.52
3	B	503	C0R	C6-C5	4.64	1.58	1.50
3	A	505	C0R	C2-C3	4.62	1.60	1.49
3	B	502	C0R	C7-C6	4.45	1.62	1.52
3	B	505	C0R	C9-C11	4.40	1.61	1.53
3	A	503	C0R	C6-C5	4.39	1.58	1.50
3	B	503	C0R	C9-C11	4.37	1.61	1.53
3	B	502	C0R	O2-C11	-4.37	1.34	1.43
3	A	505	C0R	C8-C9	4.26	1.60	1.54
3	B	505	C0R	C2-C3	4.26	1.59	1.49
3	A	503	C0R	C7-C6	4.25	1.62	1.52
3	B	505	C0R	C7-C6	4.16	1.62	1.52
3	A	504	C0R	C8-C9	4.04	1.60	1.54
3	B	502	C0R	C8-C9	3.95	1.59	1.54
3	A	502	C0R	C9-C11	3.87	1.60	1.53
2	A	501	HEM	C3C-C2C	-3.75	1.35	1.40
3	A	504	C0R	C7-C6	3.69	1.61	1.52
3	A	504	C0R	C9-C11	3.68	1.60	1.53
3	A	503	C0R	C1-C10	-3.64	1.47	1.54
3	B	503	C0R	C8-C9	3.60	1.59	1.54
3	B	504	C0R	C1-C10	-3.55	1.47	1.54
3	B	505	C0R	C1-C10	-3.47	1.47	1.54
2	A	501	HEM	C3C-CAC	3.32	1.54	1.47
2	B	501	HEM	C3C-CAC	3.30	1.54	1.47
3	B	505	C0R	C8-C9	3.22	1.58	1.54
3	A	503	C0R	C8-C9	3.17	1.58	1.54
3	A	505	C0R	C1-C10	-3.13	1.48	1.54
3	B	504	C0R	C9-C11	3.09	1.59	1.53
3	B	504	C0R	C8-C9	3.03	1.58	1.54
2	B	501	HEM	CAB-C3B	2.98	1.55	1.47
3	B	503	C0R	C1-C10	-2.98	1.48	1.54
3	B	504	C0R	C16-C15	2.94	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	C0R	C10-C5	2.94	1.58	1.52
3	B	502	C0R	C1-C10	-2.89	1.48	1.54
3	A	503	C0R	C10-C5	2.89	1.58	1.52
3	A	503	C0R	C16-C15	2.87	1.61	1.54
3	A	502	C0R	C16-C15	2.84	1.61	1.54
2	A	501	HEM	CAB-C3B	2.81	1.55	1.47
3	B	503	C0R	C16-C15	2.80	1.61	1.54
3	A	504	C0R	C16-C15	2.69	1.61	1.54
3	B	502	C0R	C16-C15	2.62	1.61	1.54
3	A	505	C0R	C10-C5	2.56	1.57	1.52
