



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:43 AM UTC

PDB ID : 4B7G / pdb_00004b7g
Title : Structure of a bacterial catalase
Authors : Gumiero, A.; Walsh, M.
Deposited on : 2012-08-20
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

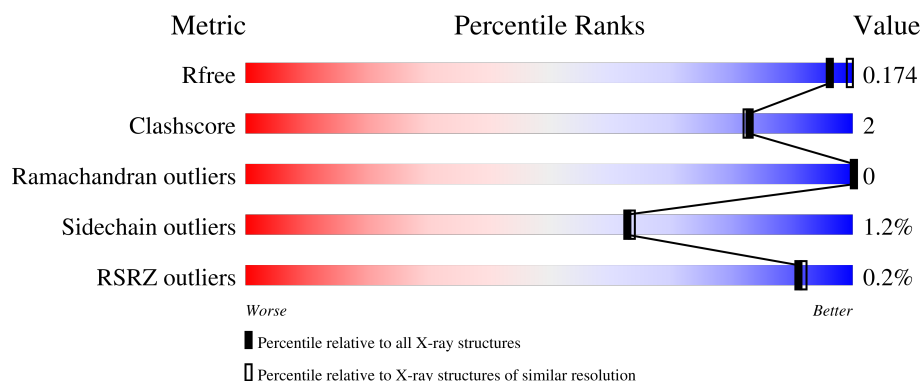
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

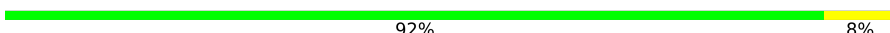
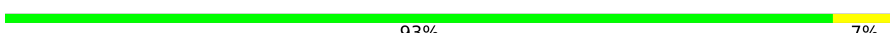
The reported resolution of this entry is 1.90 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	515	 92% 7%
1	B	515	 92% 8%
1	C	515	 93% 7%
1	D	515	 93% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19488 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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	8	0
			4178	2628	732	809	9			
1	B	514	Total	C	N	O	S	0	7	0
			4182	2628	736	809	9			
1	C	513	Total	C	N	O	S	0	5	0
			4160	2616	735	800	9			
1	D	514	Total	C	N	O	S	0	4	0
			4163	2617	735	802	9			

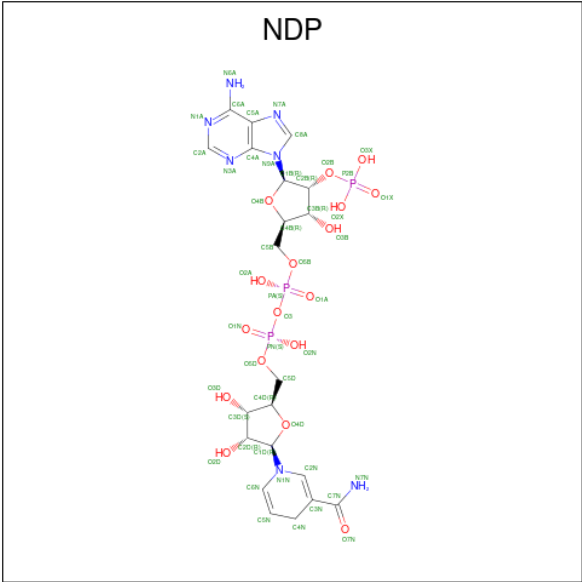
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ILE	LEU	conflict	UNP Q6M8A6
B	327	ILE	LEU	conflict	UNP Q6M8A6
C	327	ILE	LEU	conflict	UNP Q6M8A6
D	327	ILE	LEU	conflict	UNP Q6M8A6

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

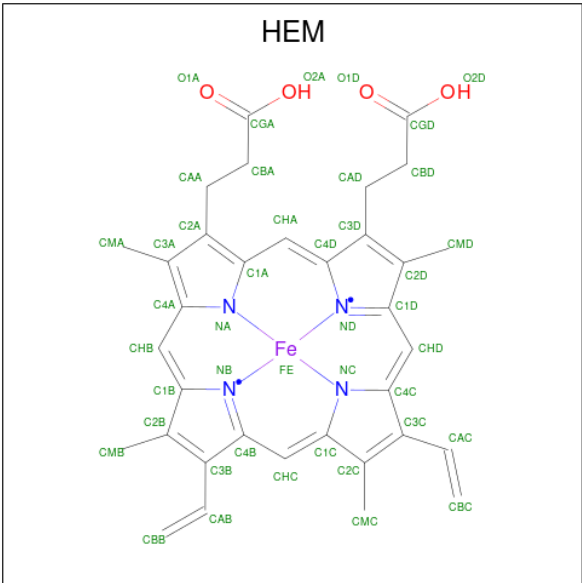
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
3	D	1	Total	C	N	O	P	0	1
			96	42	14	34	6		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

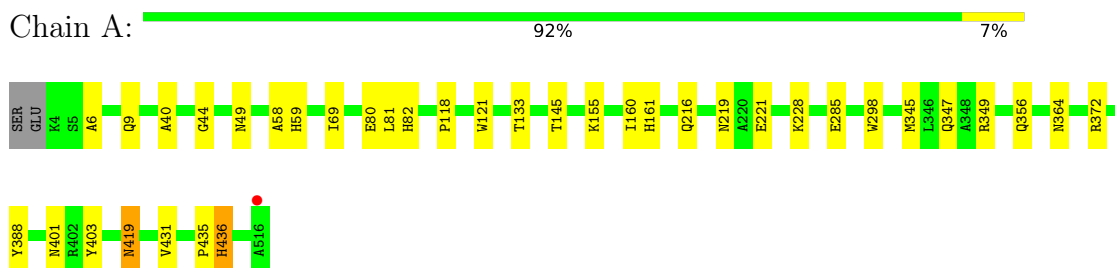
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	709	Total 709	O 709	0	0
5	B	591	Total 591	O 591	0	0
5	C	555	Total 555	O 555	0	0
5	D	488	Total 488	O 488	0	0

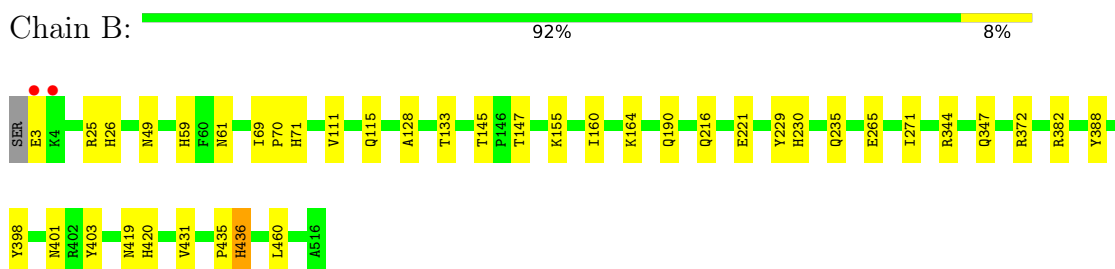
3 Residue-property plots

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.

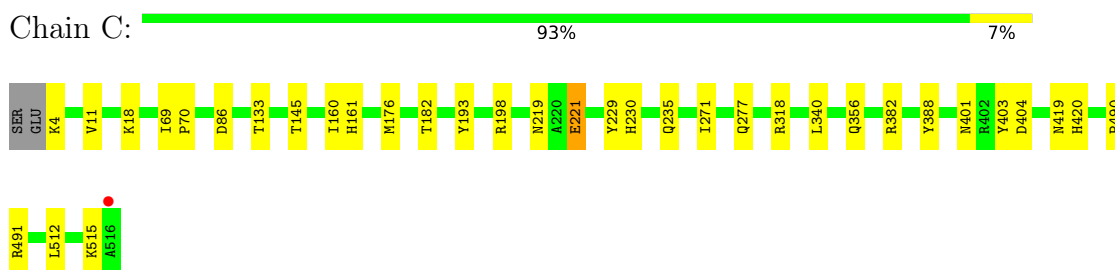
• Molecule 1: CATALASE



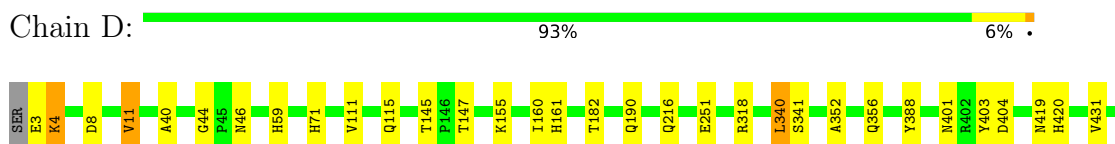
• Molecule 1: CATALASE



• Molecule 1: CATALASE



• Molecule 1: CATALASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	151.75Å 151.75Å 157.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 1.90 48.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.80-1.90) 99.5 (48.80-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.133 , 0.174 0.135 , 0.174	Depositor DCC
R_{free} test set	8067 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, HEM, CL

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	0.61	6/4318 (0.1%)	0.81	5/5866 (0.1%)
1	B	0.62	9/4313 (0.2%)	0.81	5/5859 (0.1%)
1	C	0.63	4/4291 (0.1%)	0.80	7/5829 (0.1%)
1	D	0.60	5/4291 (0.1%)	0.77	3/5829 (0.1%)
All	All	0.61	24/17213 (0.1%)	0.80	20/23383 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419	ASN	C-N	-24.56	1.01	1.33
1	D	419	ASN	C-N	-22.82	1.02	1.33
1	A	419	ASN	C-N	-17.63	1.10	1.33
1	B	419	ASN	C-N	-15.21	1.13	1.33
1	A	160	ILE	C-N	13.06	1.51	1.33
1	B	435	PRO	C-N	13.00	1.51	1.33
1	A	436	HIS	C-N	-11.33	1.17	1.33
1	C	420	HIS	C-N	-10.72	1.18	1.33
1	A	161	HIS	C-N	-10.15	1.20	1.33
1	B	436	HIS	C-N	-9.28	1.21	1.33
1	C	160	ILE	C-N	9.25	1.46	1.33
1	B	160	ILE	C-N	8.71	1.45	1.33
1	C	229	TYR	C-N	-8.50	1.23	1.33
1	B	229	TYR	C-N	-7.80	1.23	1.33
1	D	161	HIS	C-N	-7.55	1.23	1.33
1	B	420	HIS	C-N	-7.21	1.23	1.33
1	D	356	GLN	C-O	-6.90	1.15	1.24
1	B	26	HIS	C-N	-6.87	1.23	1.33
1	A	435	PRO	C-N	6.78	1.43	1.33
1	B	25	ARG	C-N	-6.50	1.25	1.33
1	B	230	HIS	C-N	-6.46	1.22	1.33
1	D	420	HIS	C-N	-6.10	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	ILE	C-N	5.72	1.41	1.33
1	A	58	ALA	C-N	-5.04	1.26	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	TYR	CA-C-N	10.22	137.52	122.39
1	B	229	TYR	C-N-CA	10.22	137.52	122.39
1	B	229	TYR	O-C-N	-9.07	112.64	123.16
1	A	161	HIS	O-C-N	-8.92	112.67	122.12
1	A	160	ILE	CA-C-N	-8.02	109.54	120.28
1	A	160	ILE	C-N-CA	-8.02	109.54	120.28
1	C	229	TYR	CA-C-N	7.51	133.50	122.39
1	C	229	TYR	C-N-CA	7.51	133.50	122.39
1	D	352	ALA	N-CA-C	6.00	118.61	111.71
1	D	419	ASN	CA-C-N	5.89	130.72	122.36
1	D	419	ASN	C-N-CA	5.89	130.72	122.36
1	C	420	HIS	O-C-N	-5.51	116.08	122.86
1	C	161	HIS	O-C-N	-5.43	116.36	122.12
1	B	435	PRO	CA-C-N	-5.37	114.62	123.05
1	B	435	PRO	C-N-CA	-5.37	114.62	123.05
1	C	229	TYR	O-C-N	-5.10	117.25	123.16
1	A	81	LEU	CA-C-N	5.09	130.18	123.05
1	A	81	LEU	C-N-CA	5.09	130.18	123.05
1	C	420	HIS	CA-C-N	5.00	128.65	121.50
1	C	420	HIS	C-N-CA	5.00	128.65	121.50

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	4178	0	3924	23	0
1	B	4182	0	3922	27	0
1	C	4160	0	3914	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4163	0	3912	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	1	0
3	C	96	0	52	4	0
3	D	96	0	52	3	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	1	0
5	A	709	0	0	5	0
5	B	591	0	0	4	0
5	C	555	0	0	3	0
5	D	488	0	0	6	0
All	All	19488	0	15948	80	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 2.

