



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:36 AM UTC

PDB ID : 8STW / pdb_00008stw
Title : K384N HUMAN CYSTATHIONINE BETA-SYNTHASE (delta 411-551)
Authors : Mascarenhas, R.; Roman, J.; Banerjee, R.
Deposited on : 2023-05-11
Resolution : 2.40 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

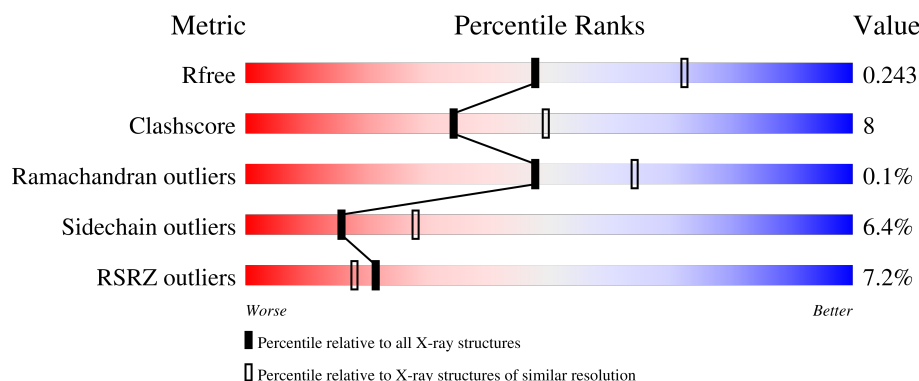
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	363	5% 82% 13% ..
1	B	363	8% 78% 17% ..
1	C	363	6% 82% 15% ..
1	D	363	9% 79% 16% ..
1	E	363	7% 75% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	363	6% 81% 14% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16481 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 Cystathionine beta-synthase, K384N variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2657	1670	468	501	18			
1	B	352	Total	C	N	O	S	0	0	0
			2670	1675	470	508	17			
1	C	358	Total	C	N	O	S	0	0	0
			2725	1710	479	518	18			
1	D	353	Total	C	N	O	S	0	0	0
			2666	1672	465	513	16			
1	E	351	Total	C	N	O	S	0	0	0
			2678	1681	474	505	18			
1	F	352	Total	C	N	O	S	0	0	0
			2663	1671	468	506	18			

There are 12 discrepancies between the modelled and reference sequences:

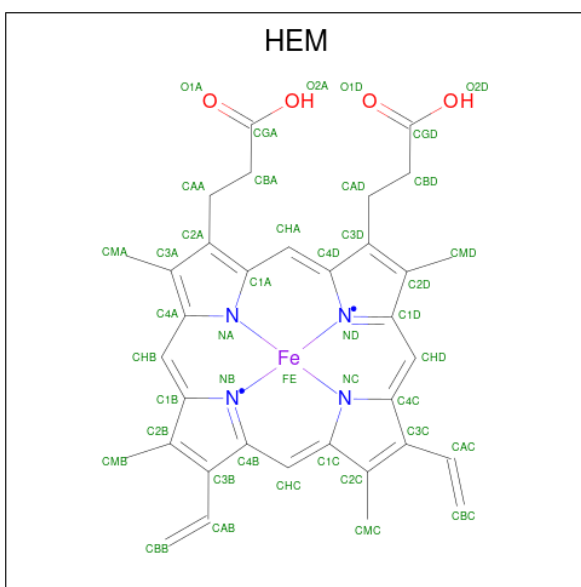
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP P35520
A	384	ASN	LYS	variant	UNP P35520
B	44	MET	-	initiating methionine	UNP P35520
B	384	ASN	LYS	variant	UNP P35520
C	44	MET	-	initiating methionine	UNP P35520
C	384	ASN	LYS	variant	UNP P35520
D	44	MET	-	initiating methionine	UNP P35520
D	384	ASN	LYS	variant	UNP P35520
E	44	MET	-	initiating methionine	UNP P35520
E	384	ASN	LYS	variant	UNP P35520
F	44	MET	-	initiating methionine	UNP P35520
F	384	ASN	LYS	variant	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

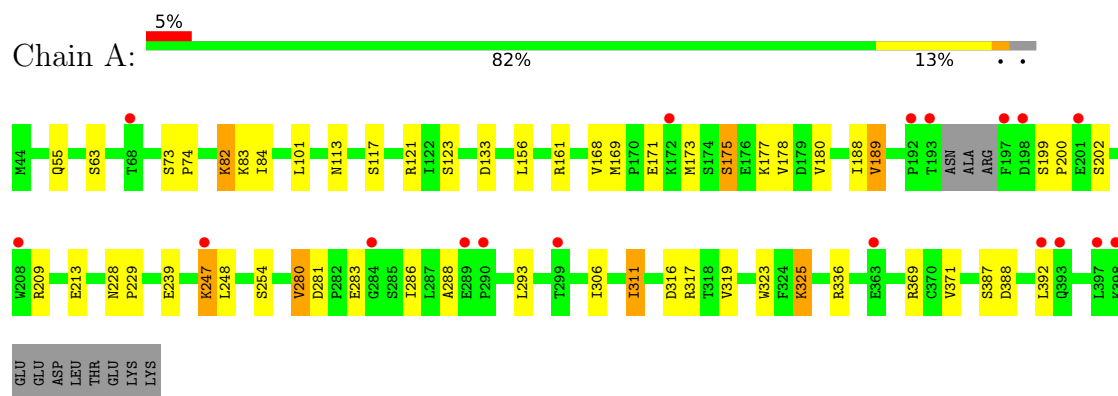
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	10	Total	O	0	0
			10	10		
4	C	16	Total	O	0	0
			16	16		
4	D	10	Total	O	0	0
			10	10		
4	E	6	Total	O	0	0
			6	6		
4	F	13	Total	O	0	0
			13	13		

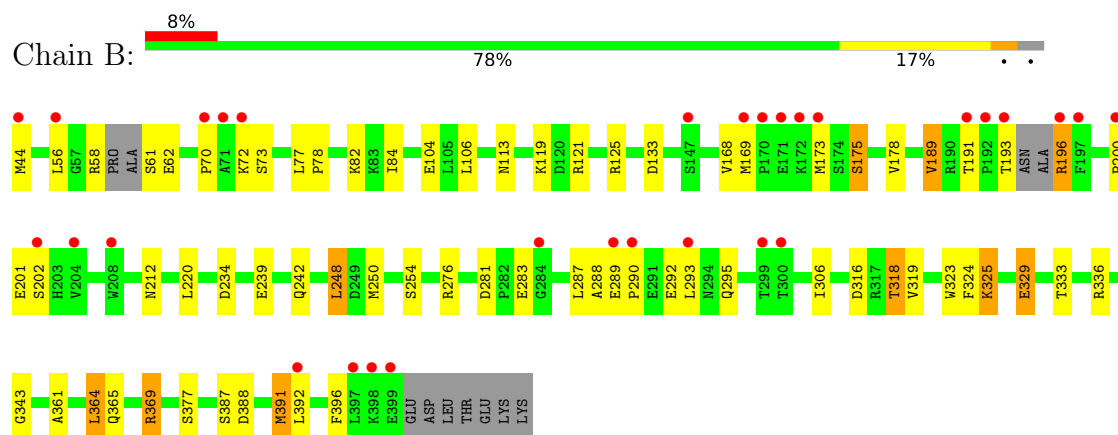
3 Residue-property plots

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.

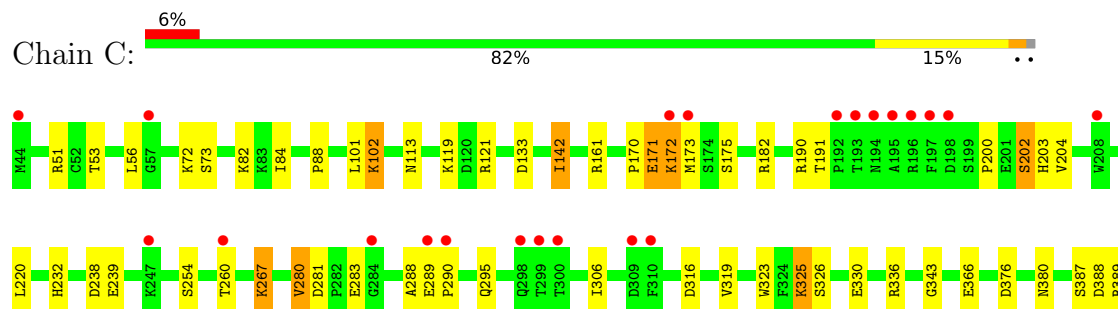
- Molecule 1: Cystathionine beta-synthase, K384N variant

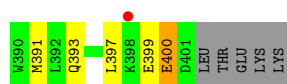


- Molecule 1: Cystathionine beta-synthase, K384N variant

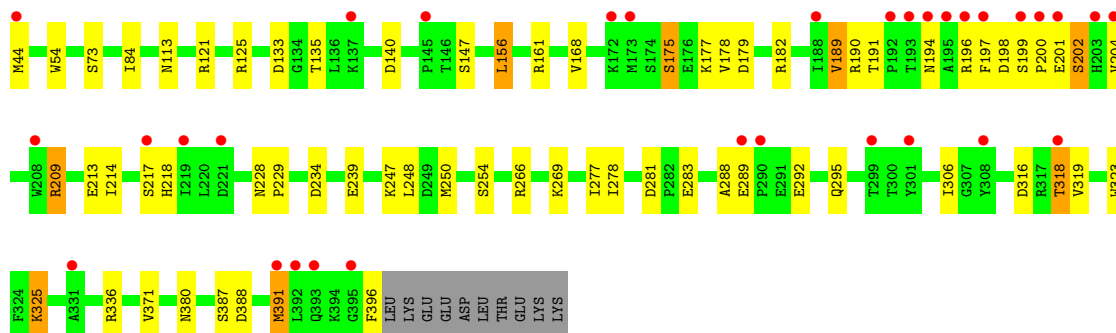
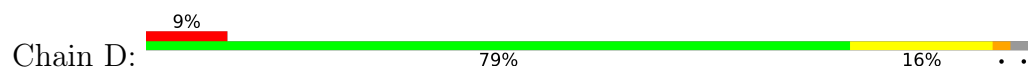


- Molecule 1: Cystathionine beta-synthase, K384N variant

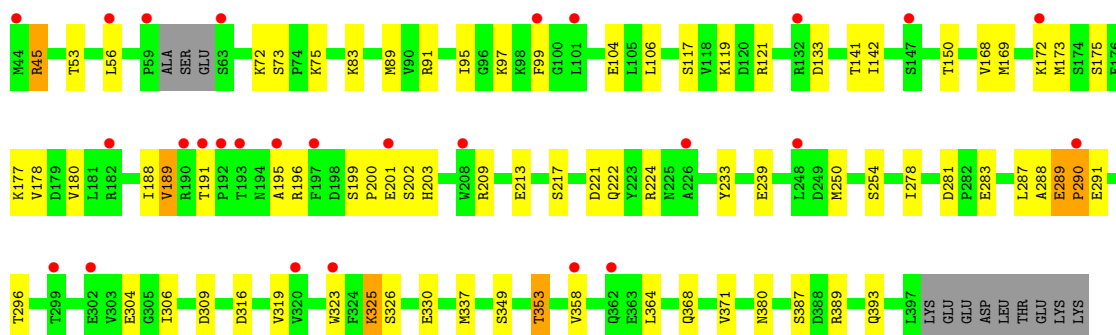
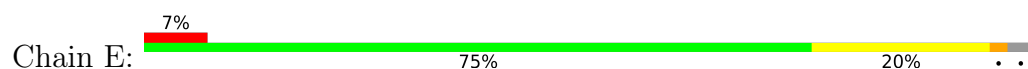