3	A	504	C0R	C1-C10	-2.51	1.49	1.54
3	A	502	C0R	C10-C5	2.50	1.57	1.52
3	A	505	C0R	C16-C15	2.49	1.60	1.54
2	A	501	HEM	CMD-C2D	2.36	1.55	1.50
3	B	505	C0R	C16-C15	2.30	1.60	1.54
2	B	501	HEM	CMB-C2B	2.27	1.55	1.50
2	A	501	HEM	CAD-C3D	2.26	1.57	1.51
3	A	502	C0R	C1-C10	-2.24	1.50	1.54
3	B	503	C0R	C7-C8	-2.17	1.49	1.53
2	B	501	HEM	CAA-C2A	2.16	1.55	1.52
2	B	501	HEM	FE-NB	-2.13	1.86	1.96
3	A	502	C0R	C19-C10	2.05	1.58	1.54

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	504	C0R	C12-C13-C14	6.48	114.40	106.94
3	A	503	C0R	C5-C4-C3	-6.09	113.84	123.67
3	B	503	C0R	C7-C8-C14	-5.82	102.14	112.08
3	B	503	C0R	C5-C4-C3	-5.65	114.55	123.67
3	B	504	C0R	C5-C4-C3	-5.47	114.85	123.67
3	B	505	C0R	C5-C4-C3	-5.28	115.16	123.67
3	A	504	C0R	C5-C4-C3	-5.00	115.60	123.67
3	B	503	C0R	C6-C7-C8	4.82	120.42	111.69
3	A	502	C0R	C1-C10-C5	4.76	117.47	108.75
3	A	504	C0R	C1-C10-C5	4.73	117.41	108.75
3	A	505	C0R	C7-C8-C14	-4.67	104.10	112.08
3	A	503	C0R	C6-C7-C8	4.65	120.12	111.69
3	A	504	C0R	C2-C1-C10	4.65	122.19	113.45
3	B	504	C0R	C12-C11-C9	-4.60	106.30	112.60
3	A	505	C0R	C12-C13-C14	4.53	112.15	106.94
3	B	503	C0R	C6-C5-C4	-4.50	113.35	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	C0R	C5-C4-C3	-4.46	116.48	123.67
3	B	502	C0R	C12-C13-C14	4.43	112.05	106.94
3	A	502	C0R	C5-C4-C3	-4.40	116.58	123.67
3	B	502	C0R	C5-C4-C3	-4.38	116.60	123.67
3	B	503	C0R	C19-C10-C1	-4.24	102.73	109.43
3	B	504	C0R	C10-C9-C11	4.14	118.72	114.47
3	A	503	C0R	C17-C13-C14	4.14	104.14	99.72