All (80) 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:B:401:ASN:HD22	1:B:403:TYR:H	1.15	0.93
1:B:216:GLN:HE22	1:B:431:VAL:H	1.08	0.91
1:D:216:GLN:HE22	1:D:431:VAL:H	1.17	0.89
1:A:401:ASN:HD22	1:A:403:TYR:H	1.14	0.89
1:C:69:ILE:H	1:C:356:GLN:HE22	1.15	0.88
1:A:216:GLN:HE22	1:A:431:VAL:H	1.16	0.88
1:C:401:ASN:HD22	1:C:403:TYR:H	1.23	0.86
1:D:401:ASN:HD22	1:D:403:TYR:H	1.19	0.85
1:A:69:ILE:H	1:A:356:GLN:HE22	1.26	0.83
1:B:235:GLN:HE22	1:B:271:ILE:H	1.34	0.74
1:A:82:HIS:HD2	5:A:2047:HOH:O	1.71	0.73
1:C:235:GLN:HE22	1:C:271:ILE:H	1.35	0.72
1:C:198:ARG:NH1	3:C:1517[B]:NDP:H72N	1.90	0.69
1:D:115:GLN:O	5:D:2141:HOH:O	2.11	0.67
3:D:1517[A]:NDP:O7N	5:D:2225:HOH:O	2.14	0.65
1:B:216:GLN:NE2	1:B:431:VAL:H	1.90	0.64
1:B:115[A]:GLN:O	5:B:2145:HOH:O	2.15	0.63
1:A:219:ASN:OD1	1:A:221[A]:GLU:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:OD1	5:A:2593:HOH:O	2.18	0.55
1:A:364:ASN:OD1	1:B:59:HIS:HE1	1.91	0.53
3:D:1517[B]:NDP:O3X	5:D:2226:HOH:O	2.17	0.52
1:B:265:GLU:OE1	5:B:2347:HOH:O	2.19	0.52
1:C:86:ASP:OD2	5:C:2113:HOH:O	2.19	0.51
1:B:401:ASN:HD22	1:B:403:TYR:N	1.97	0.51
1:C:235:GLN:NE2	1:C:271:ILE:H	2.08	0.50
1:C:491[A]:ARG:HG3	5:C:2524:HOH:O	2.12	0.50
1:A:372:ARG:NH2	5:A:2498:HOH:O	2.33	0.48
1:C:388[B]:TYR:CZ	1:D:388[B]:TYR:HB2	2.48	0.48
1:D:251:GLU:OE2	5:D:2271:HOH:O	2.20	0.48
1:A:388[B]:TYR:HB2	1:B:388[B]:TYR:CZ	2.49	0.48
4:D:3003:HEM:HMC1	4:D:3003:HEM:HBC2	1.94	0.48
1:D:11:VAL:HG13	1:D:318:ARG:HG2	1.95	0.47
1:A:82:HIS:CD2	5:A:2047:HOH:O	2.55	0.47
1:C:18:LYS:HZ1	1:D:404:ASP:HB2	1.78	0.47
1:B:147:THR:HG23	1:B:190:GLN:HE21	1.80	0.47
1:A:228:LYS:HE2	1:A:298:TRP:CE2	2.50	0.47
1:D:401:ASN:HD22	1:D:403:TYR:N	2.00	0.46
1:C:193:TYR:CD2	3:C:1517[B]:NDP:H2A	2.51	0.46
3:D:1517[A]:NDP:O1X	5:D:2226:HOH:O	2.20	0.46
1:A:401:ASN:HD22	1:A:403:TYR:N	1.97	0.46
1:C:193:TYR:CD2	3:C:1517[A]:NDP:H2A	2.51	0.46
1:D:4:LYS:HB2	1:D:8:ASP:OD2	2.15	0.46
1:C:198:ARG:HH12	3:C:1517[B]:NDP:H72N	1.61	0.46
1:D:71:HIS:CE1	1:D:111:VAL:HG22	2.50	0.46
1:C:382:ARG:O	1:D:59:HIS:HE1	1.99	0.46
1:C:490:PRO:HG2	5:C:2524:HOH:O	2.16	0.46
1:B:460:LEU:HD13	3:B:1517:NDP:H1D	1.98	0.46
1:B:69:ILE:HG13	1:B:164:LYS:HE3	1.98	0.45
1:B:235:GLN:NE2	1:B:271:ILE:H	2.09	0.45
1:B:398:TYR:CE1	1:C:176:MET:HG3	2.52	0.45
1:A:345:MET:O	1:A:349:ARG:HG3	2.17	0.45
1:C:230:HIS:HE1	1:C:277:GLN:OE1	2.01	0.44
1:A:59:HIS:HE1	1:B:382:ARG:O	2.00	0.44
5:A:2515:HOH:O	1:B:59:HIS:HD2	2.00	0.44
1:C:11:VAL:HG22	1:C:318:ARG:HG2	1.99	0.44
1:D:340:LEU:HB3	1:D:341:SER:H	1.67	0.44
1:C:182:THR:HB	1:C:491[B]:ARG:HG2	2.00	0.43
1:B:436:HIS:HD2	5:B:2503:HOH:O	2.02	0.42
1:D:40:ALA:O	1:D:44:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:HD21	1:B:347:GLN:CB	2.33	0.42
1:A:388[A]:TYR:CZ	1:B:388[A]:TYR:HB2	2.54	0.42
1:B:61:ASN:ND2	5:B:2046:HOH:O	2.52	0.42
1:B:69:ILE:HA	1:B:70:PRO:HA	1.86	0.42
1:B:128:ALA:HB2	4:B:3001:HEM:HMD3	2.01	0.42
1:A:285[A]:GLU:OE2	1:A:436:HIS:HE1	2.03	0.42
1:A:401:ASN:ND2	1:A:403:TYR:H	1.97	0.42
1:C:219:ASN:OD1	1:C:221:GLU:HG2	2.21	0.41
1:A:40:ALA:O	1:A:44:GLY:HA3	2.19	0.41
1:A:118:PRO:HD2	1:A:121:TRP:CE2	2.55	0.41
1:D:147:THR:HG23	1:D:190:GLN:HE21	1.86	0.41
1:D:182:THR:HB	1:D:491:ARG:HG2	2.02	0.41
1:A:6:ALA:HB3	1:A:80:GLU:HG2	2.02	0.41
1:D:3:GLU:OE1	5:D:2001:HOH:O	2.21	0.41
1:B:344:ARG:HG2	1:D:46:ASN:HD21	1.84	0.41
1:A:388[B]:TYR:OH	1:B:372:ARG:NH1	2.54	0.41
1:A:347:GLN:CB	1:B:49:ASN:HD21	2.34	0.40
1:C:69:ILE:HA	1:C:70:PRO:HA	1.89	0.40
1:B:216:GLN:HE22	1:B:431:VAL:N	1.93	0.40
1:C:512:LEU:HD23	1:C:512:LEU:HA	1.92	0.40
1:B:71:HIS:CE1	1:B:111:VAL:HG22	2.57	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	519/515 (101%)	499 (96%)	20 (4%)	0	100	100
1	B	519/515 (101%)	499 (96%)	20 (4%)	0	100	100
1	C	516/515 (100%)	493 (96%)	23 (4%)	0	100	100
1	D	516/515 (100%)	494 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2070/2060 (100%)	1985 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	442/436 (101%)	438 (99%)	4 (1%)	70	73
1	B	441/436 (101%)	436 (99%)	5 (1%)	65	67
1	C	439/436 (101%)	432 (98%)	7 (2%)	55	54
1	D	439/436 (101%)	434 (99%)	5 (1%)	65	67
All	All	1761/1744 (101%)	1740 (99%)	21 (1%)	63	63

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	133	THR
1	A	145	THR
1	A	155	LYS
1	B	3	GLU
1	B	133	THR
1	B	145	THR
1	B	155	LYS
1	B	221	GLU
1	C	4	LYS
1	C	133	THR
1	C	145	THR
1	C	221	GLU
1	C	340	LEU
1	C	404	ASP
1	C	515	LYS
1	D	4	LYS

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Mol	Chain	Res	Type
1	D	11	VAL
1	D	145	THR
1	D	155	LYS
1	D	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	49	ASN
1	A	61	ASN
1	A	82	HIS
1	A	115	GLN
1	A	216	GLN
1	A	300	GLN
1	A	316	ASN
1	A	356	GLN
1	A	401	ASN
1	A	436	HIS
1	A	498	ASN
1	B	49	ASN
1	B	59	HIS
1	B	61	ASN
1	B	190	GLN
1	B	216	GLN
1	B	230	HIS
1	B	235	GLN
1	B	277	GLN
1	B	316	ASN
1	B	401	ASN
1	B	420	HIS
1	B	425	GLN
1	B	436	HIS
1	B	498	ASN
1	C	9	GLN
1	C	22	ASN
1	C	49	ASN
1	C	61	ASN
1	C	75	HIS
1	C	190	GLN
1	C	230	HIS
1	C	235	GLN

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Mol	Chain	Res	Type
1	C	316	ASN
1	C	356	GLN
1	C	401	ASN
1	C	498	ASN
1	D	49	ASN
1	D	61	ASN
1	D	190	GLN
1	D	216	GLN
1	D	230	HIS
1	D	316	ASN
1	D	401	ASN
1	D	425	GLN
1	D	498	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
3	NDP	D	1517[A]	-	51,52,52	1.48	7 (13%)	71,80,80	1.57	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	A	1518	-	51,52,52	1.52	7 (13%)	71,80,80	1.56	10 (14%)
3	NDP	C	1517[B]	-	51,52,52	1.48	7 (13%)	71,80,80	1.60	10 (14%)
4	HEM	C	3002	1,5	50,50,50	1.73	9 (18%)	67,82,82	1.35	6 (8%)
4	HEM	D	3003	1,5	50,50,50	1.76	10 (20%)	67,82,82	1.31	4 (5%)
3	NDP	D	1517[B]	-	51,52,52	1.55	7 (13%)	71,80,80	1.58	10 (14%)
4	HEM	B	3001	1	50,50,50	1.76	9 (18%)	67,82,82	1.40	5 (7%)
3	NDP	C	1517[A]	-	51,52,52	1.47	7 (13%)	71,80,80	1.62	10 (14%)
4	HEM	A	3000	1	50,50,50	1.75	9 (18%)	67,82,82	1.41	6 (8%)
3	NDP	B	1517	-	51,52,52	1.54	7 (13%)	71,80,80	1.62	11 (15%)

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	NDP	D	1517[A]	-	-	12/34/77/77	0/5/5/5
3	NDP	A	1518	-	-	9/34/77/77	0/5/5/5
3	NDP	C	1517[B]	-	-	9/34/77/77	0/5/5/5
4	HEM	C	3002	1,5	-	3/14/54/54	-
4	HEM	D	3003	1,5	-	4/14/54/54	-
3	NDP	D	1517[B]	-	-	10/34/77/77	0/5/5/5
4	HEM	B	3001	1	-	3/14/54/54	-
3	NDP	C	1517[A]	-	-	11/34/77/77	0/5/5/5
4	HEM	A	3000	1	-	3/14/54/54	-
3	NDP	B	1517	-	-	8/34/77/77	0/5/5/5