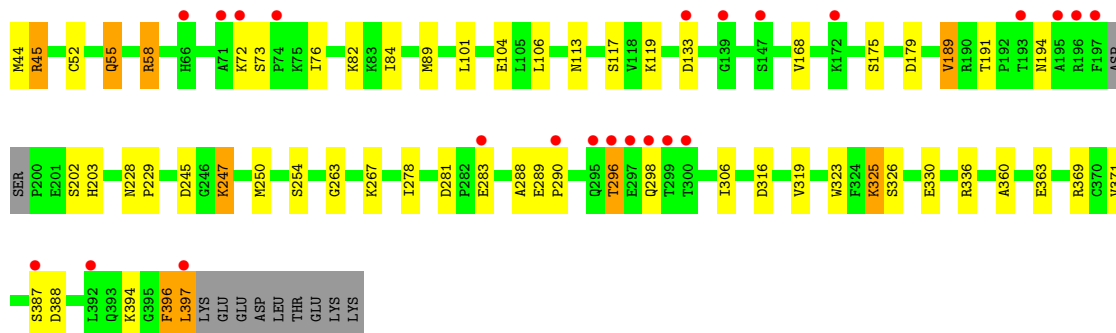
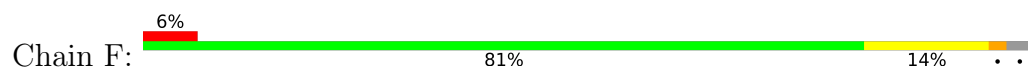
- Molecule 1: Cystathionine beta-synthase, K384N variant