3	A	503	C0R	C9-C10-C5	3.95	114.85	108.21
3	B	505	C0R	C7-C8-C14	-3.90	105.42	112.08
3	A	505	C0R	O3-C20-C17	-3.84	115.47	122.27
3	B	502	C0R	C12-C11-C9	-3.82	107.37	112.60
3	A	504	C0R	C12-C13-C14	3.82	111.33	106.94
3	A	503	C0R	C12-C13-C17	-3.82	112.34	116.15
3	B	502	C0R	C2-C1-C10	3.77	120.53	113.45
3	A	504	C0R	C7-C8-C14	-3.75	105.68	112.08
3	B	504	C0R	C1-C10-C5	3.69	115.51	108.75
3	B	502	C0R	C7-C8-C14	-3.64	105.87	112.08
3	B	504	C0R	C16-C17-C13	-3.62	100.98	104.21
3	B	505	C0R	C1-C10-C5	3.59	115.33	108.75
3	A	504	C0R	C7-C8-C9	3.53	115.92	109.64
3	B	504	C0R	C13-C14-C8	-3.52	109.17	114.38
3	A	502	C0R	C7-C6-C5	-3.50	105.35	111.93
3	A	505	C0R	C19-C10-C1	-3.49	103.92	109.43
3	A	502	C0R	C19-C10-C1	-3.48	103.93	109.43
3	A	505	C0R	C2-C1-C10	3.48	119.98	113.45
3	B	503	C0R	C6-C5-C10	3.44	123.11	116.77
3	B	502	C0R	C1-C10-C5	3.36	114.91	108.75
2	B	501	HEM	CHC-C4B-NB	3.30	128.01	124.43
2	A	501	HEM	CMA-C3A-C4A	-3.28	123.42	128.46
3	B	503	C0R	C10-C9-C11	3.28	117.83	114.47
3	A	504	C0R	C19-C10-C5	-3.24	103.11	108.34
3	B	503	C0R	C12-C13-C14	3.23	110.66	106.94
3	A	504	C0R	C16-C17-C13	-3.22	101.34	104.21
3	A	505	C0R	C1-C10-C5	3.13	114.48	108.75
3	B	503	C0R	O3-C20-C17	-3.11	116.75	122.27
3	B	505	C0R	C15-C14-C8	-3.10	113.97	119.08
3	B	505	C0R	C7-C8-C9	3.08	115.12	109.64
3	A	503	C0R	C7-C6-C5	-3.08	106.14	111.93
3	A	502	C0R	C12-C13-C14	3.07	110.47	106.94
3	A	505	C0R	C7-C8-C9	3.05	115.07	109.64
3	A	503	C0R	C19-C10-C1	-3.02	104.65	109.43