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1517	NDP	O7N-C7N	7.41	1.41	1.24
4	A	3000	HEM	C3D-C2D	7.31	1.52	1.36
3	D	1517[A]	NDP	O7N-C7N	7.27	1.41	1.24
4	C	3002	HEM	C3D-C2D	7.25	1.52	1.36
3	C	1517[B]	NDP	O7N-C7N	7.25	1.41	1.24
3	A	1518	NDP	O7N-C7N	7.22	1.41	1.24
4	D	3003	HEM	C3D-C2D	7.20	1.52	1.36
4	B	3001	HEM	C3D-C2D	7.18	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1517[B]	NDP	O7N-C7N	7.18	1.41	1.24
3	C	1517[A]	NDP	O7N-C7N	7.01	1.40	1.24
4	B	3001	HEM	FE-NC	4.56	2.10	1.95
4	A	3000	HEM	FE-ND	4.36	2.08	1.94
4	D	3003	HEM	FE-NB	3.94	2.07	1.94
4	A	3000	HEM	FE-NA	3.64	2.07	1.95
4	B	3001	HEM	FE-ND	3.59	2.06	1.94
4	C	3002	HEM	FE-NC	3.57	2.06	1.95
4	D	3003	HEM	FE-NA	3.54	2.06	1.95
4	C	3002	HEM	FE-NB	3.20	2.04	1.94
4	D	3003	HEM	FE-NC	3.19	2.05	1.95
4	B	3001	HEM	CAB-C3B	3.11	1.55	1.47
4	A	3000	HEM	FE-NB	3.11	2.04	1.94
4	C	3002	HEM	CAB-C3B	3.10	1.55	1.47
4	B	3001	HEM	FE-NB	3.00	2.04	1.94
3	A	1518	NDP	PN-O3	2.99	1.62	1.59
4	D	3003	HEM	CAC-C3C	2.96	1.55	1.47
3	D	1517[B]	NDP	PN-O3	2.95	1.62	1.59
4	D	3003	HEM	CAB-C3B	2.92	1.55	1.47
4	C	3002	HEM	FE-ND	2.90	2.03	1.94
3	B	1517	NDP	PN-O3	2.90	1.62	1.59
4	C	3002	HEM	CAC-C3C	2.89	1.55	1.47
3	D	1517[B]	NDP	C2A-N3A	2.82	1.39	1.33
3	D	1517[B]	NDP	C2A-N1A	2.82	1.38	1.33
3	A	1518	NDP	C2A-N3A	2.81	1.38	1.33
4	B	3001	HEM	FE-NA	2.78	2.04	1.95
4	A	3000	HEM	CAC-C3C	2.77	1.54	1.47
3	C	1517[A]	NDP	C2A-N1A	2.75	1.38	1.33
3	A	1518	NDP	C2A-N1A	2.75	1.38	1.33
3	B	1517	NDP	C2A-N3A	2.72	1.38	1.33
4	B	3001	HEM	CAC-C3C	2.72	1.54	1.47
3	B	1517	NDP	C2A-N1A	2.70	1.38	1.33
3	D	1517[B]	NDP	PA-O3	2.69	1.62	1.59
3	C	1517[B]	NDP	C2A-N1A	2.67	1.38	1.33
3	D	1517[A]	NDP	C2A-N3A	2.66	1.38	1.33
4	A	3000	HEM	CAB-C3B	2.64	1.54	1.47
3	B	1517	NDP	PA-O3	2.61	1.62	1.59
3	D	1517[A]	NDP	C2A-N1A	2.61	1.38	1.33
3	C	1517[B]	NDP	C2A-N3A	2.61	1.38	1.33
4	C	3002	HEM	FE-NA	2.59	2.03	1.95
3	A	1518	NDP	PA-O3	2.58	1.62	1.59
3	C	1517[A]	NDP	C2A-N3A	2.57	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	HEM	CMC-C2C	2.48	1.55	1.50
3	C	1517[B]	NDP	PN-O3	2.45	1.62	1.59
4	D	3003	HEM	FE-ND	2.43	2.02	1.94
3	C	1517[A]	NDP	PN-O3	2.41	1.62	1.59
3	D	1517[A]	NDP	PN-O3	2.40	1.62	1.59
4	A	3000	HEM	FE-NC	2.36	2.02	1.95
4	B	3001	HEM	CMC-C2C	2.33	1.55	1.50
4	D	3003	HEM	CMC-C2C	2.33	1.55	1.50
3	B	1517	NDP	C6N-C5N	2.33	1.40	1.33
3	D	1517[B]	NDP	C8A-N7A	2.31	1.36	1.31
3	D	1517[A]	NDP	PA-O3	2.31	1.62	1.59
4	C	3002	HEM	CMC-C2C	2.30	1.55	1.50
3	C	1517[A]	NDP	C8A-N7A	2.29	1.36	1.31
3	B	1517	NDP	C8A-N7A	2.27	1.36	1.31
3	C	1517[B]	NDP	C8A-N7A	2.25	1.36	1.31
3	D	1517[B]	NDP	C6N-C5N	2.24	1.39	1.33
3	C	1517[A]	NDP	PA-O3	2.22	1.61	1.59
4	C	3002	HEM	CMB-C2B	2.21	1.55	1.50
3	A	1518	NDP	C6N-C5N	2.21	1.39	1.33
3	C	1517[A]	NDP	C6N-C5N	2.21	1.39	1.33
3	A	1518	NDP	C8A-N7A	2.20	1.35	1.31
4	B	3001	HEM	CMB-C2B	2.20	1.55	1.50
3	C	1517[B]	NDP	C6N-C5N	2.18	1.39	1.33
3	C	1517[B]	NDP	PA-O3	2.17	1.61	1.59
3	D	1517[A]	NDP	C8A-N7A	2.17	1.35	1.31
4	D	3003	HEM	CMA-C3A	2.09	1.55	1.50
3	D	1517[A]	NDP	C6N-C5N	2.06	1.39	1.33
4	D	3003	HEM	CMB-C2B	2.04	1.55	1.50
4	A	3000	HEM	CMB-C2B	2.01	1.54	1.50

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3000	HEM	C4D-ND-C1D	5.63	111.88	105.21
4	B	3001	HEM	C4D-ND-C1D	5.61	111.84	105.21
3	B	1517	NDP	N3A-C2A-N1A	-5.60	120.11	128.58
3	D	1517[A]	NDP	N3A-C2A-N1A	-5.59	120.11	128.58
3	D	1517[B]	NDP	N3A-C2A-N1A	-5.53	120.21	128.58
3	C	1517[B]	NDP	N3A-C2A-N1A	-5.41	120.39	128.58
3	C	1517[A]	NDP	N3A-C2A-N1A	-5.38	120.44	128.58
3	A	1518	NDP	N3A-C2A-N1A	-5.26	120.62	128.58
4	C	3002	HEM	C4D-ND-C1D	5.04	111.18	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3003	HEM	C4D-ND-C1D	4.92	111.03	105.21
3	C	1517[A]	NDP	O4B-C1B-N9A	4.83	117.36	108.09
3	A	1518	NDP	C5A-C4A-N3A	-4.62	120.36	126.72
3	D	1517[B]	NDP	C5A-C4A-N3A	-4.56	120.43	126.72
3	D	1517[A]	NDP	C5A-C4A-N3A	-4.55	120.44	126.72
3	C	1517[B]	NDP	O4B-C1B-N9A	4.51	116.75	108.09
3	B	1517	NDP	C5A-C4A-N3A	-4.36	120.71	126.72
3	B	1517	NDP	N9A-C8A-N7A	-4.34	107.78	113.94
3	C	1517[B]	NDP	C5A-C4A-N3A	-4.16	120.98	126.72
3	C	1517[A]	NDP	C5A-C4A-N3A	-4.16	120.99	126.72
3	A	1518	NDP	O4B-C1B-N9A	4.15	116.06	108.09
3	A	1518	NDP	N9A-C8A-N7A	-4.09	108.14	113.94
3	C	1517[A]	NDP	N9A-C8A-N7A	-4.06	108.17	113.94
3	C	1517[B]	NDP	N9A-C8A-N7A	-4.06	108.17	113.94
3	D	1517[A]	NDP	N9A-C8A-N7A	-3.97	108.31	113.94
3	D	1517[B]	NDP	N9A-C8A-N7A	-3.93	108.35	113.94
3	B	1517	NDP	C5A-N7A-C8A	3.65	109.19	103.45
3	A	1518	NDP	C5A-N7A-C8A	3.65	109.18	103.45
4	B	3001	HEM	CAD-CBD-CGD	-3.57	104.19	113.67
3	B	1517	NDP	O4B-C1B-N9A	3.56	114.93	108.09
3	C	1517[B]	NDP	C5A-N7A-C8A	3.51	108.97	103.45
3	C	1517[A]	NDP	C5A-N7A-C8A	3.51	108.97	103.45
3	D	1517[A]	NDP	C5A-N7A-C8A	3.50	108.95	103.45
3	D	1517[B]	NDP	C5A-N7A-C8A	3.49	108.93	103.45
3	D	1517[B]	NDP	O4B-C1B-N9A	3.47	114.75	108.09
3	D	1517[A]	NDP	C2A-N3A-C4A	3.44	120.23	111.83
4	C	3002	HEM	CAD-CBD-CGD	-3.44	104.54	113.67
3	D	1517[B]	NDP	C2A-N3A-C4A	3.44	120.22	111.83
4	D	3003	HEM	CAD-CBD-CGD	-3.42	104.59	113.67
3	B	1517	NDP	C2A-N3A-C4A	3.37	120.06	111.83
3	A	1518	NDP	C2A-N3A-C4A	3.36	120.04	111.83
4	A	3000	HEM	CAD-CBD-CGD	-3.30	104.92	113.67
3	C	1517[A]	NDP	C2A-N3A-C4A	3.23	119.72	111.83
3	C	1517[B]	NDP	C2A-N3A-C4A	3.22	119.69	111.83
3	D	1517[A]	NDP	O4B-C1B-N9A	3.15	114.15	108.09
3	D	1517[B]	NDP	N3A-C4A-N9A	2.94	132.17	127.17
3	D	1517[A]	NDP	N3A-C4A-N9A	2.93	132.14	127.17
3	A	1518	NDP	N3A-C4A-N9A	2.91	132.12	127.17
3	B	1517	NDP	N3A-C4A-N9A	2.82	131.96	127.17
3	A	1518	NDP	C4A-C5A-N7A	-2.74	107.45	110.58
3	B	1517	NDP	C4A-C5A-N7A	-2.66	107.54	110.58
4	B	3001	HEM	CHD-C1D-ND	2.64	127.26	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1517[A]	NDP	C4A-C5A-N7A	-2.59	107.62	110.58
3	C	1517[B]	NDP	N3A-C4A-N9A	2.58	131.55	127.17
3	C	1517[B]	NDP	C4A-C5A-N7A	-2.57	107.64	110.58
3	B	1517	NDP	O2A-PA-O3	2.57	114.23	107.27
4	D	3003	HEM	CHD-C1D-ND	2.56	127.18	124.42
3	C	1517[A]	NDP	N3A-C4A-N9A	2.55	131.51	127.17
3	D	1517[B]	NDP	C4A-C5A-N7A	-2.53	107.68	110.58
3	D	1517[A]	NDP	C4A-C5A-N7A	-2.53	107.69	110.58
4	C	3002	HEM	C3B-C2B-C1B	2.48	108.27	106.41
4	B	3001	HEM	CAD-C3D-C4D	2.47	129.00	124.70
4	C	3002	HEM	CAD-C3D-C4D	2.34	128.78	124.70
4	B	3001	HEM	C3D-C4D-ND	-2.33	107.62	110.17
3	B	1517	NDP	C3D-C2D-C1D	2.31	105.83	101.46
3	B	1517	NDP	C4A-N9A-C8A	2.30	108.15	105.74
3	C	1517[B]	NDP	C3D-C2D-C1D	2.25	105.72	101.46
4	D	3003	HEM	CAD-C3D-C4D	2.22	128.56	124.70
3	C	1517[B]	NDP	O2A-PA-O3	2.21	113.24	107.27
4	A	3000	HEM	C3D-C4D-ND	-2.18	107.78	110.17
4	C	3002	HEM	CMD-C2D-C1D	2.18	128.43	125.03
4	A	3000	HEM	C2A-C1A-NA	-2.16	107.75	110.15
3	D	1517[B]	NDP	C3D-C2D-C1D	2.15	105.52	101.46
4	A	3000	HEM	CBD-CAD-C3D	-2.15	106.60	112.53
3	D	1517[A]	NDP	O2A-PA-O3	2.14	113.07	107.27
3	C	1517[A]	NDP	C3D-C2D-C1D	2.14	105.51	101.46
3	C	1517[A]	NDP	O2A-PA-O3	2.14	113.06	107.27
4	C	3002	HEM	CHD-C1D-ND	2.12	126.70	124.42
3	A	1518	NDP	C6A-C5A-C4A	2.11	120.06	117.18
4	A	3000	HEM	C3B-C2B-C1B	2.09	107.98	106.41
3	D	1517[A]	NDP	P2B-O2B-C2B	-2.05	117.96	123.43
3	D	1517[B]	NDP	O2A-PA-O3	2.04	112.79	107.27
3	A	1518	NDP	C3D-C2D-C1D	2.02	105.28	101.46

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1518	NDP	C2N-C3N-C7N-O7N
3	C	1517[A]	NDP	C5D-O5D-PN-O3
3	C	1517[A]	NDP	C5D-O5D-PN-O1N
3	C	1517[A]	NDP	C2N-C3N-C7N-O7N
3	C	1517[A]	NDP	C2N-C3N-C7N-N7N
3	D	1517[A]	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	D	1517[A]	NDP	C5D-O5D-PN-O1N
3	D	1517[B]	NDP	C5D-O5D-PN-O2N
3	D	1517[B]	NDP	C2N-C3N-C7N-O7N
3	D	1517[B]	NDP	C2N-C3N-C7N-N7N
3	C	1517[B]	NDP	C2D-C1D-N1N-C2N
3	D	1517[A]	NDP	C2D-C1D-N1N-C2N
3	A	1518	NDP	C2B-C1B-N9A-C8A
3	A	1518	NDP	C2N-C3N-C7N-N7N
3	B	1517	NDP	C2B-C1B-N9A-C8A
3	C	1517[A]	NDP	C2B-C1B-N9A-C8A
3	C	1517[B]	NDP	C2B-C1B-N9A-C8A
3	D	1517[A]	NDP	C2B-C1B-N9A-C8A
3	D	1517[B]	NDP	C2B-C1B-N9A-C8A
3	D	1517[B]	NDP	C2D-C1D-N1N-C6N
3	C	1517[B]	NDP	O4D-C1D-N1N-C2N
3	A	1518	NDP	PA-O3-PN-O1N
3	D	1517[A]	NDP	O4D-C1D-N1N-C2N
3	C	1517[A]	NDP	C2D-C1D-N1N-C6N
3	B	1517	NDP	C5B-O5B-PA-O1A
3	B	1517	NDP	C5D-O5D-PN-O3
3	C	1517[A]	NDP	C5B-O5B-PA-O1A
3	C	1517[B]	NDP	C5B-O5B-PA-O1A
3	C	1517[B]	NDP	C5D-O5D-PN-O1N
3	D	1517[A]	NDP	C5B-O5B-PA-O1A
3	D	1517[A]	NDP	C5D-O5D-PN-O2N
3	D	1517[B]	NDP	C5D-O5D-PN-O3
3	D	1517[B]	NDP	C5D-O5D-PN-O1N
3	C	1517[A]	NDP	O4D-C1D-N1N-C6N
3	D	1517[B]	NDP	O4D-C1D-N1N-C6N
3	A	1518	NDP	C2D-C1D-N1N-C6N
3	A	1518	NDP	C2B-C1B-N9A-C4A
3	B	1517	NDP	C2B-C1B-N9A-C4A
3	C	1517[B]	NDP	C2B-C1B-N9A-C4A
3	D	1517[A]	NDP	C2B-C1B-N9A-C4A
3	D	1517[B]	NDP	C2B-C1B-N9A-C4A
3	A	1518	NDP	O4D-C1D-N1N-C6N
3	B	1517	NDP	O4D-C1D-N1N-C6N
4	C	3002	HEM	CAD-CBD-CGD-O1D
3	C	1517[A]	NDP	C2B-C1B-N9A-C4A
4	A	3000	HEM	CAD-CBD-CGD-O1D
4	A	3000	HEM	CAD-CBD-CGD-O2D
4	B	3001	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
4	C	3002	HEM	CAD-CBD-CGD-O2D
4	D	3003	HEM	CAD-CBD-CGD-O2D
4	B	3001	HEM	CAD-CBD-CGD-O1D
3	C	1517[A]	NDP	PA-O3-PN-O2N
3	D	1517[A]	NDP	PA-O3-PN-O2N
4	D	3003	HEM	CAD-CBD-CGD-O1D
3	B	1517	NDP	C2D-C1D-N1N-C6N
3	B	1517	NDP	O4B-C1B-N9A-C8A
3	D	1517[A]	NDP	O4D-C1D-N1N-C6N
4	D	3003	HEM	CAA-CBA-CGA-O1A
3	D	1517[A]	NDP	O4B-C1B-N9A-C8A
3	D	1517[B]	NDP	O4B-C1B-N9A-C8A
3	D	1517[A]	NDP	C2D-C1D-N1N-C6N
3	A	1518	NDP	PA-O3-PN-O2N
3	C	1517[B]	NDP	PA-O3-PN-O2N
3	A	1518	NDP	O4B-C1B-N9A-C8A
3	C	1517[A]	NDP	O4B-C1B-N9A-C8A
3	C	1517[B]	NDP	O4B-C1B-N9A-C8A
4	D	3003	HEM	CAA-CBA-CGA-O2A
4	B	3001	HEM	CAA-CBA-CGA-O1A
3	C	1517[B]	NDP	C2N-C3N-C7N-O7N
4	C	3002	HEM	CAA-CBA-CGA-O1A
4	A	3000	HEM	CAA-CBA-CGA-O2A
3	B	1517	NDP	PA-O3-PN-O2N