- Molecule 1: Cystathionine beta-synthase, K384N variant



- Molecule 1: Cystathionine beta-synthase, K384N variant



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.46Å 90.19Å 104.22Å 106.15° 105.49° 107.47°	Depositor
Resolution (Å)	43.11 – 2.40 43.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.5 (43.11-2.40) 92.5 (43.11-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.210 , 0.243 0.214 , 0.243	Depositor DCC
R_{free} test set	4934 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16481	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, 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	1.09	1/2705 (0.0%)	1.39	5/3663 (0.1%)
1	B	1.06	0/2716	1.40	6/3676 (0.2%)
1	C	1.09	0/2774	1.40	3/3754 (0.1%)
1	D	1.07	0/2715	1.40	3/3682 (0.1%)
1	E	1.06	0/2726	1.41	8/3689 (0.2%)
1	F	1.07	0/2709	1.40	8/3666 (0.2%)
All	All	1.07	1/16345 (0.0%)	1.40	33/22130 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	GLU	C-O	5.38	1.31	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	ARG	CG-CD-NE	-8.64	93.00	112.00
1	F	363	GLU	CB-CG-CD	6.72	124.02	112.60
1	B	200	PRO	N-CA-C	6.28	121.71	113.86
1	B	292	GLU	CB-CG-CD	6.27	123.26	112.60
1	C	200	PRO	N-CA-C	5.88	122.35	114.18
1	C	133	ASP	CA-CB-CG	5.84	118.44	112.60
1	E	195	ALA	CA-C-N	5.61	129.06	120.82
1	E	195	ALA	C-N-CA	5.61	129.06	120.82
1	F	396	PHE	CA-C-N	5.60	131.78	121.70
1	F	396	PHE	C-N-CA	5.60	131.78	121.70
1	E	133	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	283	GLU	N-CA-C	-5.58	102.02	110.28
1	E	221	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	133	ASP	CA-CB-CG	5.46	118.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	369	ARG	CG-CD-NE	-5.41	100.11	112.00
1	E	353	THR	CA-CB-OG1	-5.36	101.56	109.60
1	C	283	GLU	CA-C-O	-5.33	114.90	120.55
1	B	62	GLU	CA-C-N	5.27	127.73	120.67
1	B	62	GLU	C-N-CA	5.27	127.73	120.67
1	D	283	GLU	CA-C-O	-5.24	115.00	120.55
1	E	283	GLU	N-CA-C	-5.22	102.56	110.28
1	F	133	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	117	SER	CA-C-N	5.21	129.16	120.62
1	A	117	SER	C-N-CA	5.21	129.16	120.62
1	A	283	GLU	CA-C-O	-5.20	115.04	120.55
1	F	117	SER	CA-C-N	5.19	129.14	120.62
1	F	117	SER	C-N-CA	5.19	129.14	120.62
1	D	133	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	391	MET	CA-CB-CG	-5.16	103.77	114.10
1	F	283	GLU	CA-C-O	-5.13	115.11	120.55
1	E	117	SER	CA-C-N	5.09	128.96	120.62
1	E	117	SER	C-N-CA	5.09	128.96	120.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2657	0	2652	32	0
1	B	2670	0	2660	45	0
1	C	2725	0	2733	45	0
1	D	2666	0	2643	37	0
1	E	2678	0	2693	50	0
1	F	2663	0	2671	35	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	7	4	0
2	D	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	15	0	6	1	0
2	F	15	0	6	1	0
3	A	43	0	30	5	0
3	B	43	0	30	2	0
3	C	43	0	30	12	0
3	D	43	0	30	4	0
3	E	43	0	30	5	0
3	F	43	0	30	4	0
4	A	19	0	0	3	0
4	B	10	0	0	1	0
4	C	16	0	0	1	0
4	D	10	0	0	1	0
4	E	6	0	0	1	0
4	F	13	0	0	0	0
All	All	16481	0	16269	249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (249) 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:175:SER:HA	1:B:178:VAL:HG22	1.47	0.96
1:E:150:THR:HG21	1:E:222:GLN:OE1	1.75	0.86
1:E:99:PHE:CB	1:E:358:VAL:HG21	2.09	0.81
3:C:502:HEM:HMB1	3:C:502:HEM:HBB2	1.63	0.80
3:C:502:HEM:HMC1	3:C:502:HEM:HBC2	1.62	0.80
1:E:349:SER:O	1:E:353:THR:HG23	1.83	0.79
1:C:260:THR:HG23	2:C:501:PLP:O2P	1.84	0.77
1:E:233:TYR:CE1	3:E:502:HEM:HBB1	2.20	0.77
1:E:99:PHE:CB	1:E:358:VAL:CG2	2.63	0.76
1:B:391:MET:HE3	1:B:396:PHE:HB2	1.68	0.76
1:E:91:ARG:NH2	1:F:76:ILE:HD11	2.00	0.76
1:C:102:LYS:H	1:C:102:LYS:HE2	1.52	0.74
1:C:391:MET:HB3	1:C:397:LEU:HD22	1.67	0.74
1:E:104:GLU:HG2	1:E:106:LEU:HD11	1.69	0.74
3:A:502:HEM:HMC1	3:A:502:HEM:HBC2	1.70	0.73
1:B:125:ARG:NH2	1:B:234:ASP:OD2	2.22	0.73
1:E:99:PHE:HB2	1:E:358:VAL:CG2	2.18	0.73
1:A:254:SER:HA	1:A:280:VAL:HG22	1.71	0.72
1:E:99:PHE:HB2	1:E:358:VAL:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:ASP:O	1:F:247:LYS:HD2	1.90	0.72
1:C:53:THR:CG2	3:C:502:HEM:HHB	2.20	0.71
1:C:254:SER:HA	1:C:280:VAL:HG22	1.72	0.71
1:F:76:ILE:O	1:F:76:ILE:HD12	1.91	0.71
1:B:289:GLU:HB3	1:B:290:PRO:HD3	1.73	0.71
1:B:290:PRO:HD2	1:B:293:LEU:CD1	2.22	0.69
1:B:175:SER:HA	1:B:178:VAL:CG2	2.23	0.69
1:D:269:LYS:HE2	1:D:277:ILE:HD13	1.74	0.69
1:C:53:THR:HG22	3:C:502:HEM:HHB	1.73	0.68
1:A:63:SER:HB2	3:A:502:HEM:CBB	2.23	0.67
1:A:209:ARG:HD2	1:A:213:GLU:OE2	1.93	0.67
1:B:391:MET:CE	1:B:396:PHE:HB2	2.25	0.67
1:E:233:TYR:CZ	3:E:502:HEM:HBB1	2.31	0.66
1:C:289:GLU:HB3	1:C:290:PRO:HD3	1.79	0.65
1:C:391:MET:CB	1:C:397:LEU:HD22	2.26	0.65
1:E:209:ARG:HD2	1:E:213:GLU:OE2	1.96	0.65
1:D:125:ARG:NH2	1:D:234:ASP:OD2	2.30	0.63
1:F:289:GLU:HB3	1:F:290:PRO:HD3	1.79	0.63
1:A:293:LEU:HA	1:E:389:ARG:HG2	1.80	0.63
1:B:388:ASP:OD2	1:D:182:ARG:NH1	2.32	0.63
1:B:336:ARG:NH2	1:B:388:ASP:OD1	2.32	0.63
1:B:391:MET:HE3	1:B:396:PHE:CB	2.29	0.63
3:E:502:HEM:HHC	3:E:502:HEM:HBB2	1.80	0.63
3:A:502:HEM:HBC2	3:A:502:HEM:CMC	2.29	0.62
1:B:196:ARG:NE	1:B:196:ARG:HA	2.14	0.62
1:B:391:MET:CE	1:B:396:PHE:CB	2.77	0.62
1:C:102:LYS:HE2	1:C:102:LYS:N	2.13	0.62
1:F:76:ILE:HD12	1:F:76:ILE:C	2.25	0.61
1:E:91:ARG:NH2	1:F:76:ILE:CD1	2.64	0.60
3:D:502:HEM:HBB2	3:D:502:HEM:HMB2	1.82	0.60
1:B:78:PRO:HD2	1:B:82:LYS:HD3	1.82	0.60
1:E:91:ARG:HH22	1:F:76:ILE:HD11	1.67	0.60
1:D:269:LYS:HE2	1:D:277:ILE:CD1	2.32	0.59
1:C:171:GLU:OE1	1:C:172:LYS:N	2.32	0.59
1:E:99:PHE:CG	1:E:358:VAL:HG21	2.37	0.59
1:B:329:GLU:O	1:B:333:THR:HG23	2.02	0.59
3:C:502:HEM:HBB2	3:C:502:HEM:CMB	2.32	0.59
1:E:141:THR:OG1	1:E:217:SER:HA	2.02	0.59
1:E:89:MET:HE1	1:E:371:VAL:HG13	1.85	0.59
1:D:254:SER:HB2	1:D:306:ILE:HG21	1.85	0.58
3:D:502:HEM:HBC2	3:D:502:HEM:HMC2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:N	1:E:106:LEU:HD12	2.19	0.58
1:F:89:MET:HE1	1:F:371:VAL:HG13	1.86	0.58
1:A:254:SER:HB2	1:A:306:ILE:HG21	1.86	0.57
1:E:254:SER:HB2	1:E:306:ILE:HG21	1.85	0.57
1:C:53:THR:HG22	3:C:502:HEM:CHB	2.35	0.57
1:B:290:PRO:HD2	1:B:293:LEU:HD12	1.86	0.57
1:E:380:ASN:ND2	4:E:602:HOH:O	2.36	0.57
1:F:254:SER:HB2	1:F:306:ILE:HG21	1.87	0.57
1:D:336:ARG:NH2	1:D:388:ASP:OD1	2.31	0.56
1:B:254:SER:HB2	1:B:306:ILE:HG21	1.88	0.56
1:C:53:THR:HG22	3:C:502:HEM:CMA	2.36	0.56
1:E:99:PHE:HB3	1:E:358:VAL:CG2	2.35	0.56
1:B:169:MET:HE2	1:B:173:MET:CB	2.35	0.56
1:E:389:ARG:NH2	1:F:179:ASP:OD2	2.40	0.55
1:A:199:SER:OG	1:A:200:PRO:O	2.25	0.55
2:E:501:PLP:O4P	2:E:501:PLP:C4A	2.55	0.55
1:D:147:SER:O	1:D:177:LYS:HE3	2.07	0.55
1:F:278:ILE:HD13	1:F:360:ALA:HB1	1.87	0.55
1:A:84:ILE:O	1:A:113:ASN:OD1	2.25	0.55
1:B:84:ILE:O	1:B:113:ASN:OD1	2.25	0.55
1:B:377:SER:HB2	4:B:609:HOH:O	2.07	0.55
1:D:84:ILE:O	1:D:113:ASN:OD1	2.24	0.55
1:C:84:ILE:O	1:C:113:ASN:OD1	2.25	0.55
1:E:104:GLU:HG2	1:E:106:LEU:CD1	2.37	0.55
1:C:254:SER:HB2	1:C:306:ILE:HG21	1.90	0.54
1:F:106:LEU:HD11	1:F:369:ARG:HD3	1.89	0.54
1:B:343:GLY:HA3	1:D:156:LEU:CD2	2.38	0.54
3:B:502:HEM:HMC1	3:B:502:HEM:HBC2	1.90	0.53
1:C:238:ASP:OD1	1:C:267:LYS:HE2	2.07	0.53
1:C:51:ARG:HB2	3:C:502:HEM:O2A	2.08	0.53
1:F:84:ILE:O	1:F:113:ASN:OD1	2.24	0.53
1:D:191:THR:HG23	1:D:201:GLU:O	2.09	0.53
1:D:202:SER:OG	1:D:204:VAL:HG12	2.09	0.53
1:A:177:LYS:O	1:A:180:VAL:HG12	2.09	0.53
1:B:106:LEU:HD11	1:B:369:ARG:HD2	1.90	0.52