3	B	504	C0R	C9-C8-C14	-3.01	103.97	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	C0R	C9-C8-C14	2.97	114.41	109.23
3	B	503	C0R	C9-C10-C5	2.96	113.17	108.21
2	A	501	HEM	C4C-CHD-C1D	2.95	126.45	122.56
2	B	501	HEM	CHD-C1D-ND	2.91	127.59	124.43
3	B	505	C0R	C12-C13-C14	2.88	110.25	106.94
3	B	504	C0R	C8-C9-C11	-2.86	106.11	113.41
3	B	505	C0R	C13-C17-C20	2.85	119.56	115.47
3	B	504	C0R	C7-C8-C9	2.83	114.67	109.64
3	B	505	C0R	C16-C17-C20	-2.82	108.46	113.89
3	A	503	C0R	C1-C10-C5	2.81	113.89	108.75
3	B	502	C0R	C18-C13-C12	-2.80	106.58	110.76
3	A	503	C0R	C13-C14-C8	-2.79	110.25	114.38
3	A	502	C0R	C2-C1-C10	2.74	118.59	113.45
3	A	503	C0R	C10-C9-C11	2.73	117.27	114.47
3	A	502	C0R	C6-C5-C10	2.73	121.81	116.77
3	A	504	C0R	C13-C14-C8	-2.73	110.34	114.38
3	B	502	C0R	C9-C8-C14	2.72	113.99	109.23
3	A	502	C0R	C7-C8-C14	-2.72	107.43	112.08
2	A	501	HEM	O1D-CGD-CBD	-2.72	114.34	123.08
3	B	502	C0R	C7-C6-C5	-2.71	106.83	111.93
3	B	502	C0R	C16-C17-C13	-2.69	101.81	104.21
3	B	504	C0R	C9-C10-C5	-2.67	103.74	108.21
3	A	505	C0R	C10-C9-C11	2.66	117.19	114.47
3	A	502	C0R	C15-C16-C17	-2.60	101.02	105.30
3	A	505	C0R	C16-C15-C14	-2.59	100.00	105.13
3	A	502	C0R	O4-C21-C20	-2.58	105.72	112.66
3	B	505	C0R	O3-C20-C17	-2.57	117.71	122.27
3	B	502	C0R	C16-C15-C14	-2.56	100.05	105.13
3	A	505	C0R	C16-C17-C13	-2.53	101.96	104.21
3	A	503	C0R	C16-C17-C13	-2.52	101.96	104.21
3	A	505	C0R	C2-C3-C4	-2.52	112.86	116.74
2	A	501	HEM	CMC-C2C-C3C	2.48	129.32	124.68
3	A	503	C0R	C9-C8-C14	2.47	113.56	109.23