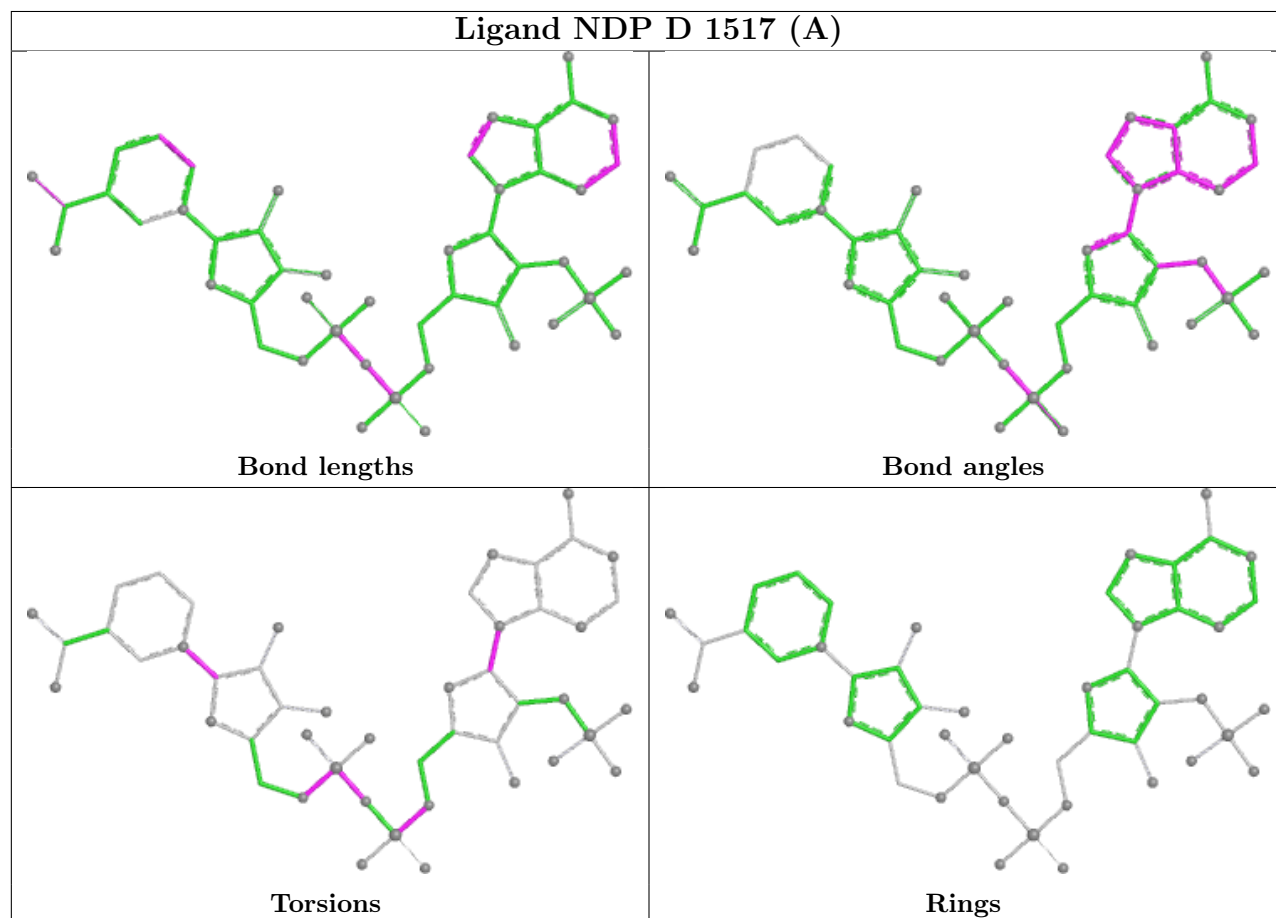
There are no ring outliers.

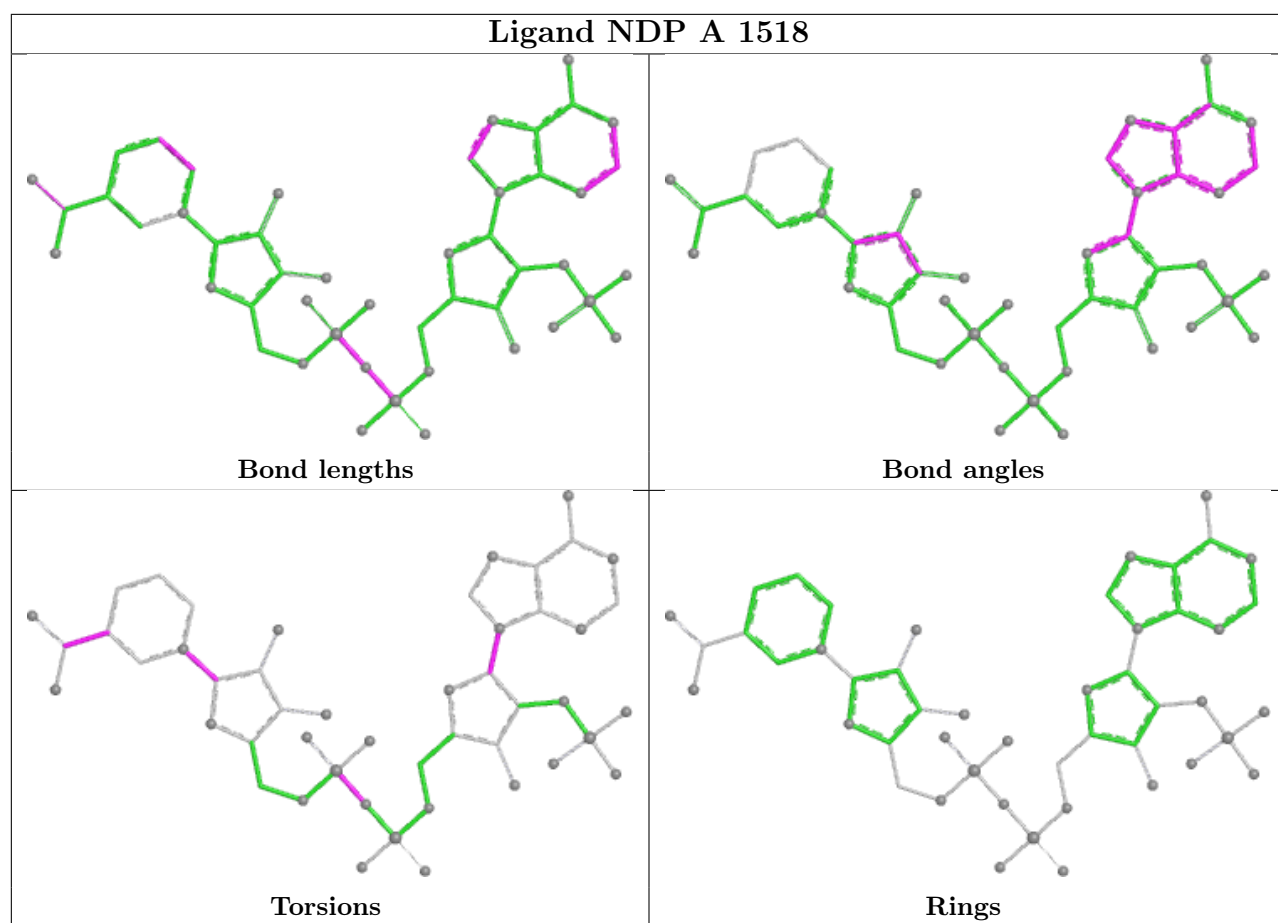
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1517[A]	NDP	2	0
3	C	1517[B]	NDP	3	0
4	D	3003	HEM	1	0
3	D	1517[B]	NDP	1	0
4	B	3001	HEM	1	0
3	C	1517[A]	NDP	1	0
3	B	1517	NDP	1	0

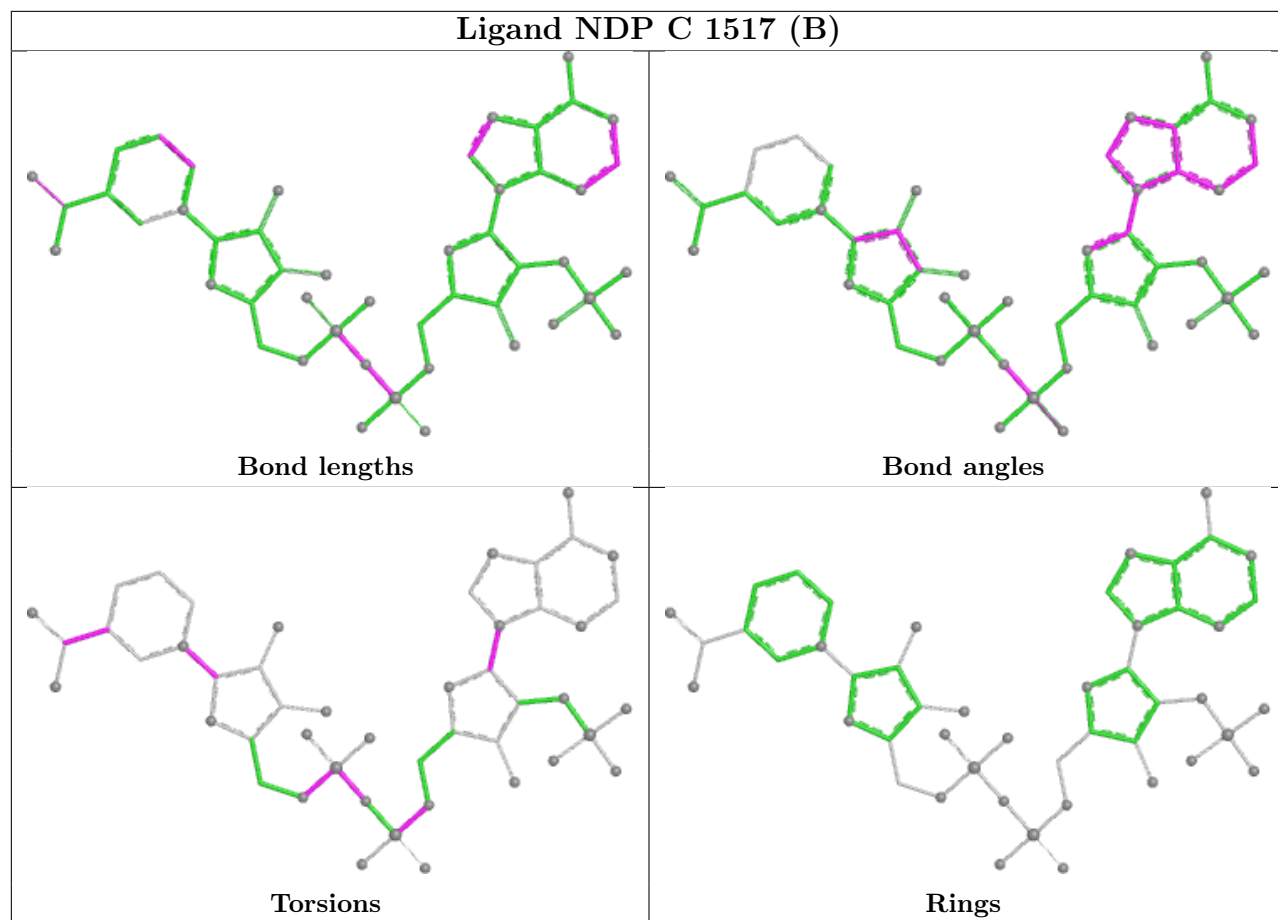
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