3:C:502:HEM:HBA2	3:C:502:HEM:HHA	1.91	0.52
1:A:311:ILE:CD1	1:A:317:ARG:CZ	2.87	0.52
1:D:140:ASP:OD2	1:D:218:HIS:HE1	1.92	0.52
1:C:202:SER:OG	1:C:204:VAL:HG12	2.09	0.52
1:F:52:CYS:HA	3:F:502:HEM:C1A	2.43	0.52
1:A:175:SER:HB3	1:B:295:GLN:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:THR:HG23	3:C:502:HEM:HHB	1.92	0.52
1:C:397:LEU:HD23	1:C:397:LEU:O	2.10	0.52
1:D:380:ASN:ND2	4:D:603:HOH:O	2.43	0.52
1:E:289:GLU:O	1:E:291:GLU:N	2.43	0.52
1:F:336:ARG:NH2	1:F:388:ASP:OD1	2.31	0.51
1:F:250:MET:SD	1:F:278:ILE:CD1	2.99	0.51
1:C:171:GLU:OE2	1:C:190:ARG:HD3	2.10	0.51
3:F:502:HEM:HMC1	3:F:502:HEM:HBC2	1.93	0.51
1:D:175:SER:O	1:D:179:ASP:OD1	2.29	0.51
1:A:311:ILE:CD1	1:A:317:ARG:NH2	2.74	0.50
3:C:502:HEM:HBC2	3:C:502:HEM:CMC	2.36	0.50
1:D:199:SER:OG	1:D:200:PRO:O	2.27	0.50
1:D:135:THR:HG22	1:D:218:HIS:CD2	2.46	0.50
1:C:56:LEU:C	1:C:56:LEU:HD23	2.37	0.50
1:B:168:VAL:HG22	1:B:189:VAL:HG22	1.93	0.50
1:B:248:LEU:HD21	1:B:250:MET:O	2.12	0.49
1:B:191:THR:HG23	1:B:201:GLU:O	2.11	0.49
1:E:104:GLU:CG	1:E:106:LEU:HD11	2.42	0.49
1:F:44:MET:HE2	1:F:45:ARG:NH1	2.28	0.49
1:F:104:GLU:OE1	1:F:369:ARG:NH1	2.45	0.49
1:E:75:LYS:NZ	1:F:245:ASP:OD2	2.46	0.49
1:A:168:VAL:HG22	1:A:189:VAL:HG22	1.95	0.49
1:B:343:GLY:HA3	1:D:156:LEU:HD21	1.95	0.48
1:D:250:MET:HG3	1:D:278:ILE:HD13	1.95	0.48
1:E:309:ASP:OD2	1:E:309:ASP:N	2.41	0.48
1:C:336:ARG:NH2	1:C:388:ASP:OD1	2.35	0.48
1:D:214:ILE:HB	1:D:217:SER:OG	2.14	0.48
1:C:400:GLU:HA	1:C:400:GLU:OE1	2.13	0.48
1:D:168:VAL:HG22	1:D:189:VAL:HG22	1.96	0.48
3:E:502:HEM:HBC2	3:E:502:HEM:CMC	2.44	0.48
1:B:196:ARG:NE	1:B:196:ARG:CA	2.77	0.47
1:B:361:ALA:HA	1:B:364:LEU:CD2	2.43	0.47
3:B:502:HEM:HBC2	3:B:502:HEM:CMC	2.44	0.47
1:E:250:MET:HG3	1:E:278:ILE:HD13	1.95	0.47
1:D:288:ALA:HA	1:D:323:TRP:CD2	2.49	0.47
1:E:99:PHE:HB3	1:E:358:VAL:HG22	1.95	0.47
1:E:121:ARG:HH22	1:E:239:GLU:CD	2.22	0.47
1:C:232:HIS:CE1	1:C:260:THR:HG22	2.49	0.47
1:E:288:ALA:HA	1:E:323:TRP:CD2	2.50	0.47
1:F:245:ASP:O	1:F:247:LYS:CD	2.62	0.47
1:D:121:ARG:HH22	1:D:239:GLU:CD	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:HD13	1:A:317:ARG:CZ	2.44	0.47
1:B:288:ALA:HA	1:B:323:TRP:CD2	2.50	0.46
3:D:502:HEM:HBB2	3:D:502:HEM:CMB	2.45	0.46
1:F:296:THR:HG22	1:F:298:GLN:H	1.80	0.46
1:A:169:MET:HE2	1:A:173:MET:HG3	1.98	0.46
1:A:288:ALA:HA	1:A:323:TRP:CD2	2.51	0.46
1:B:293:LEU:HD23	1:C:389:ARG:HD2	1.97	0.46
1:F:288:ALA:HA	1:F:323:TRP:CD2	2.51	0.46
1:B:281:ASP:O	1:B:325:LYS:HA	2.15	0.46
1:B:121:ARG:HH22	1:B:239:GLU:CD	2.23	0.46
1:B:361:ALA:HA	1:B:364:LEU:HD22	1.97	0.46
1:E:200:PRO:O	1:E:201:GLU:HB2	2.16	0.46
1:C:376:ASP:CG	2:C:501:PLP:H2A2	2.41	0.46
1:A:121:ARG:HH22	1:A:239:GLU:CD	2.23	0.46
1:C:121:ARG:HH22	1:C:239:GLU:CD	2.23	0.46
1:D:197:PHE:O	1:D:204:VAL:HG11	2.16	0.46
1:E:119:LYS:HD2	1:E:150:THR:HG22	1.97	0.46
1:F:191:THR:HG21	1:F:203:HIS:HA	1.97	0.46
1:D:281:ASP:O	1:D:325:LYS:HA	2.16	0.46
1:E:169:MET:HE3	1:E:188:ILE:CG2	2.46	0.46
1:C:288:ALA:HA	1:C:323:TRP:CD2	2.50	0.46
1:C:119:LYS:NZ	2:C:501:PLP:O3	2.49	0.45
1:D:182:ARG:NH1	1:D:182:ARG:HB3	2.30	0.45
1:E:45:ARG:HE	1:E:45:ARG:HA	1.81	0.45
1:E:172:LYS:O	1:E:173:MET:HE2	2.16	0.45
1:A:247:LYS:HE3	4:A:608:HOH:O	2.16	0.45
1:A:83:LYS:HE3	1:C:88:PRO:HG3	1.99	0.45
3:A:502:HEM:HMC1	3:A:502:HEM:CBC	2.44	0.45
1:B:316:ASP:O	1:B:319:VAL:HG22	2.16	0.45
1:C:254:SER:CA	1:C:280:VAL:HG22	2.43	0.45
1:E:281:ASP:O	1:E:325:LYS:HA	2.16	0.45
1:F:316:ASP:O	1:F:319:VAL:HG22	2.15	0.45
1:B:193:THR:C	1:B:196:ARG:NH1	2.74	0.45
1:E:289:GLU:HB3	1:E:290:PRO:HD3	1.99	0.45
1:D:54:TRP:HB3	1:D:266:ARG:NH2	2.32	0.45
1:D:135:THR:CG2	1:D:218:HIS:CD2	3.00	0.45
3:E:502:HEM:HBC2	3:E:502:HEM:HMC1	1.98	0.45
1:A:336:ARG:NH2	1:A:388:ASP:OD1	2.30	0.45
1:B:391:MET:CE	1:B:396:PHE:HB3	2.46	0.45
1:D:277:ILE:HD12	1:D:277:ILE:N	2.32	0.45
1:E:168:VAL:HG22	1:E:189:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HG2	1:D:213:GLU:OE1	2.17	0.44
1:B:104:GLU:OE1	1:B:369:ARG:CD	2.65	0.44
1:F:168:VAL:HG22	1:F:189:VAL:HG22	1.98	0.44
1:F:55:GLN:HG3	1:F:58:ARG:HB2	1.99	0.44
1:A:281:ASP:O	1:A:325:LYS:HA	2.16	0.44
1:C:281:ASP:O	1:C:325:LYS:HA	2.18	0.44
1:C:316:ASP:O	1:C:319:VAL:HG22	2.18	0.44
1:E:316:ASP:O	1:E:319:VAL:HG22	2.18	0.44
1:A:316:ASP:O	1:A:319:VAL:HG22	2.17	0.44
1:C:53:THR:HG22	3:C:502:HEM:HMA3	2.00	0.44
1:C:170:PRO:HB2	1:C:173:MET:HE2	1.99	0.44
1:A:247:LYS:NZ	4:A:608:HOH:O	2.51	0.44
1:A:178:VAL:HG13	1:A:188:ILE:HD12	2.00	0.44
1:E:191:THR:HG21	1:E:203:HIS:HA	2.00	0.43
1:D:306:ILE:CG2	2:D:501:PLP:H6	2.48	0.43
1:D:316:ASP:O	1:D:319:VAL:HG22	2.18	0.43
1:E:364:LEU:HD22	1:E:368:GLN:NE2	2.34	0.43
1:B:324:PHE:CD2	1:C:393:GLN:HG3	2.53	0.43
1:E:254:SER:HB3	1:E:353:THR:HG22	1.99	0.43
1:A:74:PRO:HD3	1:A:82:LYS:HE2	2.00	0.43
1:C:171:GLU:O	1:C:172:LYS:HG3	2.19	0.43
1:C:191:THR:HG21	1:C:203:HIS:HA	2.01	0.43
1:F:263:GLY:HA2	3:F:502:HEM:HBC1	2.00	0.43
3:D:502:HEM:HBC2	3:D:502:HEM:CMC	2.47	0.43
1:E:177:LYS:NZ	1:E:304:GLU:OE2	2.52	0.43
2:C:501:PLP:O4P	2:C:501:PLP:C4A	2.67	0.43
1:D:316:ASP:OD1	1:D:318:THR:HG22	2.18	0.43
1:A:63:SER:HB2	3:A:502:HEM:HBB2	1.98	0.42
1:F:281:ASP:O	1:F:325:LYS:HA	2.19	0.42
1:F:396:PHE:O	1:F:397:LEU:O	2.37	0.42
1:C:380:ASN:ND2	4:C:603:HOH:O	2.48	0.42
1:B:104:GLU:OE1	1:B:369:ARG:HD3	2.18	0.42
1:B:119:LYS:HA	1:B:119:LYS:HD3	1.92	0.42
1:A:123:SER:HB2	4:A:609:HOH:O	2.18	0.42
1:A:156:LEU:CD1	1:C:343:GLY:HA3	2.50	0.42
1:D:248:LEU:HD13	1:D:371:VAL:HG23	2.01	0.42
1:F:250:MET:HG3	1:F:278:ILE:HD12	2.01	0.42
1:C:171:GLU:HG2	1:C:190:ARG:HB3	2.02	0.42
1:E:119:LYS:HE2	1:E:150:THR:HG23	2.00	0.42
1:E:250:MET:SD	1:E:278:ILE:HD13	2.60	0.42
1:F:326:SER:HA	1:F:330:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:394:LYS:HB3	1:F:396:PHE:CE2	2.55	0.41
1:A:248:LEU:HD13	1:A:371:VAL:HG23	2.01	0.41
1:F:228:ASN:HB3	1:F:229:PRO:CD	2.51	0.41
1:E:169:MET:HE3	1:E:188:ILE:HG23	2.01	0.41
1:F:76:ILE:O	1:F:76:ILE:CD1	2.67	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.94	0.41
1:A:228:ASN:HB3	1:A:229:PRO:CD	2.50	0.41
1:B:175:SER:CA	1:B:178:VAL:HG22	2.32	0.41
1:B:212:ASN:N	1:B:212:ASN:HD22	2.19	0.41
1:A:156:LEU:CD1	1:C:343:GLY:CA	2.99	0.41
1:D:196:ARG:HH12	1:D:198:ASP:HB2	1.85	0.41
1:D:228:ASN:HB3	1:D:229:PRO:CD	2.51	0.41
1:E:95:ILE:HG23	1:E:337:MET:CE	2.50	0.41
1:C:326:SER:HA	1:C:330:GLU:OE2	2.20	0.41
1:D:178:VAL:O	1:D:182:ARG:HG3	2.21	0.41
1:E:178:VAL:HG13	1:E:188:ILE:CD1	2.51	0.41
1:E:326:SER:HA	1:E:330:GLU:OE2	2.21	0.41
1:B:290:PRO:CD	1:B:293:LEU:HD12	2.50	0.40
1:F:119:LYS:NZ	2:F:501:PLP:O3	2.54	0.40
3:F:502:HEM:HBC2	3:F:502:HEM:CMC	2.50	0.40
1:A:156:LEU:HD11	1:C:343:GLY:O	2.20	0.40
1:B:70:PRO:HG2	1:B:242:GLN:HE22	1.86	0.40
1:B:316:ASP:OD1	1:B:318:THR:HG22	2.21	0.40
1:C:142:ILE:CD1	1:C:220:LEU:HD11	2.52	0.40
1:D:391:MET:HE3	1:D:396:PHE:HB3	2.04	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	348/363 (96%)	333 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	346/363 (95%)	330 (95%)	16 (5%)	0	100	100
1	C	356/363 (98%)	336 (94%)	19 (5%)	1 (0%)	36	50
1	D	351/363 (97%)	332 (95%)	19 (5%)	0	100	100
1	E	347/363 (96%)	328 (94%)	18 (5%)	1 (0%)	36	50
1	F	348/363 (96%)	331 (95%)	17 (5%)	0	100	100
All	All	2096/2178 (96%)	1990 (95%)	104 (5%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	399	GLU
1	E	290	PRO