3	A	502	C0R	C16-C17-C13	-2.47	102.00	104.21
3	B	504	C0R	C12-C13-C17	-2.46	113.69	116.15
3	B	504	C0R	C18-C13-C12	-2.46	107.08	110.76
3	A	503	C0R	C19-C10-C9	-2.45	108.58	112.65
3	B	503	C0R	O3-C20-C21	2.44	124.35	120.13
3	A	503	C0R	C6-C5-C4	-2.44	116.79	120.87
3	B	505	C0R	C15-C16-C17	-2.44	101.28	105.30
3	A	505	C0R	O3-C20-C21	2.43	124.34	120.13
3	B	503	C0R	C16-C15-C14	-2.43	100.31	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CBA-CAA-C2A	-2.40	108.52	112.62
3	B	503	C0R	C9-C8-C14	2.39	113.41	109.23
3	A	504	C0R	C15-C16-C17	-2.39	101.36	105.30
3	B	505	C0R	C2-C1-C10	2.38	117.93	113.45
3	B	502	C0R	C6-C5-C4	-2.38	116.88	120.87
3	A	502	C0R	C18-C13-C12	-2.38	107.21	110.76
3	A	502	C0R	C6-C5-C4	-2.36	116.91	120.87
3	B	505	C0R	C16-C17-C13	-2.35	102.11	104.21
3	B	505	C0R	C18-C13-C17	2.32	114.00	110.24
3	A	504	C0R	C1-C2-C3	2.32	116.59	111.62
3	B	503	C0R	C15-C16-C17	-2.28	101.55	105.30
3	A	502	C0R	C19-C10-C5	-2.28	104.66	108.34
3	B	504	C0R	C10-C9-C8	2.27	117.27	113.63
2	A	501	HEM	O2D-CGD-CBD	2.26	121.30	114.03
3	B	502	C0R	C16-C17-C20	-2.23	109.59	113.89
3	B	504	C0R	C6-C7-C8	-2.23	107.66	111.69
3	B	502	C0R	C6-C5-C10	2.21	120.86	116.77
3	A	505	C0R	C6-C7-C8	2.21	115.69	111.69
3	B	503	C0R	C16-C17-C13	-2.20	102.25	104.21
3	B	504	C0R	C16-C15-C14	-2.19	100.79	105.13
3	B	505	C0R	C2-C3-C4	-2.16	113.40	116.74
3	B	505	C0R	C7-C6-C5	-2.16	107.86	111.93
3	A	504	C0R	C8-C9-C11	-2.16	107.90	113.41
3	B	503	C0R	C1-C10-C5	2.15	112.69	108.75