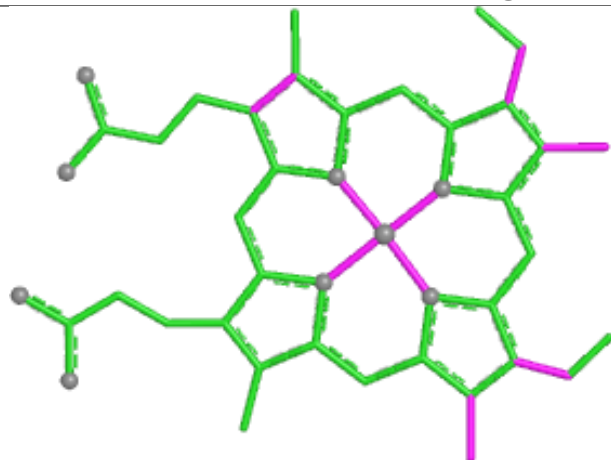




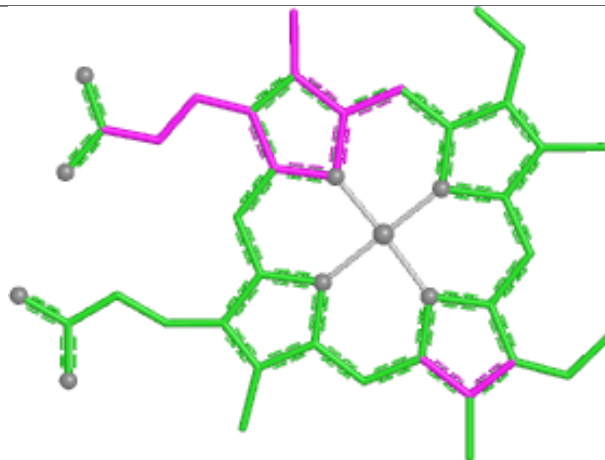
Ligand NDP C 1517 (B)