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	283/304 (93%)	269 (95%)	14 (5%)	22	39
1	B	286/304 (94%)	262 (92%)	24 (8%)	10	17
1	C	293/304 (96%)	274 (94%)	19 (6%)	15	27
1	D	285/304 (94%)	268 (94%)	17 (6%)	17	31
1	E	289/304 (95%)	268 (93%)	21 (7%)	13	22
1	F	286/304 (94%)	270 (94%)	16 (6%)	19	33
All	All	1722/1824 (94%)	1611 (94%)	111 (6%)	16	28

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	73	SER
1	A	82	LYS
1	A	161	ARG

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Mol	Chain	Res	Type
1	A	175	SER
1	A	189	VAL
1	A	202	SER
1	A	247	LYS
1	A	280	VAL
1	A	286	ILE
1	A	311	ILE
1	A	325	LYS
1	A	387	SER
1	A	392	LEU
1	B	44	MET
1	B	56	LEU
1	B	58	ARG
1	B	61	SER
1	B	72	LYS
1	B	73	SER
1	B	77	LEU
1	B	175	SER
1	B	189	VAL
1	B	196	ARG
1	B	202	SER
1	B	220	LEU
1	B	248	LEU
1	B	276	ARG
1	B	287	LEU
1	B	318	THR
1	B	325	LYS
1	B	329	GLU
1	B	364	LEU
1	B	365	GLN
1	B	369	ARG
1	B	387	SER
1	B	391	MET
1	B	392	LEU
1	C	72	LYS
1	C	73	SER
1	C	82	LYS
1	C	101	LEU
1	C	102	LYS
1	C	142	ILE
1	C	161	ARG
1	C	171	GLU

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Mol	Chain	Res	Type
1	C	172	LYS
1	C	175	SER
1	C	182	ARG
1	C	202	SER
1	C	267	LYS
1	C	280	VAL
1	C	295	GLN
1	C	325	LYS
1	C	366	GLU
1	C	387	SER
1	C	400	GLU
1	D	44	MET
1	D	73	SER
1	D	156	LEU
1	D	161	ARG
1	D	175	SER
1	D	189	VAL
1	D	190	ARG
1	D	194	ASN
1	D	202	SER
1	D	209	ARG
1	D	247	LYS
1	D	289	GLU
1	D	292	GLU
1	D	295	GLN
1	D	318	THR
1	D	325	LYS
1	D	387	SER
1	E	45	ARG
1	E	53	THR
1	E	56	LEU
1	E	72	LYS
1	E	73	SER
1	E	83	LYS
1	E	97	LYS
1	E	142	ILE
1	E	175	SER
1	E	180	VAL
1	E	189	VAL
1	E	196	ARG
1	E	199	SER
1	E	202	SER

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Mol	Chain	Res	Type
1	E	224	ARG
1	E	287	LEU
1	E	289	GLU
1	E	296	THR
1	E	325	LYS
1	E	387	SER
1	E	393	GLN
1	F	45	ARG
1	F	55	GLN
1	F	72	LYS
1	F	73	SER
1	F	82	LYS
1	F	101	LEU
1	F	175	SER
1	F	189	VAL
1	F	194	ASN
1	F	202	SER
1	F	247	LYS
1	F	267	LYS
1	F	296	THR
1	F	325	LYS
1	F	387	SER
1	F	397	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	212	ASN
1	A	380	ASN
1	B	149	ASN
1	B	212	ASN
1	B	242	GLN
1	B	295	GLN
1	B	298	GLN
1	B	380	ASN
1	C	212	ASN
1	C	298	GLN
1	D	149	ASN
1	D	218	HIS
1	D	380	ASN
1	D	393	GLN

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Mol	Chain	Res	Type
1	E	149	ASN
1	E	368	GLN
1	E	380	ASN
1	F	149	ASN
1	F	212	ASN
1	F	380	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
2	PLP	B	501	1	15,15,16	0.95	1 (6%)	21,22,23	1.05	2 (9%)
2	PLP	E	501	1	15,15,16	0.82	1 (6%)	21,22,23	0.73	1 (4%)
3	HEM	E	502	1	50,50,50	1.58	8 (16%)	67,82,82	2.03	20 (29%)
2	PLP	C	501	1	15,15,16	0.90	0	21,22,23	1.23	2 (9%)
3	HEM	C	502	1	50,50,50	1.65	11 (22%)	67,82,82	1.96	14 (20%)
3	HEM	B	502	1	50,50,50	1.70	11 (22%)	67,82,82	1.53	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	F	502	1	50,50,50	1.73	8 (16%)	67,82,82	1.60	11 (16%)
2	PLP	F	501	1	15,15,16	0.91	1 (6%)	21,22,23	1.02	2 (9%)
3	HEM	D	502	1	50,50,50	1.81	10 (20%)	67,82,82	1.46	13 (19%)
3	HEM	A	502	1	50,50,50	1.72	9 (18%)	67,82,82	1.85	18 (26%)
2	PLP	A	501	1	15,15,16	0.88	1 (6%)	21,22,23	1.30	4 (19%)
2	PLP	D	501	1	15,15,16	0.97	1 (6%)	21,22,23	1.03	1 (4%)