2	B	501	HEM	CBA-CAA-C2A	-2.14	108.97	112.62
3	A	503	C0R	C12-C13-C14	2.14	109.40	106.94
3	A	502	C0R	C12-C11-C9	-2.13	109.69	112.60
3	A	503	C0R	C7-C8-C14	-2.12	108.45	112.08
3	B	502	C0R	C9-C10-C5	2.12	111.77	108.21
3	B	504	C0R	C19-C10-C1	-2.12	106.09	109.43
3	B	503	C0R	C2-C1-C10	2.11	117.42	113.45
3	B	503	C0R	C8-C9-C11	-2.10	108.04	113.41
3	B	502	C0R	C18-C13-C17	2.10	113.65	110.24
3	A	504	C0R	C10-C9-C8	2.10	116.98	113.63
3	B	504	C0R	C15-C16-C17	-2.07	101.89	105.30
3	A	502	C0R	C7-C8-C9	2.07	113.31	109.64
3	B	504	C0R	C2-C1-C10	2.06	117.32	113.45
3	A	504	C0R	C18-C13-C12	-2.05	107.69	110.76
3	A	505	C0R	C18-C13-C12	-2.05	107.70	110.76
3	A	505	C0R	C9-C8-C14	2.04	112.79	109.23
3	B	505	C0R	C18-C13-C12	-2.02	107.74	110.76
3	A	504	C0R	C7-C6-C5	-2.01	108.15	111.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	C0R	O3-C20-C21-O4
3	B	504	C0R	O3-C20-C21-O4
3	B	504	C0R	C17-C20-C21-O4
3	B	503	C0R	O3-C20-C21-O4
3	A	504	C0R	O3-C20-C21-O4
2	B	501	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	C0R	3	0
2	B	501	HEM	1	0
3	B	502	C0R	2	0
3	B	503	C0R	7	0
3	A	503	C0R	11	0
3	B	505	C0R	2	0
3	A	504	C0R	7	0
2	A	501	HEM	4	0
3	B	504	C0R	6	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 C0R A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R A 505

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R A 504

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand C0R B 504

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(Å²)	Q<0.9