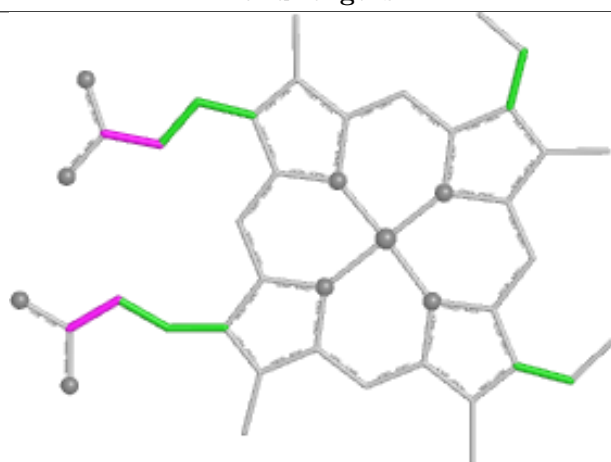
Ligand HEM C 3002



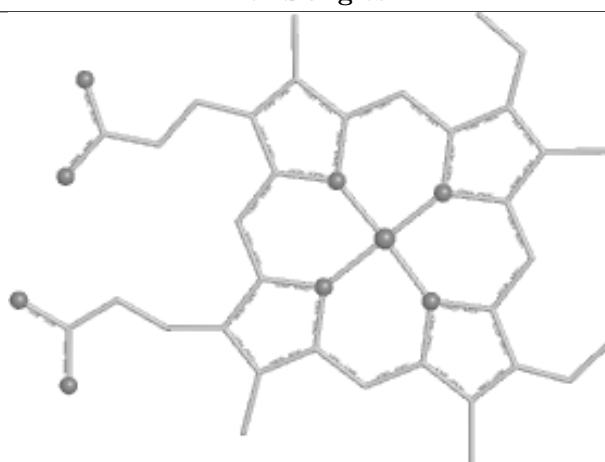
Bond lengths



Bond angles

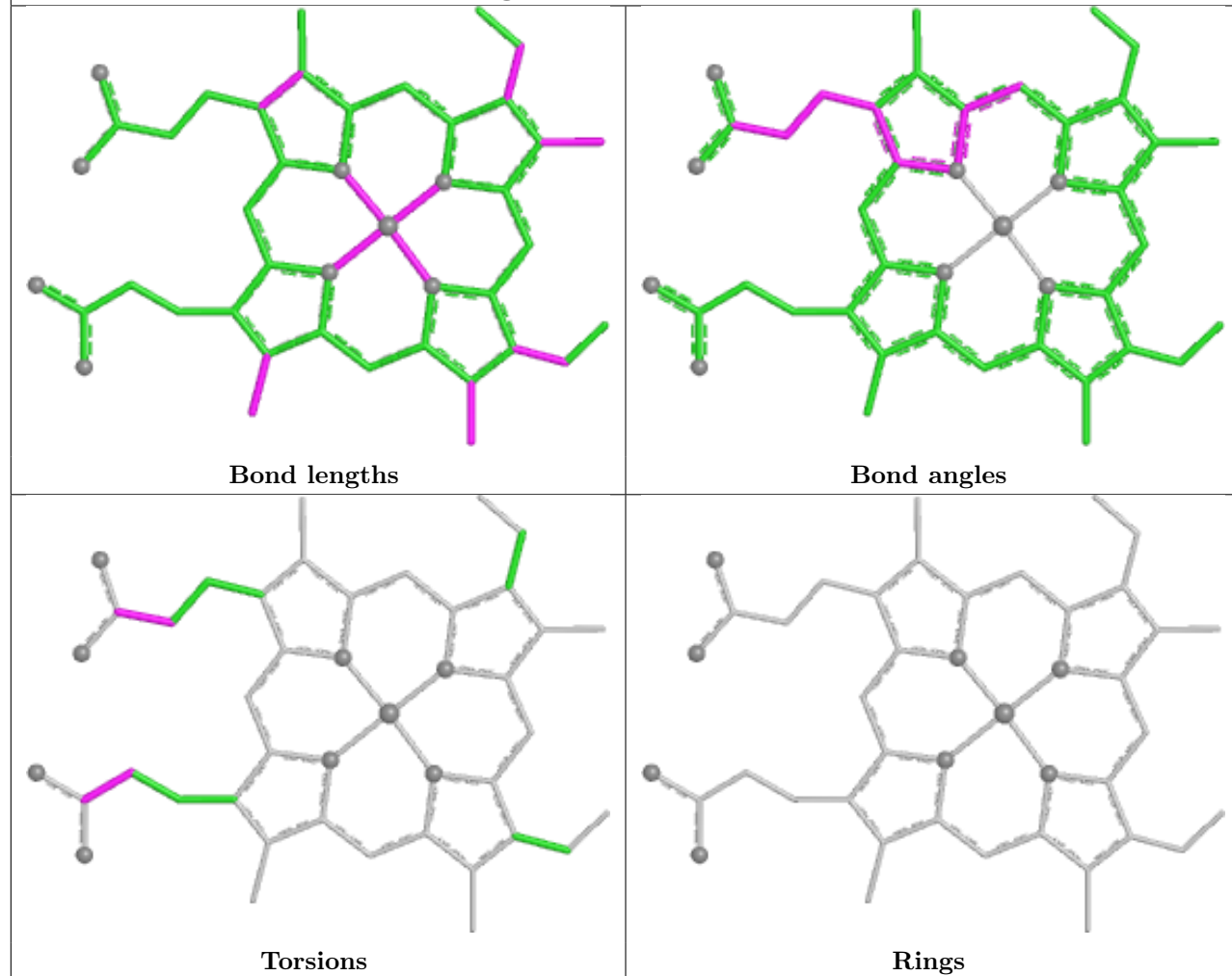


Torsions

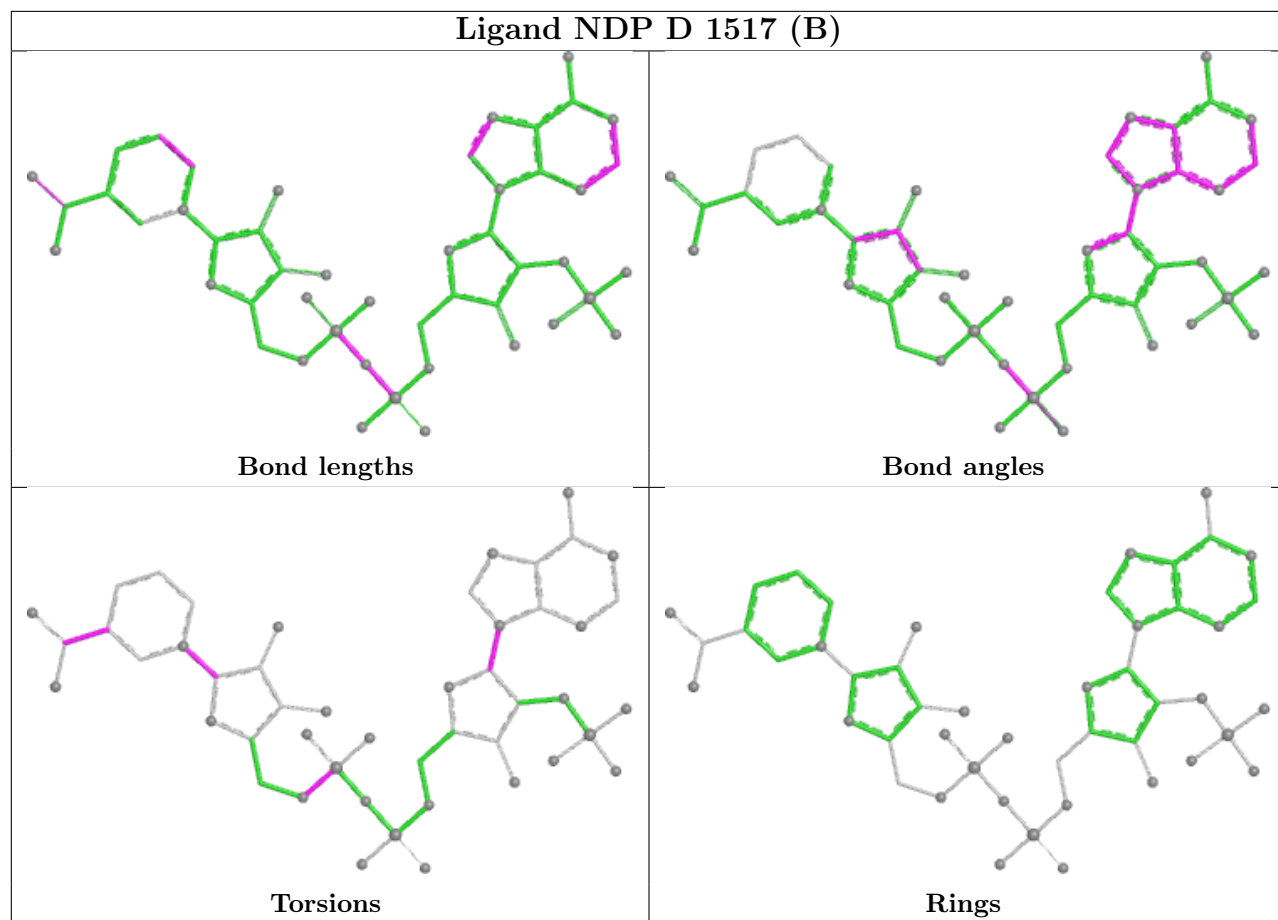


Rings

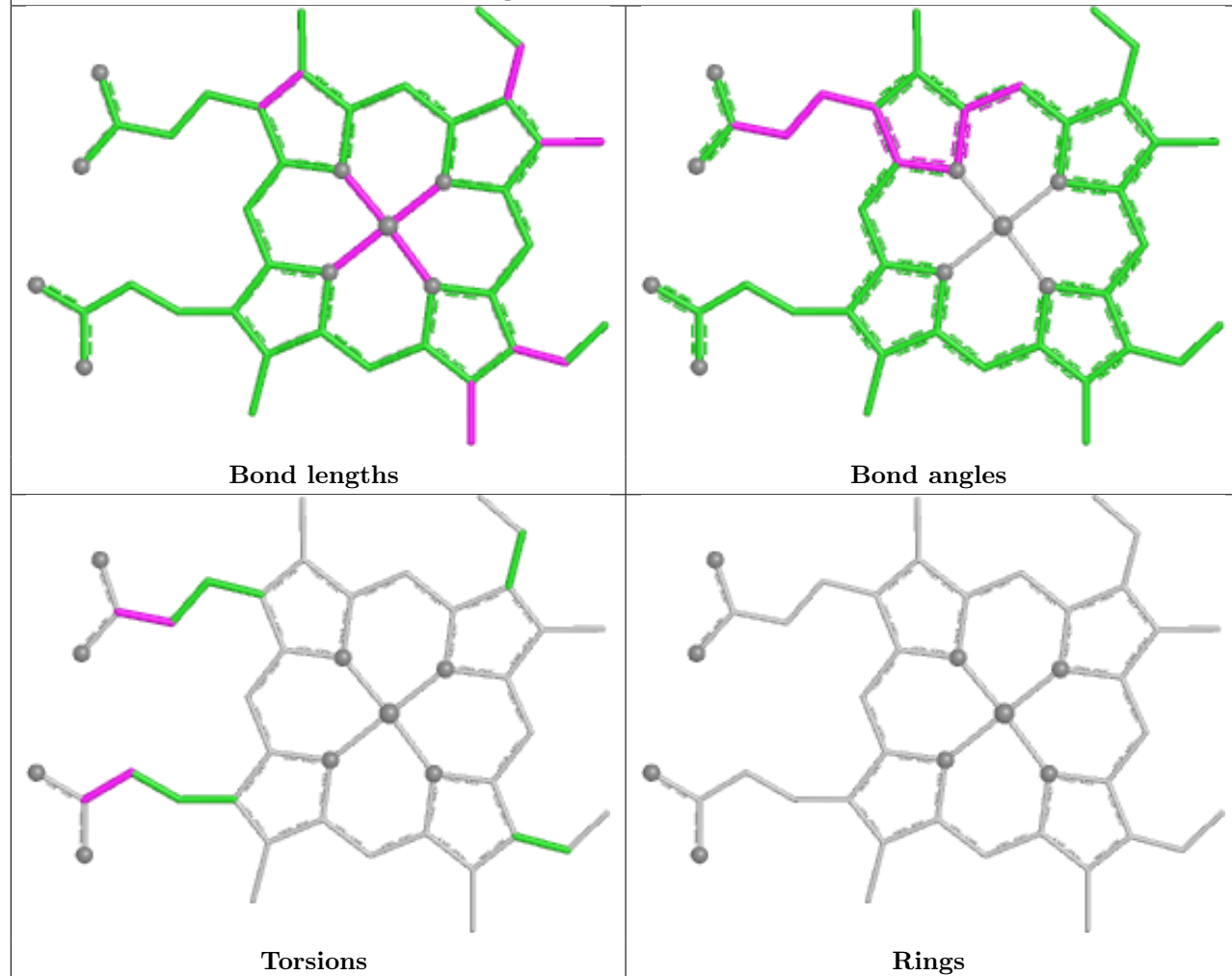
Ligand HEM D 3003



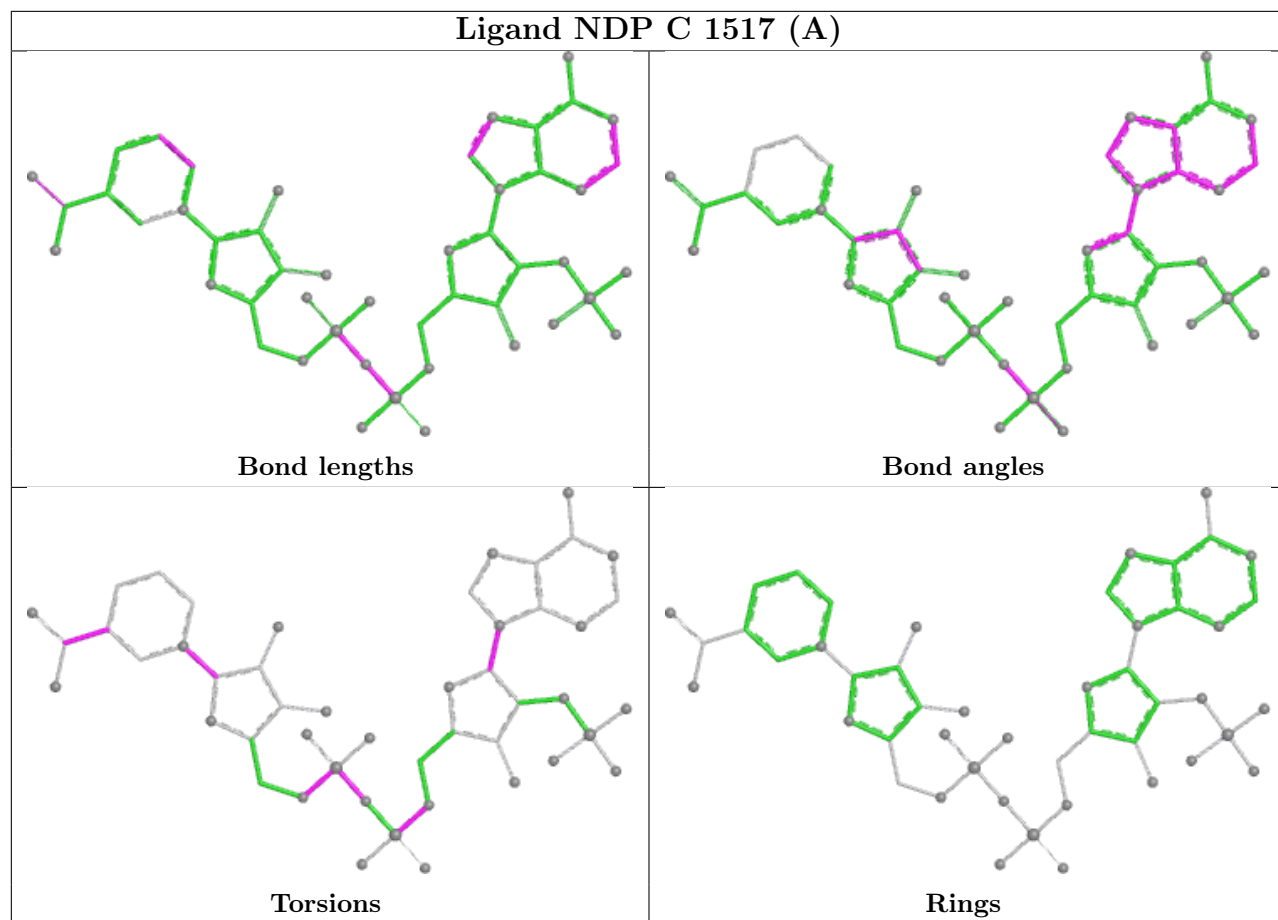
Ligand NDP D 1517 (B)



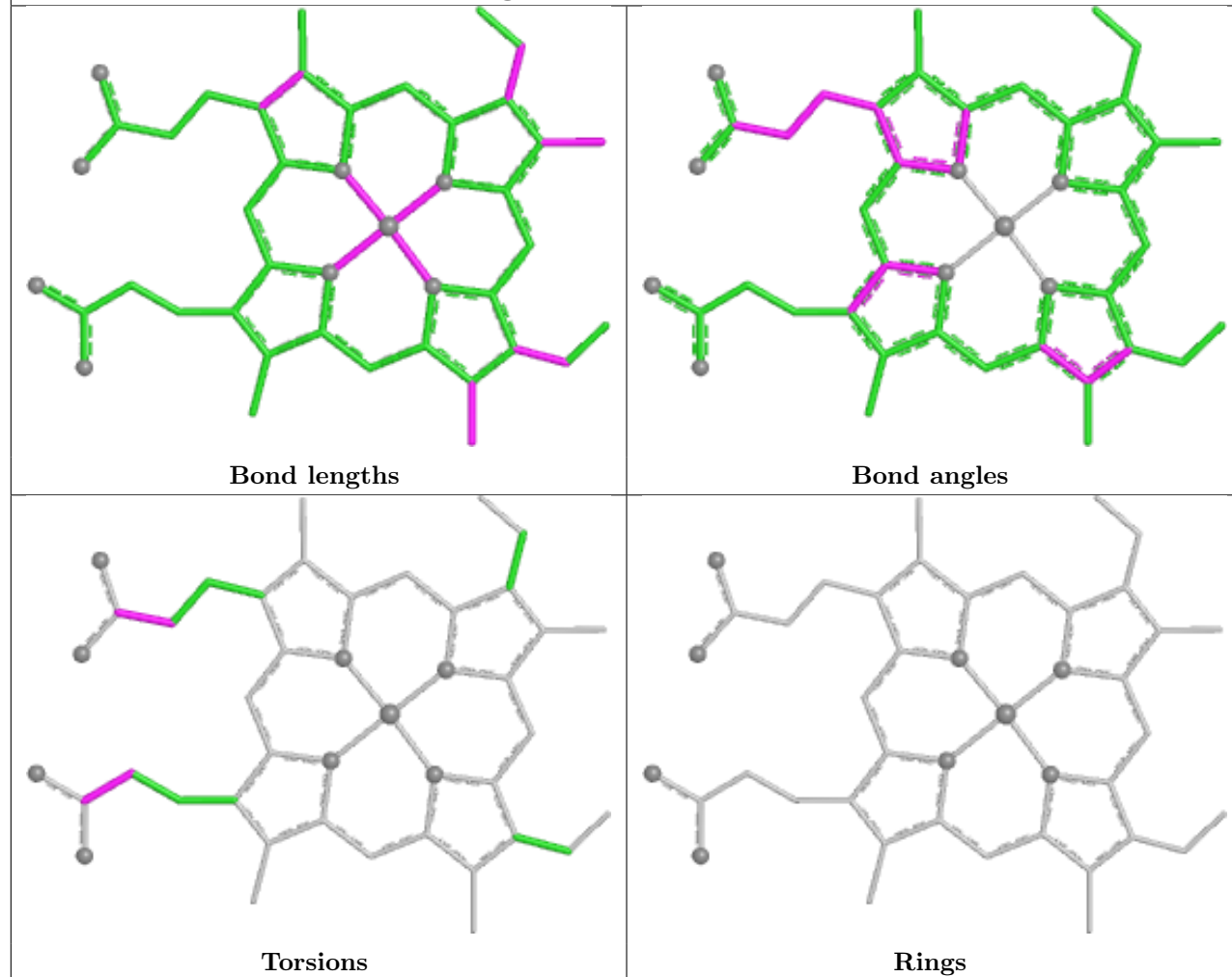
Ligand HEM B 3001

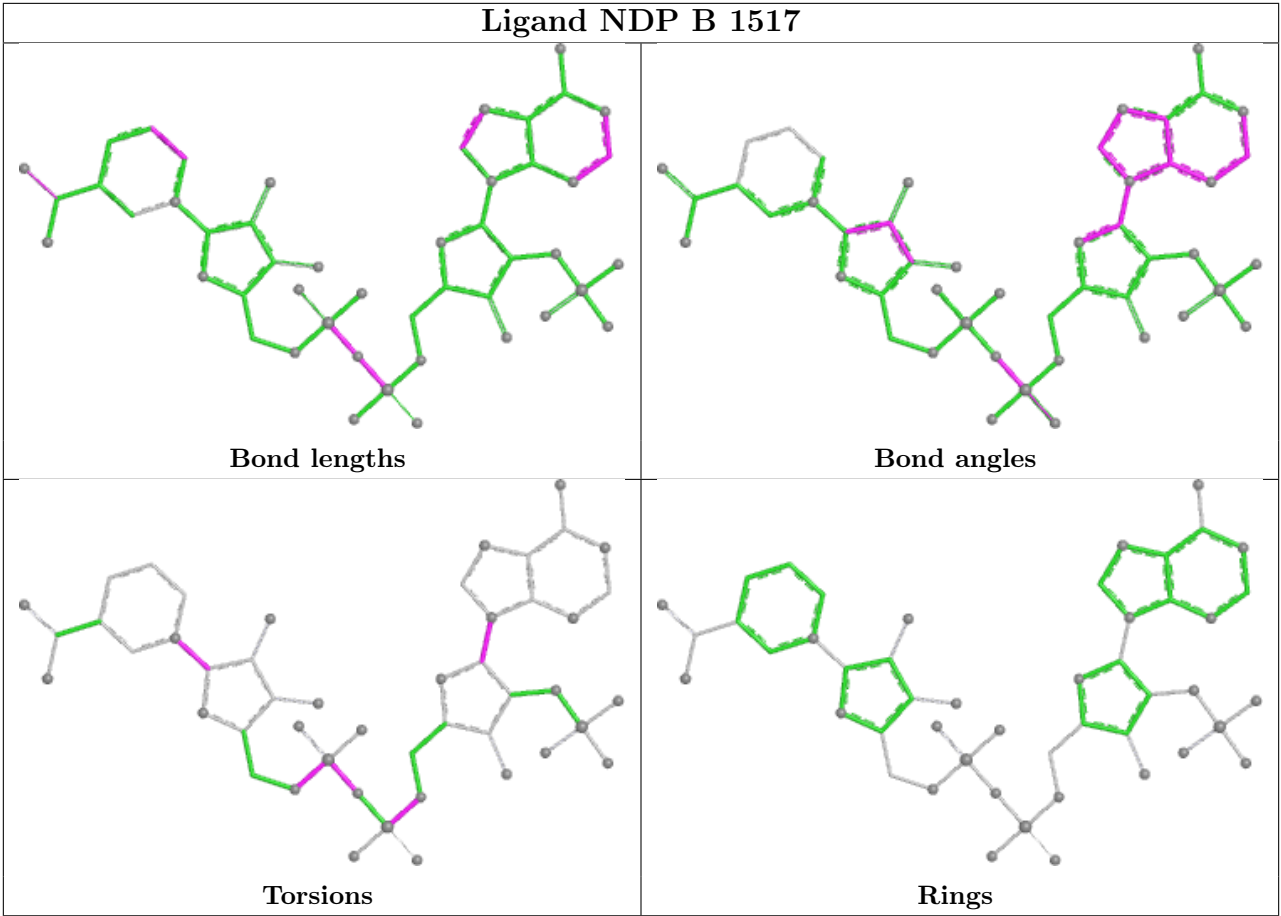


Ligand NDP C 1517 (A)



Ligand HEM A 3000





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	C	2
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	161:HIS	C	162:SER	N	1.19
1	C	420:HIS	C	421:THR	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	436:HIS	C	437:GLY	N	1.17
1	B	419:ASN	C	420:HIS	N	1.13
1	A	419:ASN	C	420:HIS	N	1.10
1	D	419:ASN	C	420:HIS	N	1.02
1	C	419:ASN	C	420:HIS	N	1.01