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	PLP	B	501	1	-	0/6/6/8	0/1/1/1
2	PLP	E	501	1	-	5/6/6/8	0/1/1/1
3	HEM	E	502	1	-	4/14/54/54	-
2	PLP	C	501	1	-	4/6/6/8	0/1/1/1
3	HEM	C	502	1	-	5/14/54/54	-
3	HEM	B	502	1	-	4/14/54/54	-
3	HEM	F	502	1	-	2/14/54/54	-
2	PLP	F	501	1	-	0/6/6/8	0/1/1/1
3	HEM	D	502	1	-	2/14/54/54	-
3	HEM	A	502	1	-	3/14/54/54	-
2	PLP	A	501	1	-	5/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	FE-NB	5.36	2.11	1.94
3	C	502	HEM	FE-NB	5.21	2.10	1.94
3	F	502	HEM	FE-NC	5.12	2.12	1.95
3	F	502	HEM	FE-NB	4.74	2.09	1.94
3	D	502	HEM	C4D-ND	-4.71	1.32	1.40
3	C	502	HEM	C1B-NB	-4.57	1.32	1.40
3	E	502	HEM	FE-NB	4.46	2.08	1.94
3	B	502	HEM	C4B-NB	-4.37	1.30	1.38
3	D	502	HEM	FE-NC	4.36	2.09	1.95
3	A	502	HEM	C1B-NB	-4.34	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	HEM	C4D-ND	-4.29	1.32	1.40
3	F	502	HEM	C4D-ND	-4.23	1.32	1.40
3	A	502	HEM	FE-NC	4.09	2.08	1.95
3	D	502	HEM	FE-NB	3.85	2.06	1.94
3	E	502	HEM	FE-NC	3.83	2.07	1.95
3	A	502	HEM	C4D-ND	-3.61	1.34	1.40
3	B	502	HEM	C1C-NC	-3.56	1.32	1.39
3	B	502	HEM	FE-NB	3.46	2.05	1.94
3	D	502	HEM	C1B-NB	-3.45	1.34	1.40
3	D	502	HEM	C4B-NB	-3.38	1.32	1.38
3	E	502	HEM	C4B-NB	-3.31	1.32	1.38
3	B	502	HEM	C4D-ND	-3.25	1.34	1.40
3	B	502	HEM	FE-NC	3.24	2.05	1.95
3	C	502	HEM	C4D-ND	-3.23	1.34	1.40
3	F	502	HEM	C3B-C4B	3.19	1.51	1.44
3	F	502	HEM	C1B-NB	-3.14	1.34	1.40
3	D	502	HEM	C1D-ND	-3.09	1.32	1.38
3	D	502	HEM	C1C-NC	-3.05	1.33	1.39
3	E	502	HEM	C3B-C4B	2.92	1.50	1.44
3	C	502	HEM	C1D-ND	-2.91	1.33	1.38
3	B	502	HEM	C1B-NB	-2.91	1.35	1.40
3	B	502	HEM	C3B-C4B	2.85	1.50	1.44
3	A	502	HEM	C3B-C4B	2.84	1.50	1.44
3	E	502	HEM	C1D-ND	-2.79	1.33	1.38
3	B	502	HEM	C1C-C2C	-2.77	1.39	1.45
3	A	502	HEM	C4A-NA	-2.75	1.34	1.39
2	D	501	PLP	C4A-C4	-2.73	1.46	1.51
2	B	501	PLP	C4A-C4	-2.68	1.46	1.51
2	E	501	PLP	C4A-C4	-2.66	1.46	1.51
3	C	502	HEM	FE-NC	2.62	2.03	1.95
3	D	502	HEM	FE-ND	-2.48	1.87	1.94
2	A	501	PLP	C4A-C4	-2.46	1.46	1.51
2	F	501	PLP	C4A-C4	-2.44	1.46	1.51
3	E	502	HEM	FE-ND	-2.43	1.87	1.94
3	B	502	HEM	O1A-CGA	2.42	1.30	1.22
3	B	502	HEM	C1D-ND	-2.40	1.34	1.38
3	C	502	HEM	FE-ND	-2.38	1.87	1.94
3	A	502	HEM	C1B-C2B	-2.32	1.39	1.44
3	D	502	HEM	C3B-C4B	2.31	1.49	1.44
3	D	502	HEM	C4C-NC	-2.30	1.35	1.39
3	C	502	HEM	C1C-NC	-2.25	1.35	1.39
3	A	502	HEM	CMA-C3A	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	HEM	C4B-NB	-2.21	1.34	1.38
3	F	502	HEM	C1A-NA	-2.19	1.35	1.39
3	E	502	HEM	C1C-NC	-2.13	1.35	1.39
3	C	502	HEM	C4B-NB	-2.11	1.34	1.38
3	C	502	HEM	C4C-NC	-2.10	1.35	1.39
3	A	502	HEM	FE-NA	2.09	2.02	1.95
3	F	502	HEM	C4A-NA	-2.09	1.35	1.39
3	C	502	HEM	C3C-C4C	-2.04	1.42	1.46
3	C	502	HEM	C1A-C2A	-2.01	1.40	1.44
3	B	502	HEM	O1D-CGD	2.00	1.28	1.22

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	HEM	CAA-C2A-C1A	5.71	136.09	124.94
3	A	502	HEM	C3B-C4B-NB	-5.39	105.60	109.47
3	E	502	HEM	C3B-C4B-NB	-4.82	106.01	109.47
3	F	502	HEM	CBA-CAA-C2A	4.69	125.49	112.53
3	C	502	HEM	CAA-C2A-C3A	-4.65	116.63	127.07
3	A	502	HEM	CHD-C1D-ND	4.63	129.41	124.42
3	C	502	HEM	CBA-CAA-C2A	4.51	125.01	112.53
3	E	502	HEM	CMC-C2C-C1C	4.38	132.44	124.73
3	E	502	HEM	CHC-C1C-NC	-4.38	119.69	124.45
3	C	502	HEM	CHD-C1D-ND	4.35	129.10	124.42
3	E	502	HEM	C1B-NB-C4B	4.24	110.23	105.21
3	E	502	HEM	CHC-C4B-NB	4.18	128.92	124.42
3	E	502	HEM	CMB-C2B-C1B	4.12	131.47	125.03
3	F	502	HEM	C1B-NB-C4B	4.11	110.08	105.21
3	F	502	HEM	CHC-C4B-NB	4.00	128.73	124.42
3	E	502	HEM	CAD-C3D-C2D	3.97	135.30	127.87
3	B	502	HEM	CHB-C1B-NB	3.89	129.18	124.37
3	D	502	HEM	CBD-CAD-C3D	-3.70	102.31	112.53
3	B	502	HEM	C1B-NB-C4B	3.64	109.51	105.21
3	A	502	HEM	CHB-C1B-NB	3.59	128.80	124.37
3	F	502	HEM	CHD-C1D-ND	3.56	128.25	124.42
3	A	502	HEM	CAB-C3B-C2B	-3.54	116.92	128.43
3	D	502	HEM	CHB-C1B-NB	3.48	128.68	124.37
3	C	502	HEM	CHD-C1D-C2D	-3.47	119.56	125.03
3	C	502	HEM	CHA-C4D-ND	3.44	128.63	124.37
3	B	502	HEM	CBD-CAD-C3D	-3.44	103.02	112.53
3	F	502	HEM	CAA-CBA-CGA	-3.41	104.62	113.67
3	D	502	HEM	C1B-NB-C4B	3.41	109.25	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	HEM	CHA-C4D-C3D	-3.35	119.05	125.23
3	D	502	HEM	CHD-C1D-ND	3.35	128.02	124.42
3	D	502	HEM	O2A-CGA-CBA	3.32	124.48	114.00
3	B	502	HEM	CHD-C1D-C2D	-3.27	119.87	125.03
3	C	502	HEM	O2D-CGD-CBD	3.25	124.27	114.00
3	B	502	HEM	CHC-C4B-NB	3.22	127.89	124.42
3	E	502	HEM	CHB-C1B-NB	3.22	128.34	124.37
3	A	502	HEM	C4C-NC-C1C	3.20	111.04	105.82
3	A	502	HEM	C1B-NB-C4B	3.16	108.95	105.21
3	E	502	HEM	CHA-C4D-ND	3.15	128.27	124.37
3	F	502	HEM	CHA-C4D-ND	3.13	128.24	124.37
3	B	502	HEM	CHD-C1D-ND	3.13	127.79	124.42
3	F	502	HEM	C3B-C4B-NB	-3.08	107.26	109.47
3	B	502	HEM	CHD-C4C-NC	3.06	127.79	124.45
3	A	502	HEM	CHD-C4C-NC	3.03	127.75	124.45
2	B	501	PLP	O4P-C5A-C5	2.97	114.93	109.36
2	C	501	PLP	C4A-C4-C5	-2.94	117.91	120.94
3	A	502	HEM	CHA-C4D-ND	2.88	127.93	124.37
3	F	502	HEM	CHB-C1B-NB	2.88	127.93	124.37
3	E	502	HEM	CAB-C3B-C2B	-2.87	119.09	128.43
3	A	502	HEM	CHB-C1B-C2B	-2.87	118.80	126.95
3	E	502	HEM	O2D-CGD-CBD	2.86	123.03	114.00
3	C	502	HEM	CHD-C4C-NC	2.86	127.56	124.45
3	C	502	HEM	CAA-CBA-CGA	-2.82	106.18	113.67
3	E	502	HEM	C3C-C2C-C1C	-2.81	104.39	107.05
3	A	502	HEM	O2D-CGD-O1D	-2.79	116.16	123.33
3	F	502	HEM	CHA-C4D-C3D	-2.76	120.13	125.23
2	A	501	PLP	O4P-P-O1P	-2.75	99.01	106.44
2	D	501	PLP	O4P-C5A-C5	2.73	114.48	109.36
3	A	502	HEM	CBD-CAD-C3D	-2.69	105.09	112.53
3	C	502	HEM	CHC-C4B-NB	2.66	127.29	124.42
3	A	502	HEM	CAB-C3B-C4B	2.66	136.14	124.39
3	B	502	HEM	C3B-C4B-NB	-2.64	107.57	109.47
3	D	502	HEM	CHC-C4B-NB	2.63	127.26	124.42
3	A	502	HEM	O2D-CGD-CBD	2.63	122.31	114.00
3	D	502	HEM	C4D-C3D-C2D	-2.61	103.09	106.89
3	B	502	HEM	CHB-C1B-C2B	-2.59	119.57	126.95
3	A	502	HEM	C3C-C2C-C1C	2.57	109.48	107.05
3	D	502	HEM	O2A-CGA-O1A	-2.54	116.81	123.33
3	F	502	HEM	CHD-C1D-C2D	-2.54	121.03	125.03
3	C	502	HEM	C4C-NC-C1C	2.53	109.95	105.82
3	C	502	HEM	CHC-C1C-NC	2.53	127.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	HEM	C1A-CHA-C4D	-2.52	120.33	126.25
3	B	502	HEM	CAD-C3D-C4D	2.51	129.08	124.70
2	A	501	PLP	O3-C3-C4	2.50	124.63	118.10
3	B	502	HEM	C4C-NC-C1C	2.48	109.87	105.82
3	E	502	HEM	CAD-C3D-C4D	-2.43	120.47	124.70
2	A	501	PLP	O3P-P-O4P	-2.39	100.44	106.67
3	A	502	HEM	C4C-CHD-C1D	-2.31	121.10	126.02
3	E	502	HEM	CBD-CAD-C3D	2.31	118.93	112.53
3	B	502	HEM	CAA-CBA-CGA	-2.30	107.57	113.67
3	D	502	HEM	C4C-NC-C1C	2.27	109.51	105.82
3	F	502	HEM	C4B-C3B-C2B	-2.25	105.21	107.28
3	D	502	HEM	CHD-C1D-C2D	-2.24	121.49	125.03
3	E	502	HEM	CMB-C2B-C3B	-2.23	123.03	128.43
3	D	502	HEM	CHB-C1B-C2B	-2.21	120.66	126.95
3	C	502	HEM	C4B-C3B-C2B	-2.21	105.25	107.28
2	C	501	PLP	O4P-C5A-C5	2.20	113.48	109.36
3	E	502	HEM	O1D-CGD-CBD	-2.19	116.16	123.09
3	E	502	HEM	CMC-C2C-C3C	-2.17	123.17	128.43
3	A	502	HEM	CMB-C2B-C1B	2.17	128.42	125.03
3	E	502	HEM	C3D-C4D-ND	2.16	112.54	110.17
3	D	502	HEM	CHD-C4C-C3C	2.16	128.85	125.21
2	F	501	PLP	O3-C3-C4	2.15	123.71	118.10
3	E	502	HEM	C4A-CHB-C1B	-2.13	121.24	126.25
2	A	501	PLP	O4P-C5A-C5	2.12	113.33	109.36
3	A	502	HEM	C2B-C1B-NB	2.11	112.27	109.84
3	A	502	HEM	C4D-ND-C1D	2.07	107.66	105.21
2	F	501	PLP	O4P-C5A-C5	2.07	113.24	109.36
2	E	501	PLP	O3-C3-C4	2.06	123.49	118.10
2	B	501	PLP	O2P-P-O4P	-2.05	101.33	106.67
3	B	502	HEM	C2D-C1D-ND	2.03	112.25	109.90
3	D	502	HEM	C4B-C3B-C2B	-2.01	105.43	107.28