1	A	391/410 (95%)	-0.53	2 (0%)	91	90	23, 36, 60, 109	0
1	B	389/410 (94%)	-0.19	9 (2%)	60	58	26, 42, 69, 99	0
All	All	780/820 (95%)	-0.36	11 (1%)	75	73	23, 39, 67, 109	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	GLU	5.2
1	B	22	ARG	4.0
1	B	21	GLU	3.1
1	B	43	GLU	2.9
1	B	20	GLU	2.7
1	B	405	HIS	2.5
1	B	406	HIS	2.4
1	B	27	SER	2.3
1	B	34	ASN	2.1
1	B	35	THR	2.1
1	A	19	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (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
3	C0R	A	503	25/25	0.73	0.28	61,77,89,94	0
3	C0R	A	504	25/25	0.81	0.22	47,79,98,101	0
3	C0R	B	503	25/25	0.81	0.19	47,61,74,79	0
3	C0R	B	504	25/25	0.84	0.21	55,77,92,99	0
3	C0R	A	502	25/25	0.89	0.14	37,44,54,58	0
3	C0R	A	505	25/25	0.89	0.13	45,54,59,75	0
3	C0R	B	502	25/25	0.92	0.13	32,41,47,48	0
3	C0R	B	505	25/25	0.93	0.13	41,47,55,72	0
2	HEM	A	501	43/43	0.98	0.11	19,25,27,28	0
2	HEM	B	501	43/43	0.98	0.13	22,26,31,35	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.
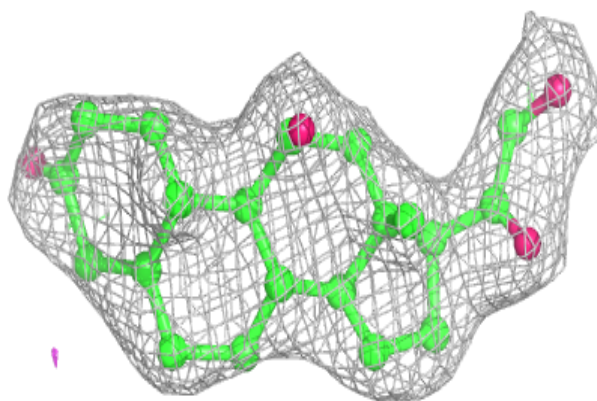

Electron density around C0R A 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
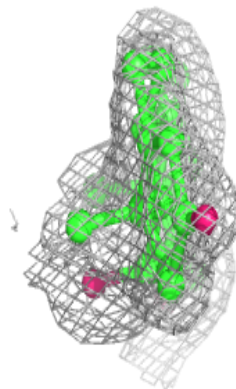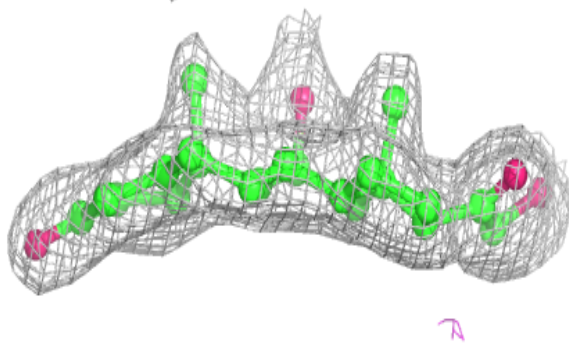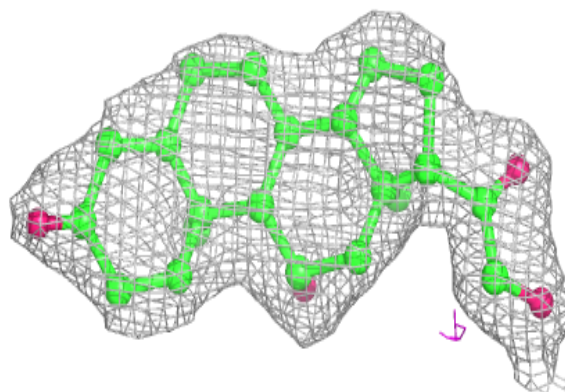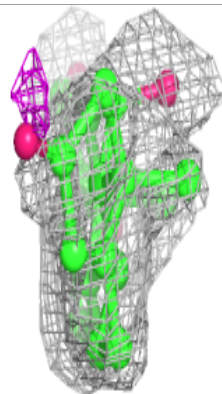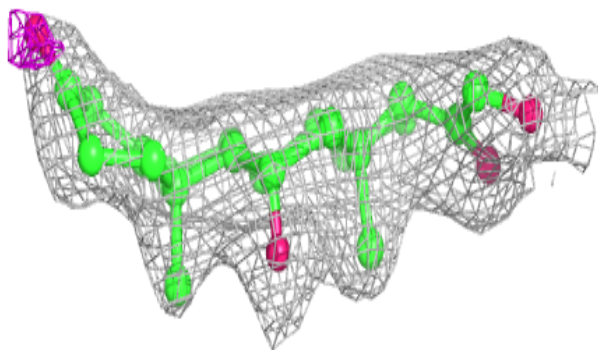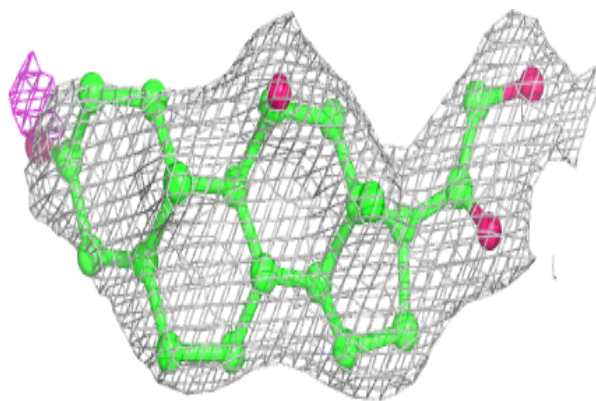mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
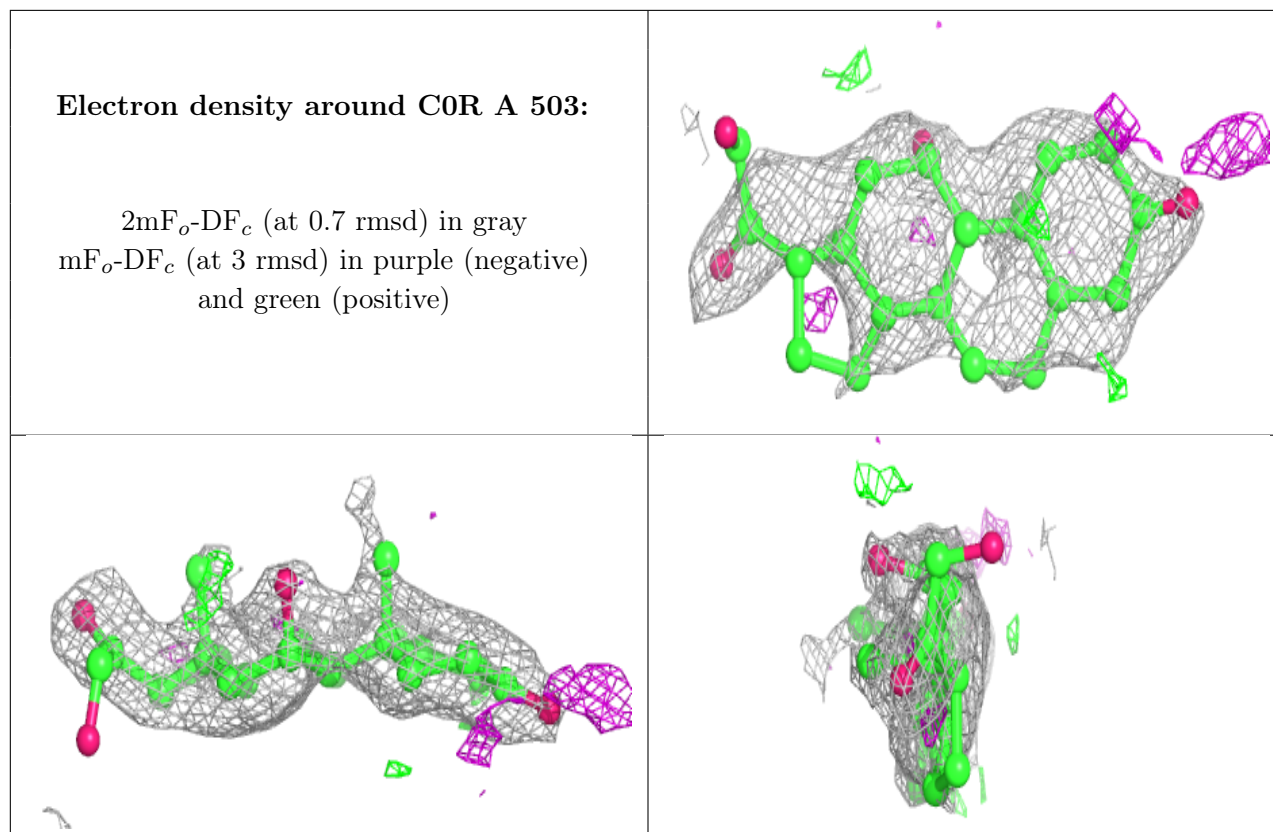