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/515 (99%)	-0.83	1 (0%) 91 92	8, 16, 25, 74	8 (1%)
1	B	514/515 (99%)	-0.75	2 (0%) 88 90	8, 17, 28, 70	7 (1%)
1	C	513/515 (99%)	-0.80	1 (0%) 91 92	8, 16, 26, 67	5 (0%)
1	D	514/515 (99%)	-0.79	1 (0%) 91 92	8, 16, 26, 78	4 (0%)
All	All	2054/2060 (99%)	-0.79	5 (0%) 91 92	8, 16, 26, 78	24 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	ALA	3.9
1	C	516	ALA	3.3
1	D	516	ALA	3.1
1	B	3	GLU	2.8
1	B	4	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

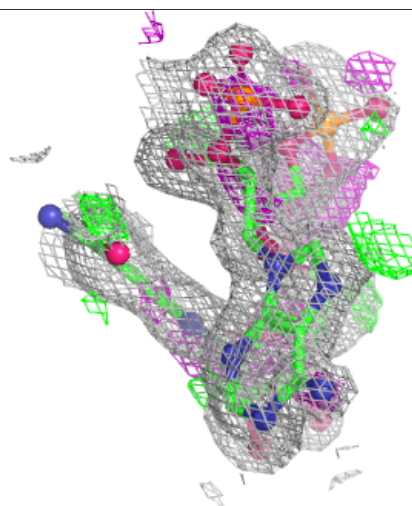
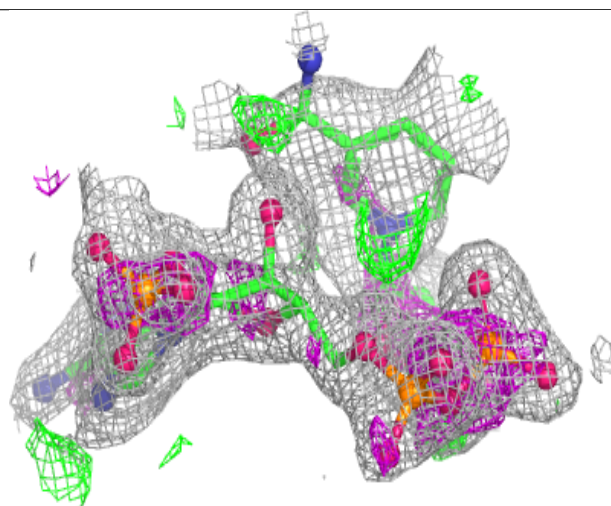
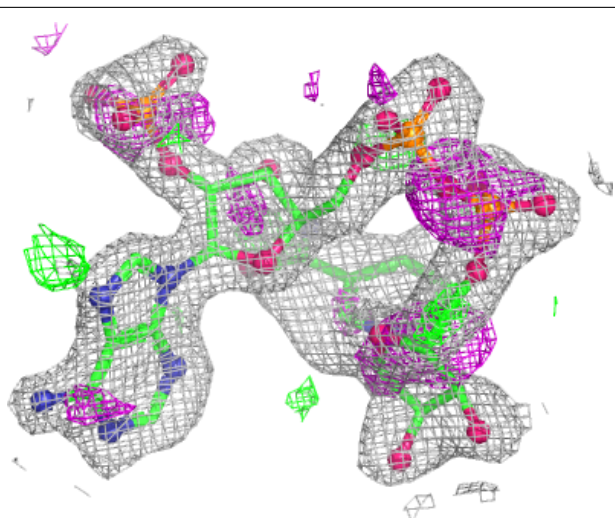
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	D	1517[A]	48/48	0.68	0.13	26,34,42,45	48
3	NDP	D	1517[B]	48/48	0.68	0.13	24,35,42,46	48
3	NDP	C	1517[A]	48/48	0.70	0.14	23,39,49,54	48
3	NDP	C	1517[B]	48/48	0.70	0.14	28,39,49,54	48
3	NDP	B	1517	48/48	0.88	0.09	27,33,41,44	0
3	NDP	A	1518	48/48	0.92	0.08	21,29,34,38	0
4	HEM	A	3000	43/43	0.98	0.05	10,13,16,18	0
2	CL	B	1518	1/1	0.99	0.04	16,16,16,16	0
4	HEM	B	3001	43/43	0.99	0.04	10,14,17,18	0
4	HEM	C	3002	43/43	0.99	0.04	10,13,16,17	0
4	HEM	D	3003	43/43	0.99	0.04	7,13,17,17	0
2	CL	A	1517	1/1	1.00	0.04	18,18,18,18	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.

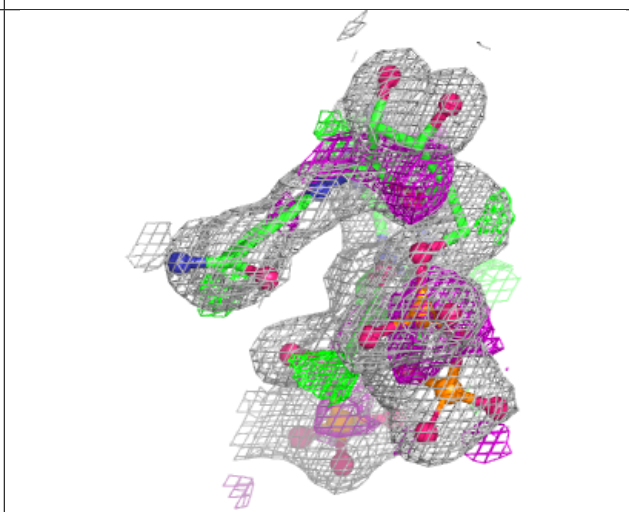
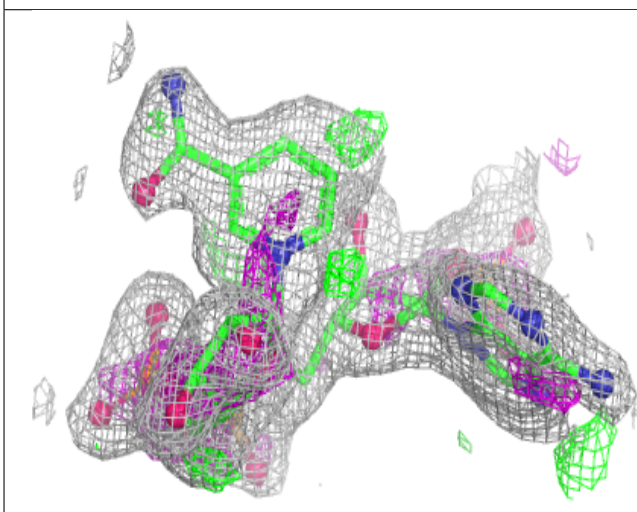
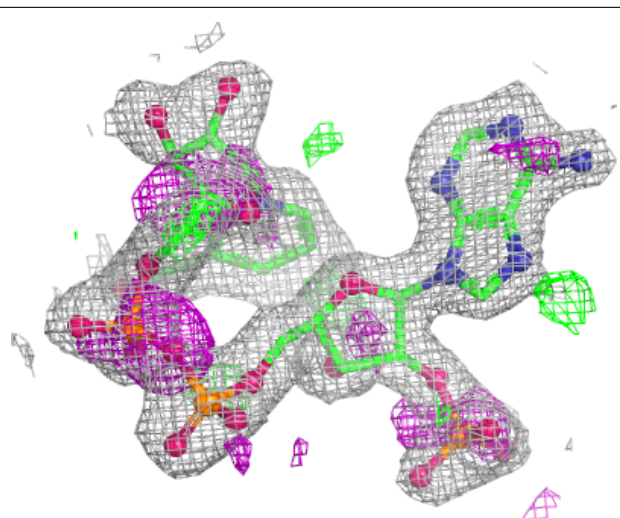
Electron density around NDP D 1517 (A):

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



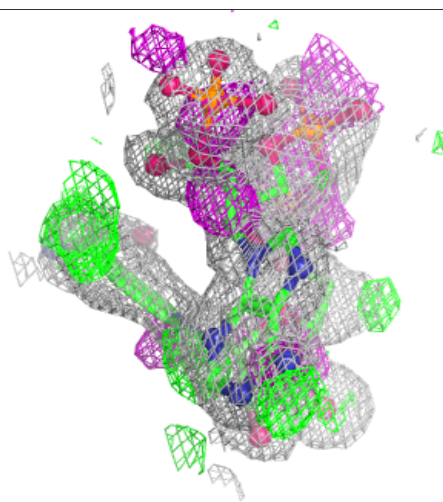
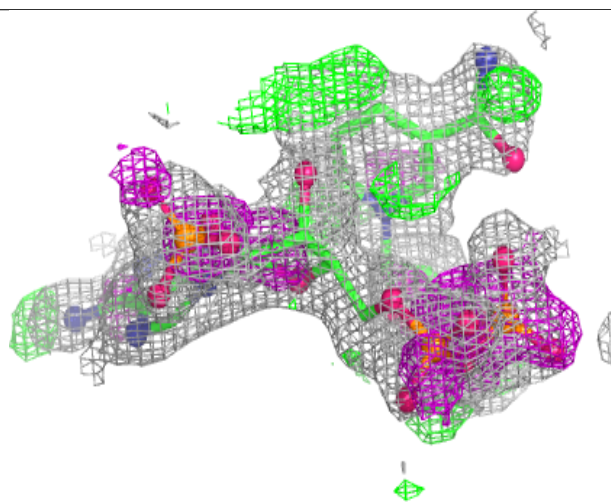
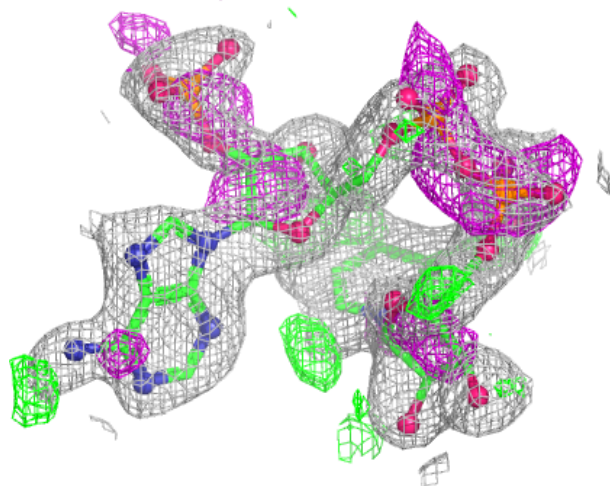
Electron density around NDP D 1517 (B):

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



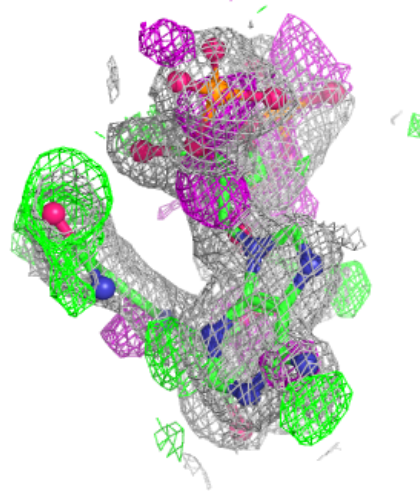
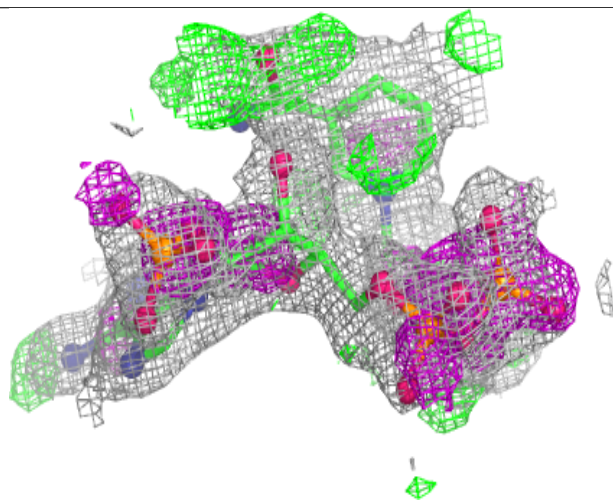
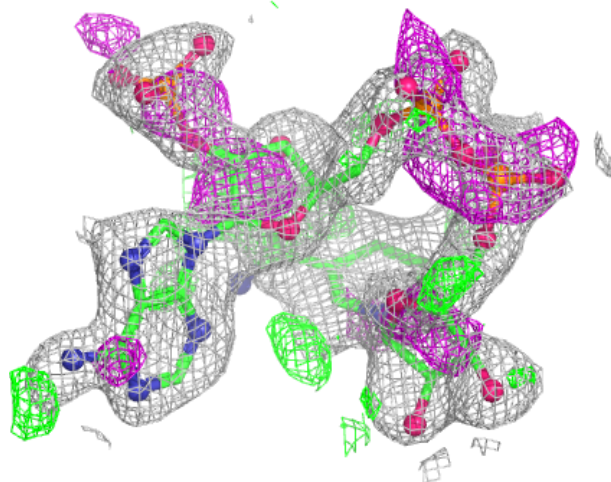
Electron density around NDP C 1517 (A):