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C4-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P
2	C	501	PLP	C4-C5-C5A-O4P
2	C	501	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	C	501	PLP	C5A-O4P-P-O2P
2	C	501	PLP	C5A-O4P-P-O3P
2	E	501	PLP	C4-C5-C5A-O4P
2	E	501	PLP	C6-C5-C5A-O4P
2	E	501	PLP	C5A-O4P-P-O2P
2	E	501	PLP	C5A-O4P-P-O3P
3	C	502	HEM	C1A-C2A-CAA-CBA
3	E	502	HEM	C4D-C3D-CAD-CBD
3	E	502	HEM	C2D-C3D-CAD-CBD
3	C	502	HEM	C2A-CAA-CBA-CGA
3	B	502	HEM	C2A-CAA-CBA-CGA
3	C	502	HEM	C3A-C2A-CAA-CBA
2	A	501	PLP	C5A-O4P-P-O1P
2	E	501	PLP	C5A-O4P-P-O1P
3	E	502	HEM	C4B-C3B-CAB-CBB
3	A	502	HEM	C4B-C3B-CAB-CBB
3	D	502	HEM	CAA-CBA-CGA-O1A
3	D	502	HEM	CAA-CBA-CGA-O2A
3	C	502	HEM	CAA-CBA-CGA-O1A
3	A	502	HEM	CAA-CBA-CGA-O1A
3	B	502	HEM	CAA-CBA-CGA-O1A
3	B	502	HEM	C3D-CAD-CBD-CGD
3	A	502	HEM	CAA-CBA-CGA-O2A
3	F	502	HEM	CAA-CBA-CGA-O1A
3	F	502	HEM	CAA-CBA-CGA-O2A
3	C	502	HEM	CAA-CBA-CGA-O2A
3	B	502	HEM	CAA-CBA-CGA-O2A
3	E	502	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

10 monomers are involved in 39 short contacts:

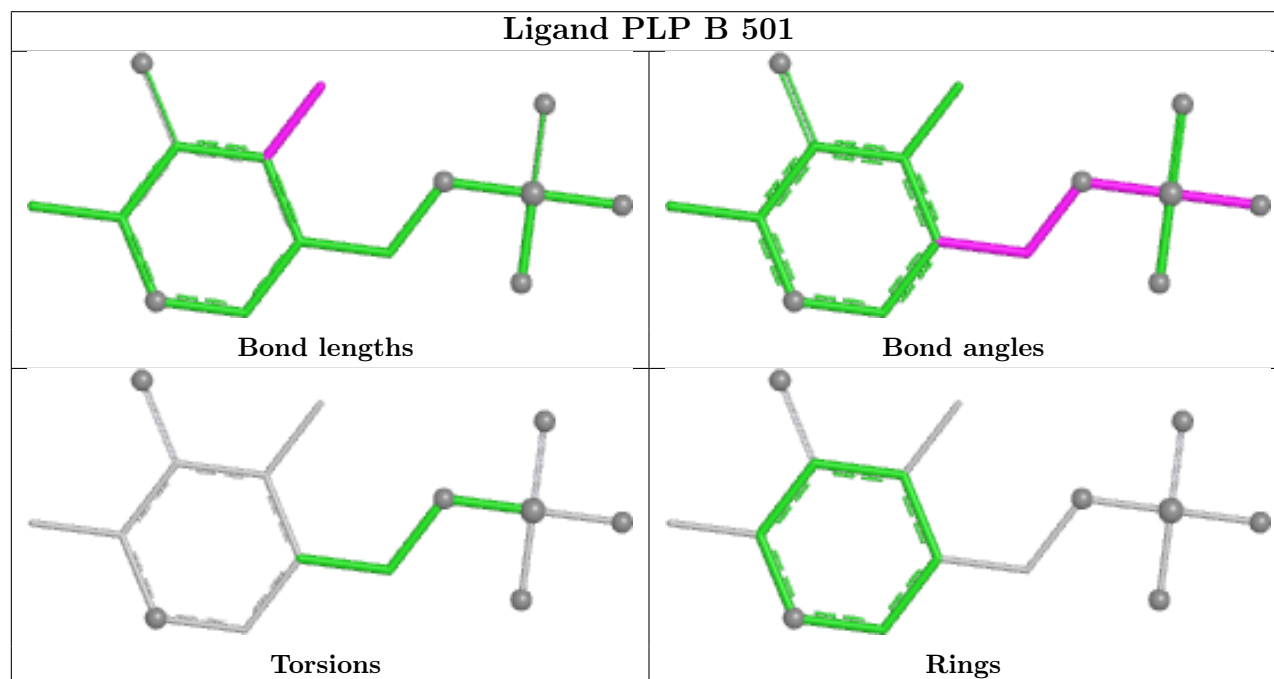
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	PLP	1	0
3	E	502	HEM	5	0
2	C	501	PLP	4	0
3	C	502	HEM	12	0
3	B	502	HEM	2	0
3	F	502	HEM	4	0
2	F	501	PLP	1	0
3	D	502	HEM	4	0
3	A	502	HEM	5	0

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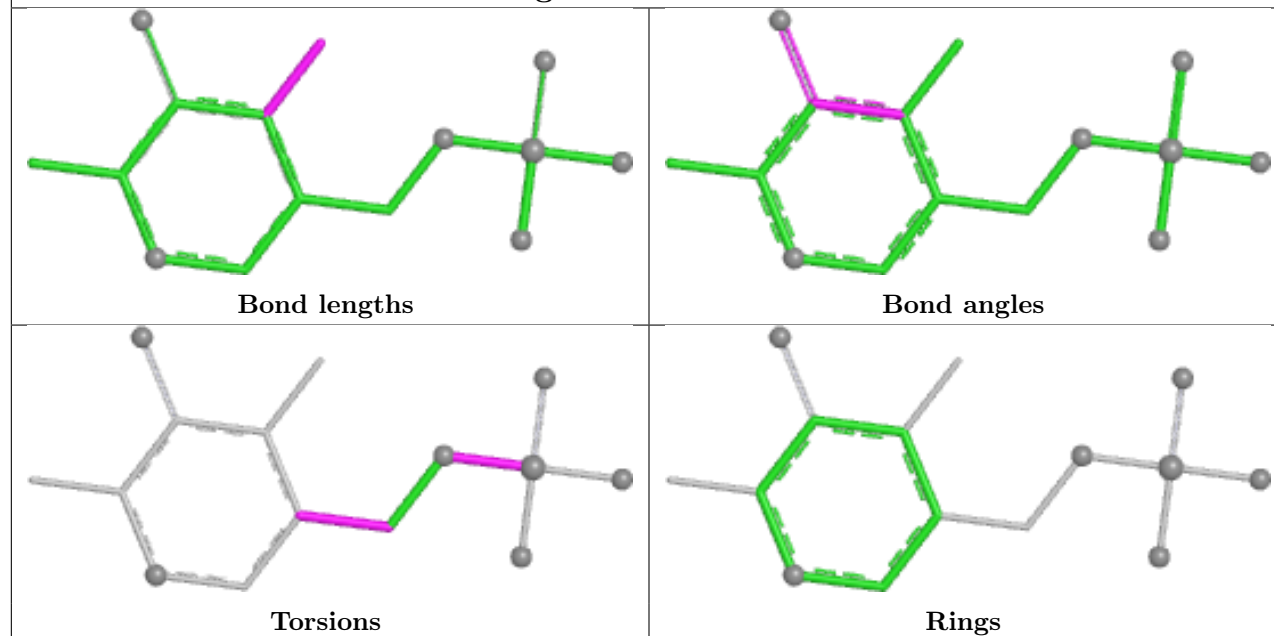
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PLP	1	0

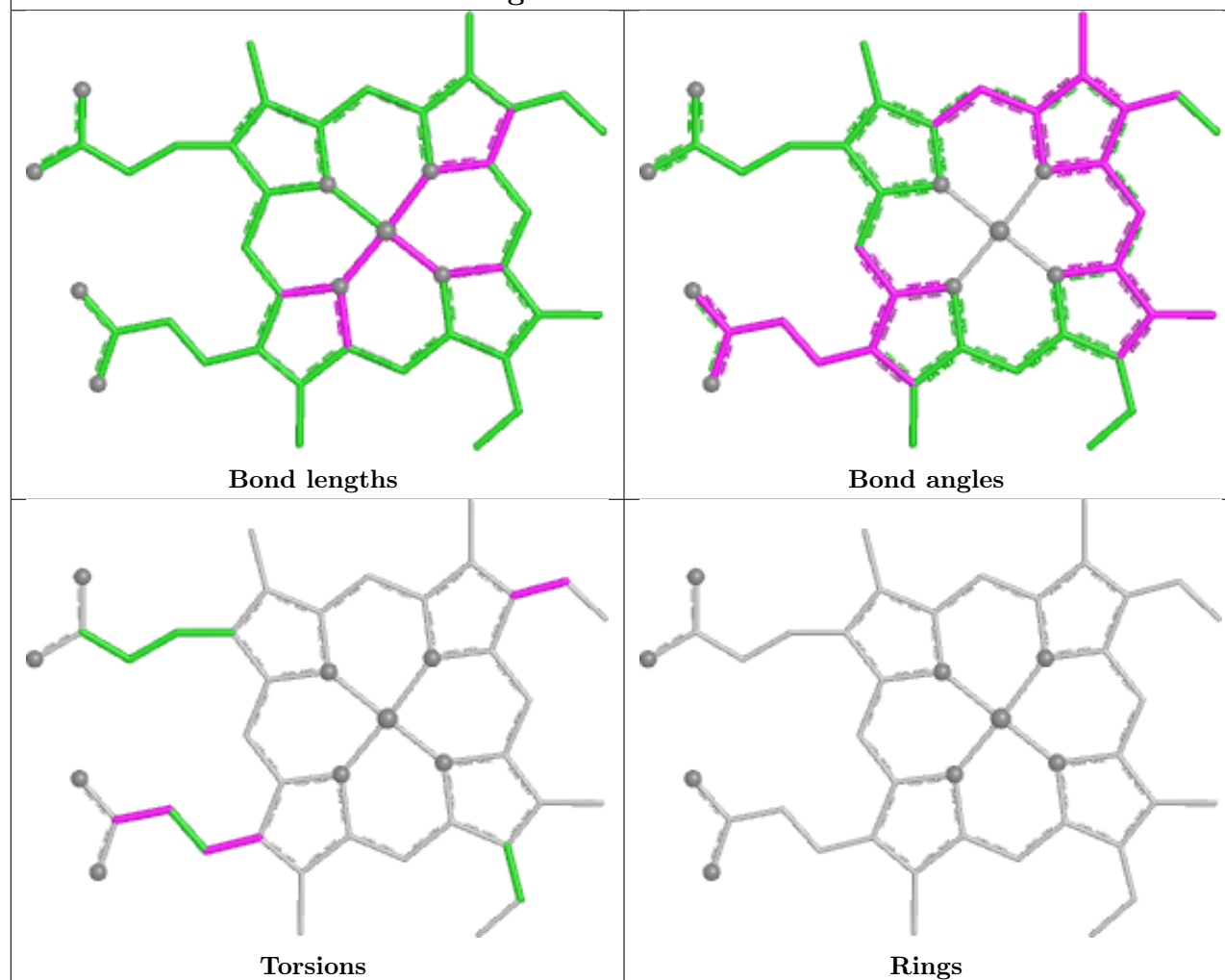
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