Electron density around C0R A 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
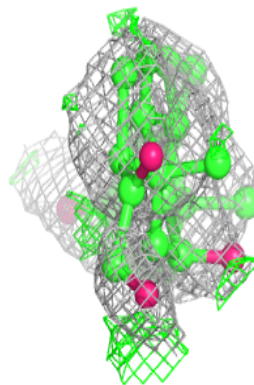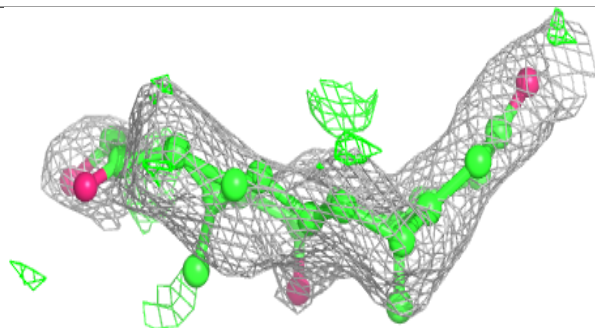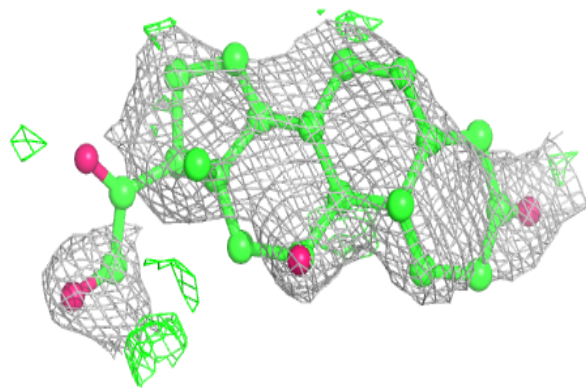
Electron density around C0R B 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
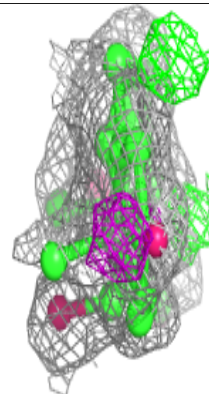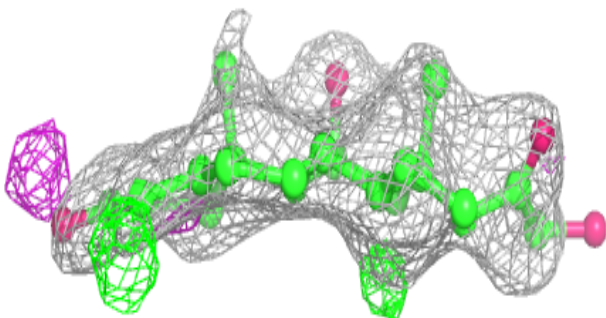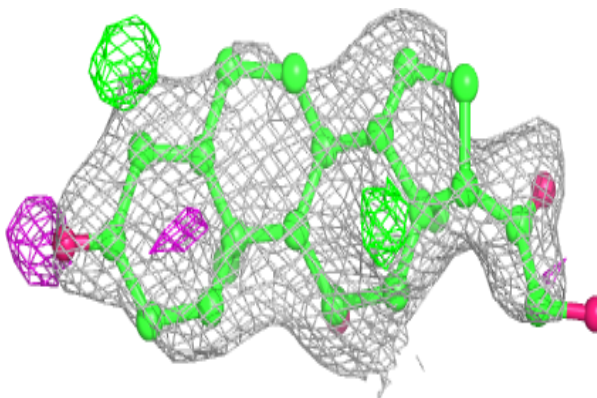
Electron density around C0R B 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
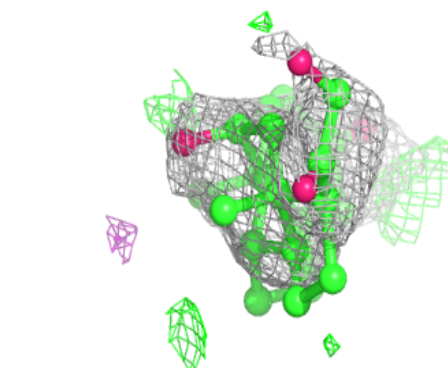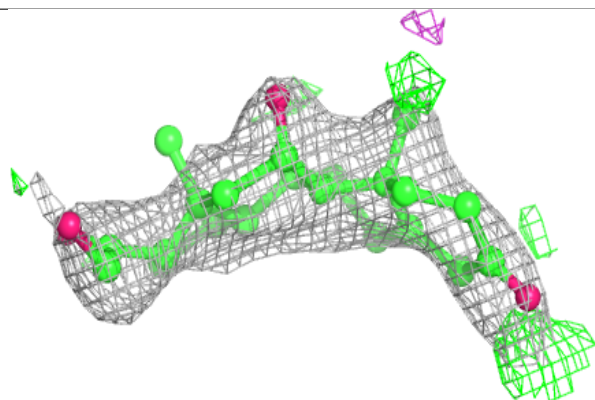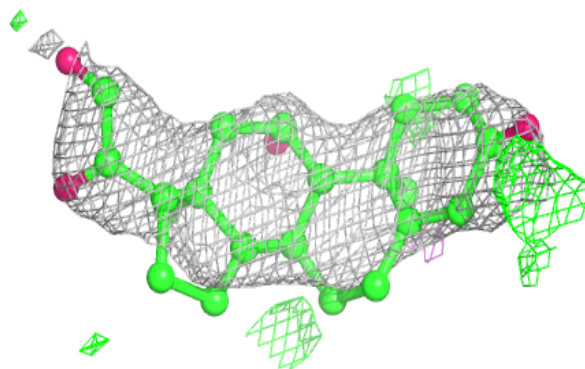
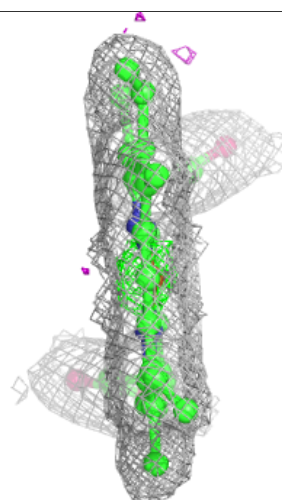

Electron density around C0R A 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
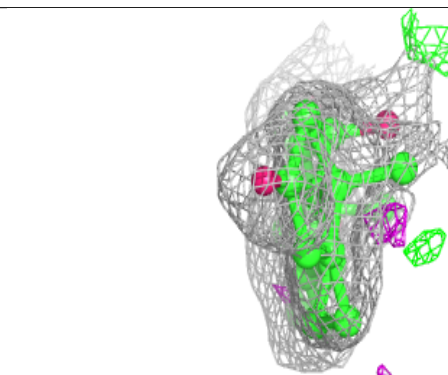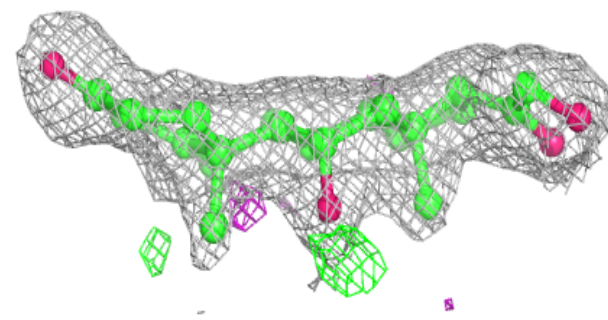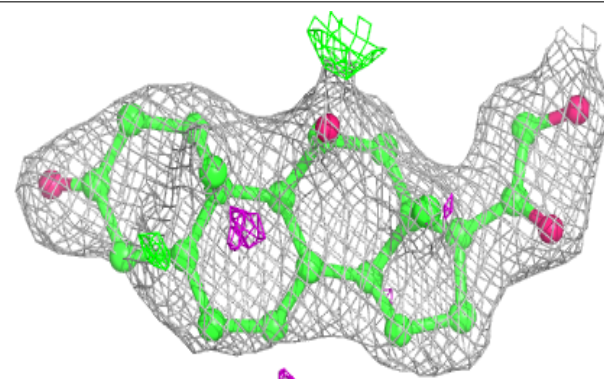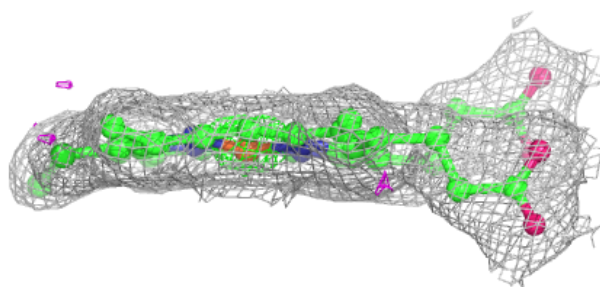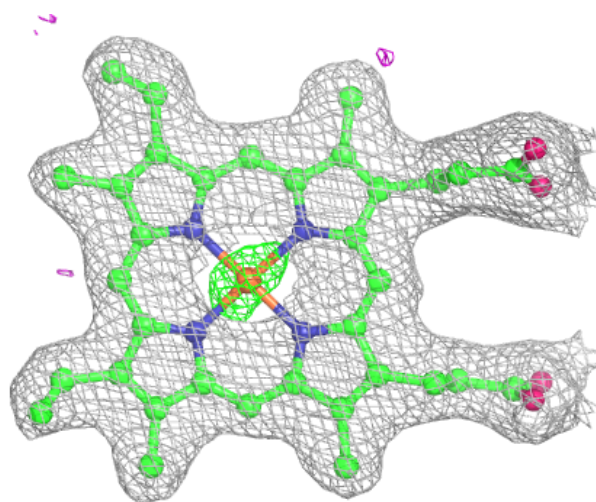
Electron density around C0R A 505:

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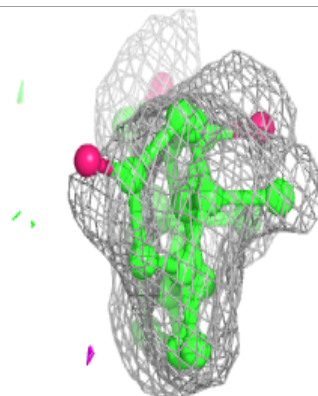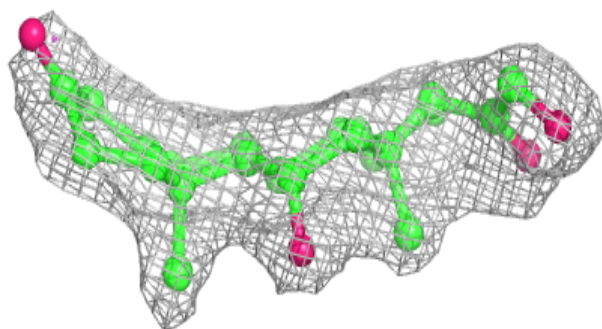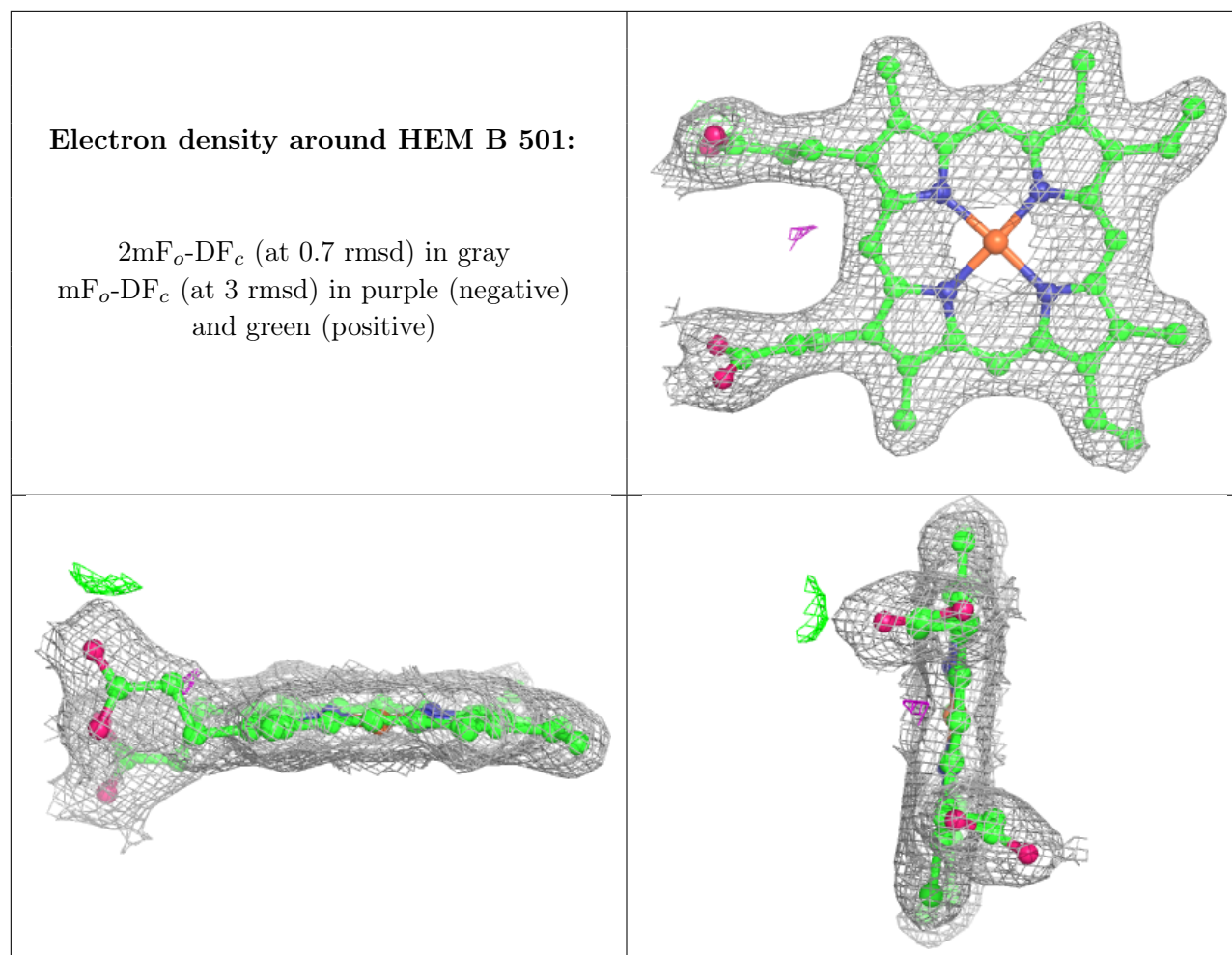

Electron density around C0R B 502:

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

Electron density around C0R B 505:

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

Electron density around HEM A 501:

$2mF_o$-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 B 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.