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



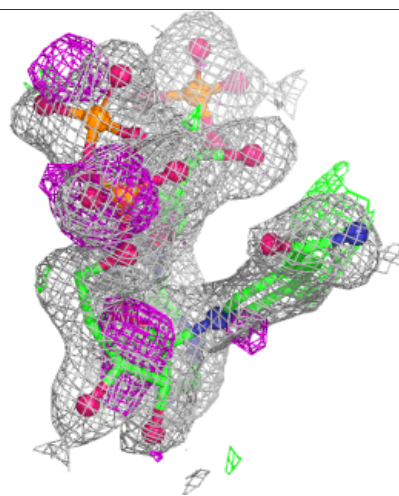
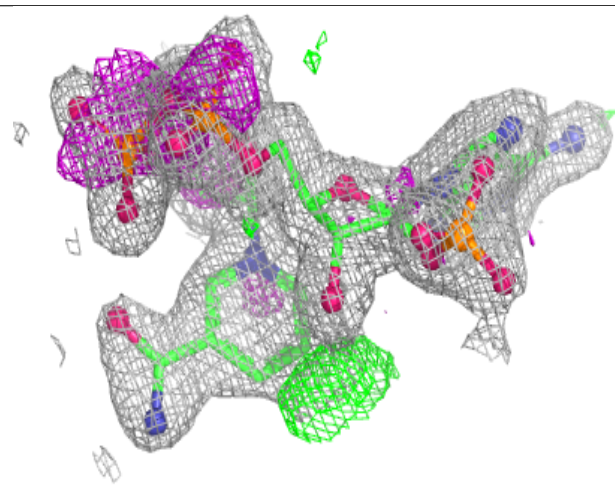
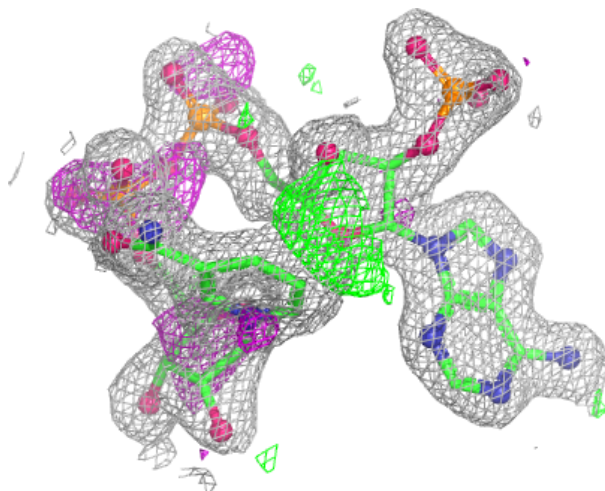
Electron density around NDP C 1517 (B):

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



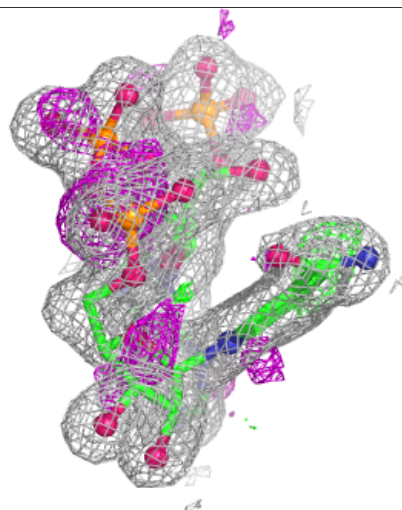
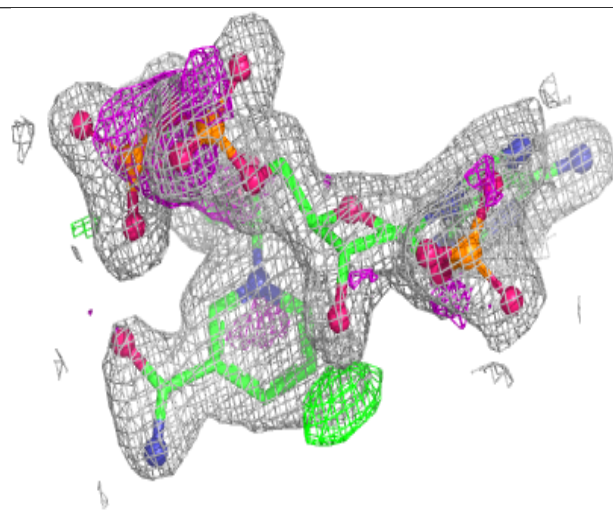
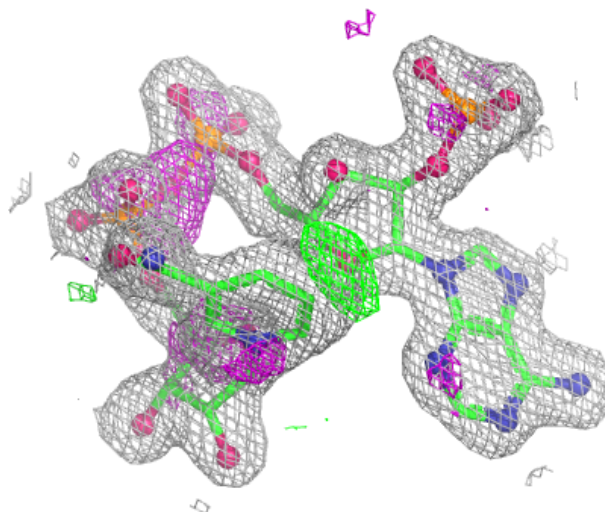
Electron density around NDP B 1517:

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



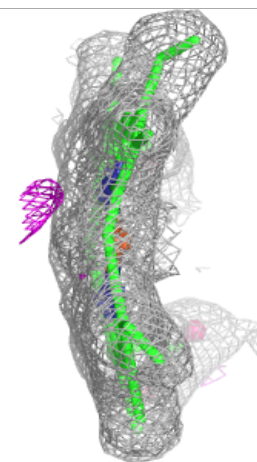
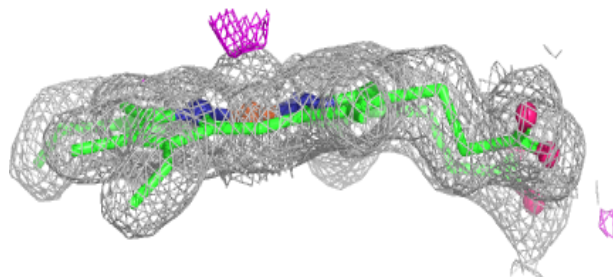
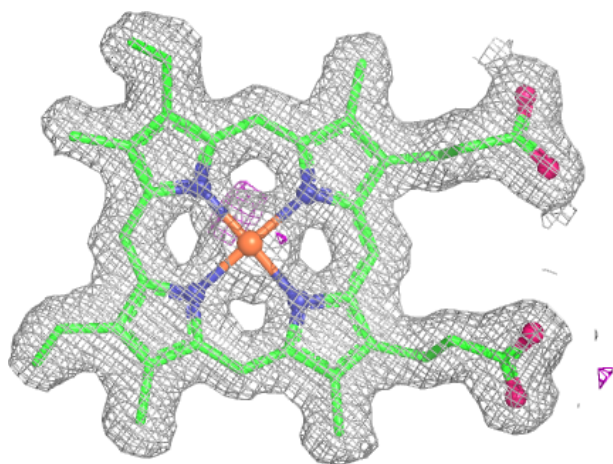
Electron density around NDP A 1518:

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



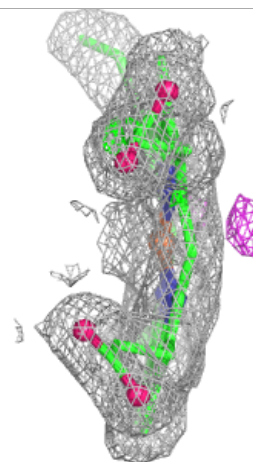
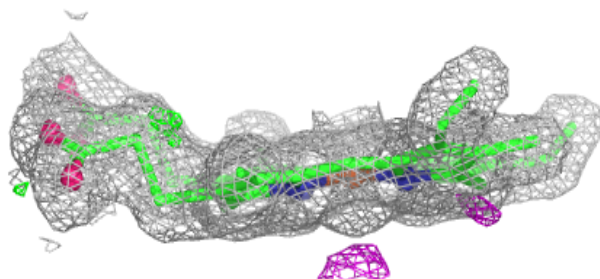
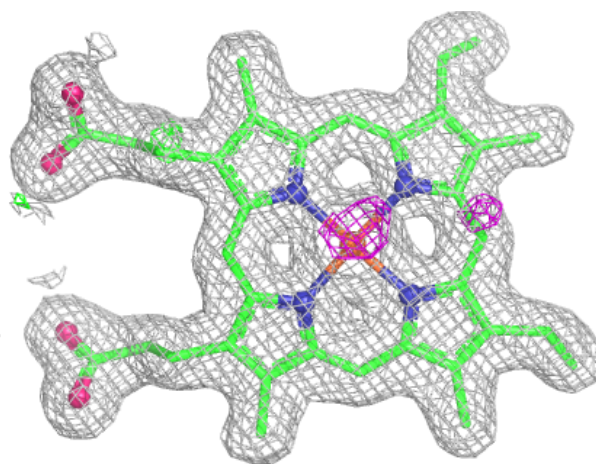
Electron density around HEM A 3000:

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and green (positive)



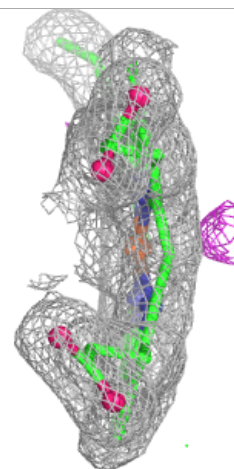
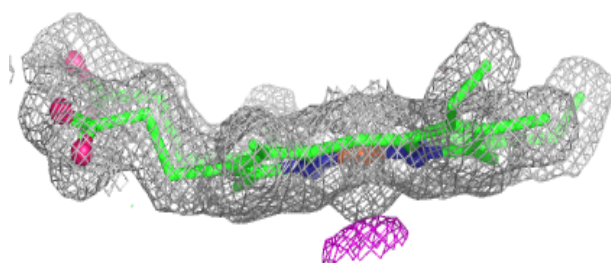
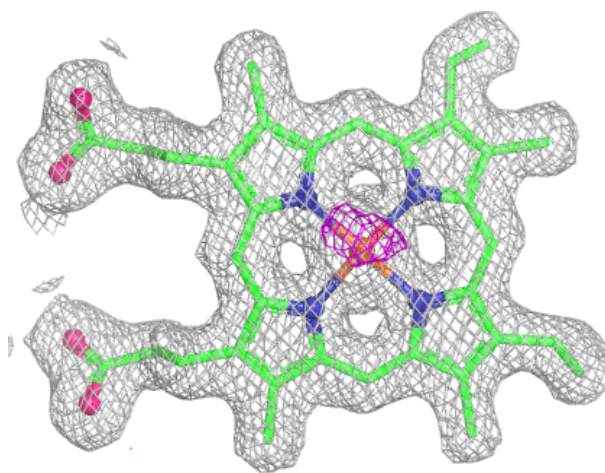
Electron density around HEM B 3001:

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and green (positive)



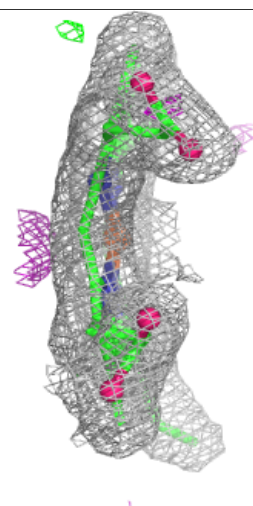
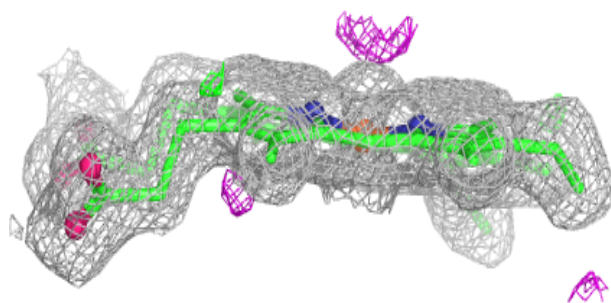
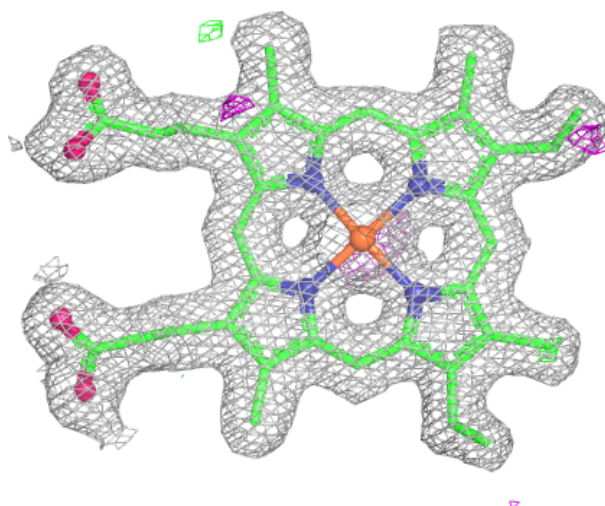
Electron density around HEM C 3002:

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



Electron density around HEM D 3003:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.