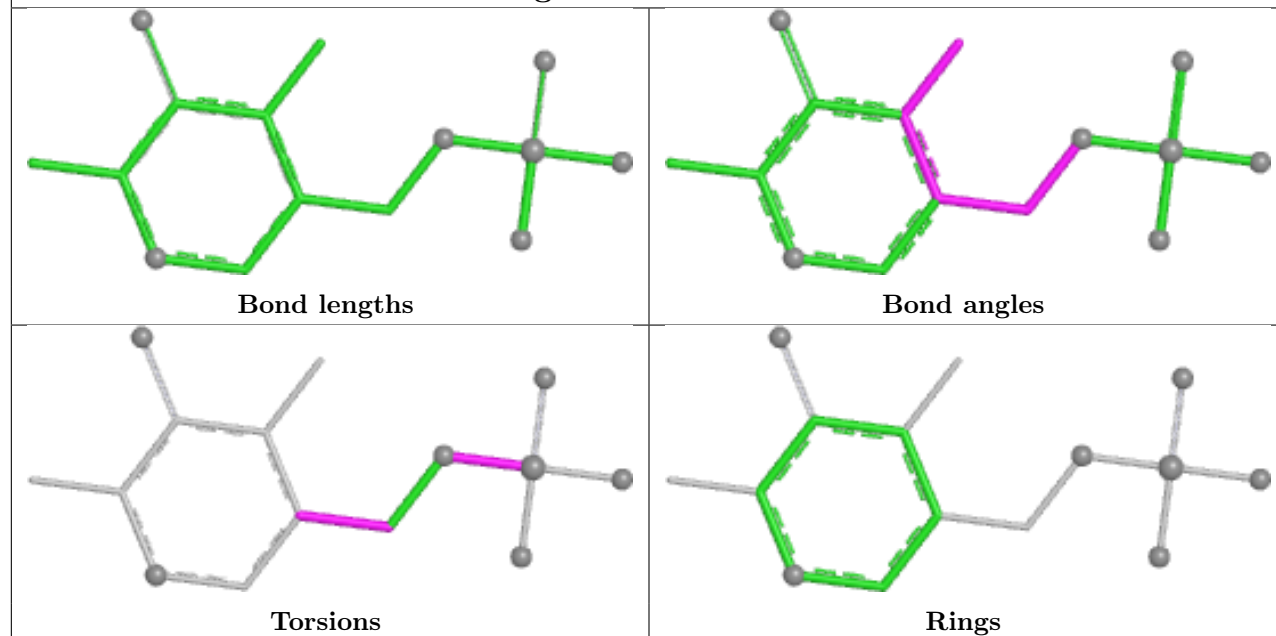
Ligand PLP E 501



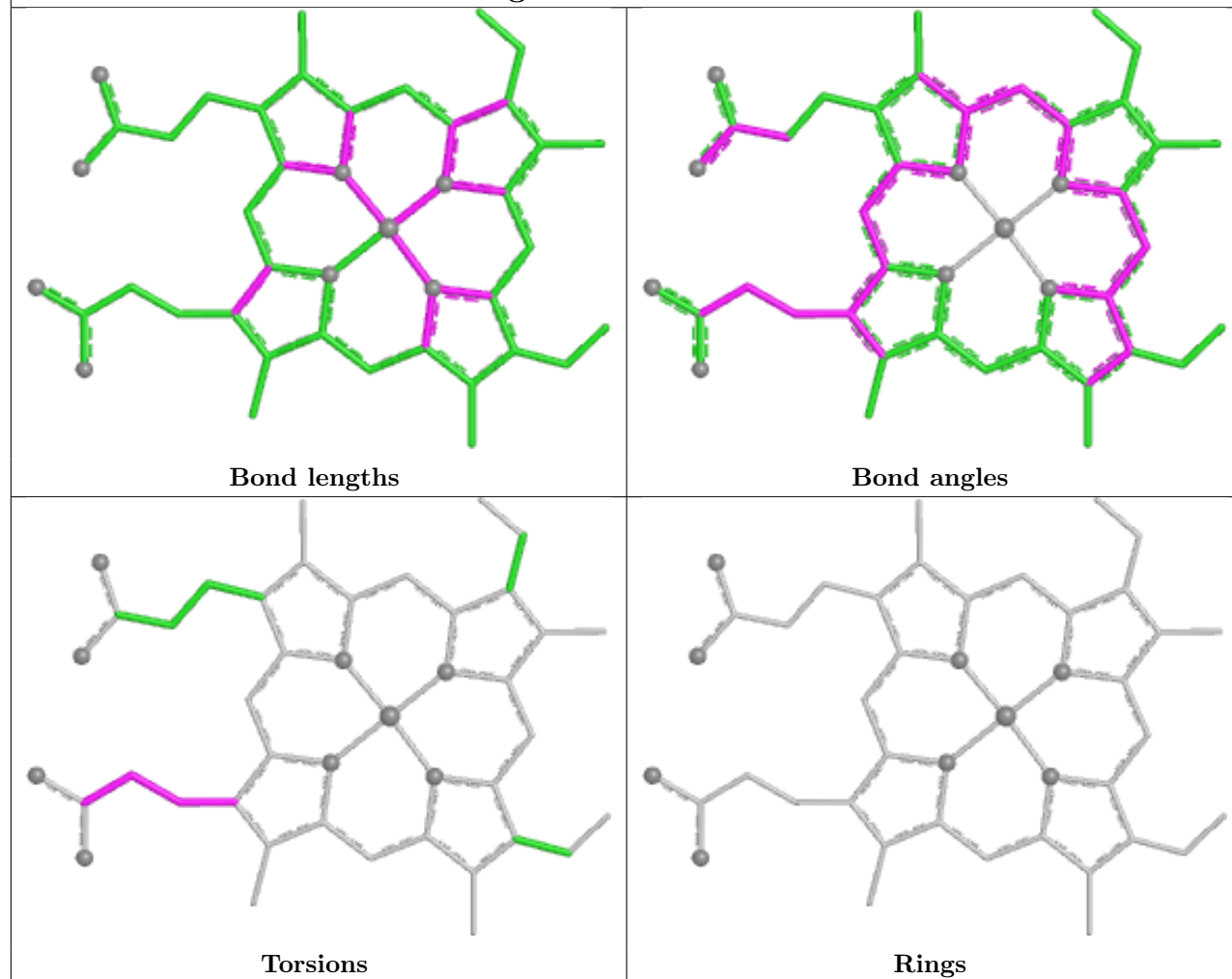
Ligand HEM E 502

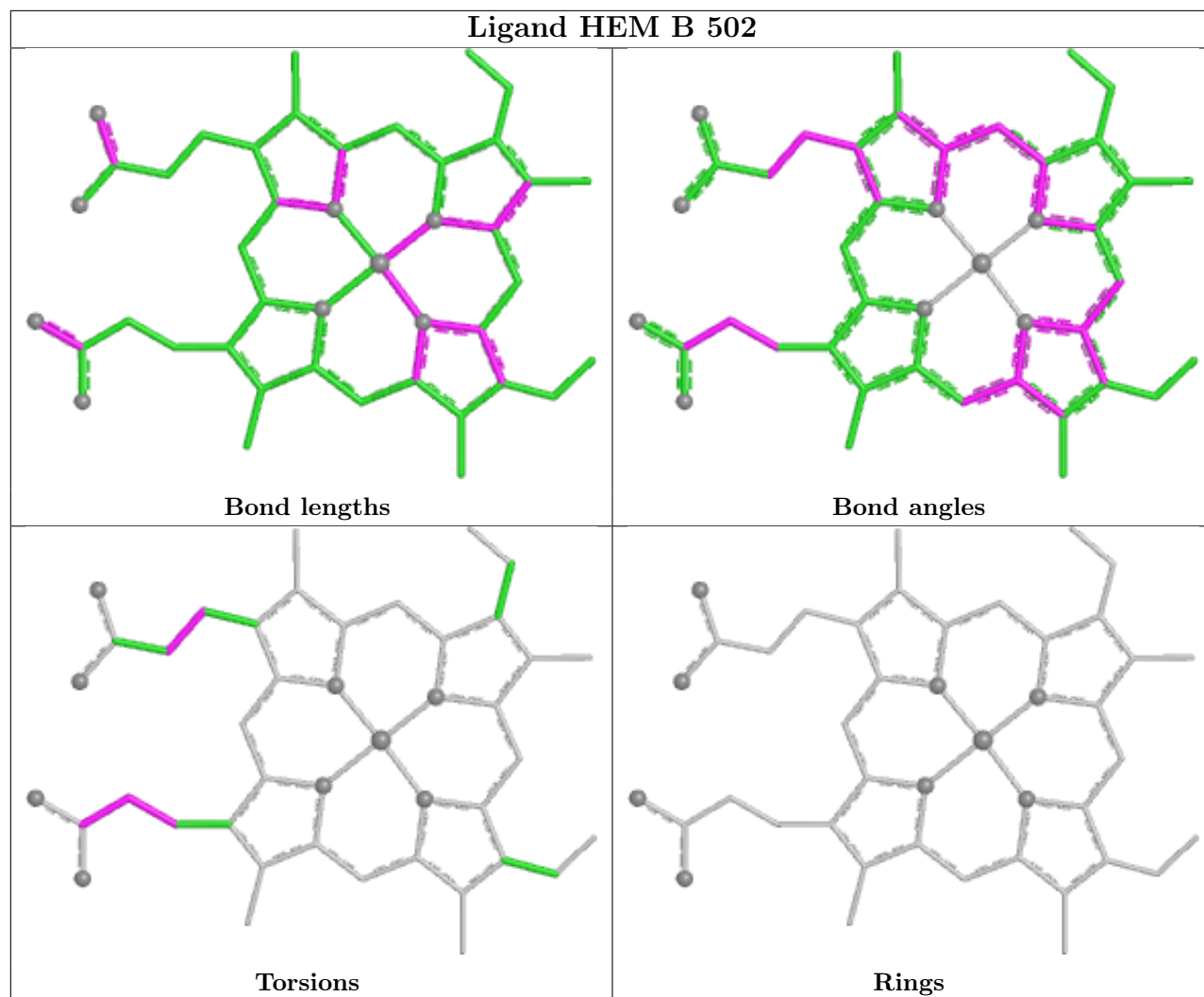


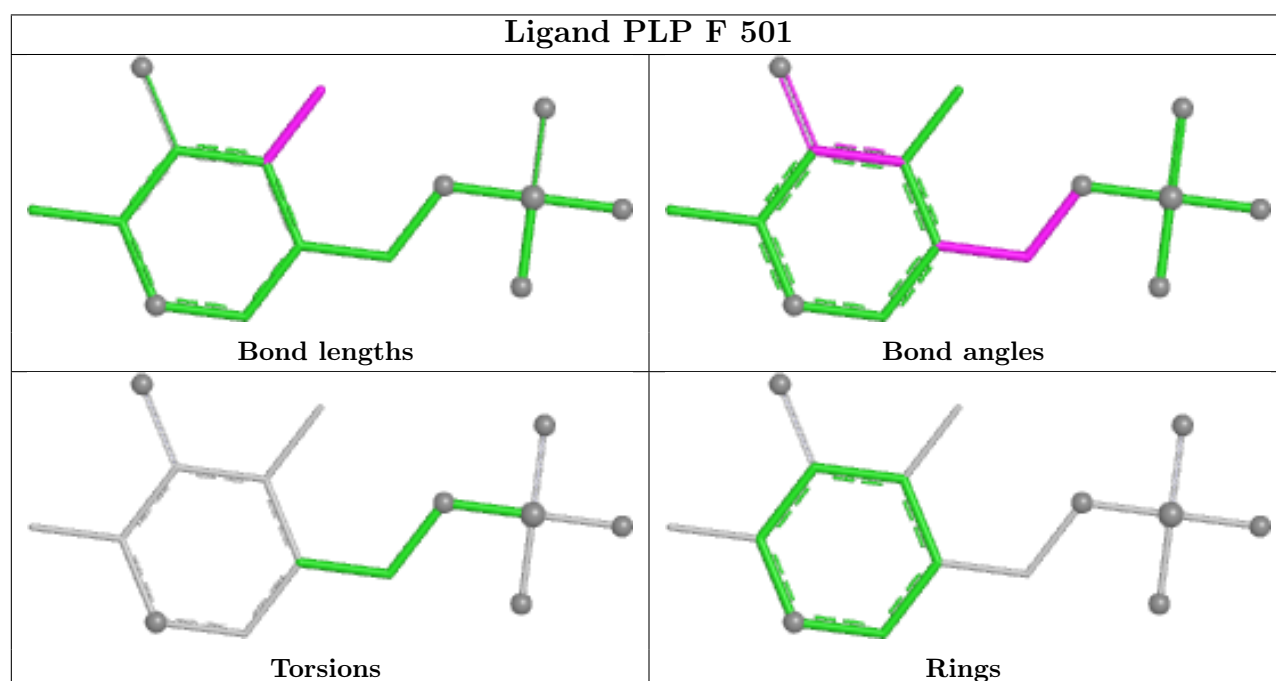
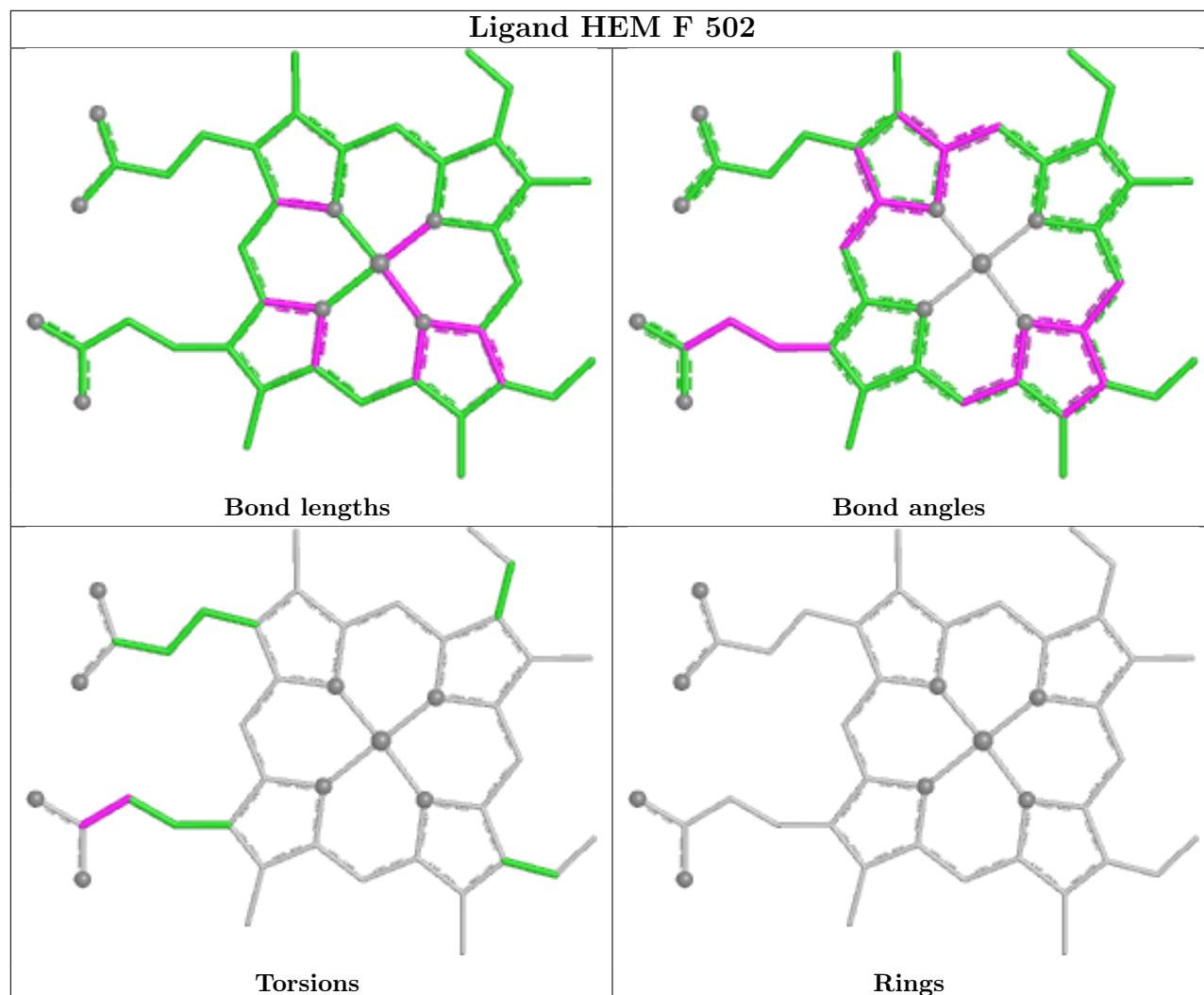
Ligand PLP C 501

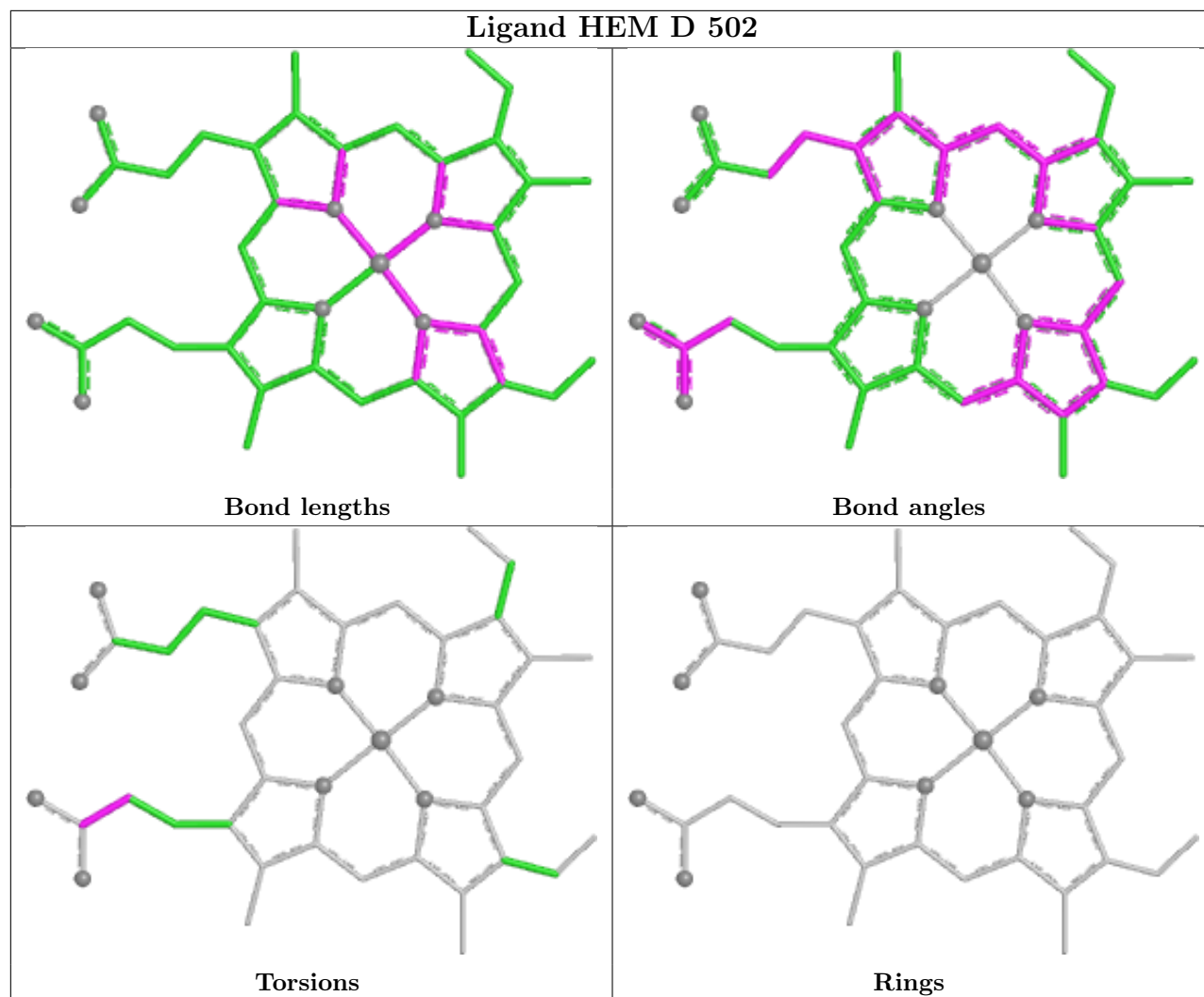


Ligand HEM C 502

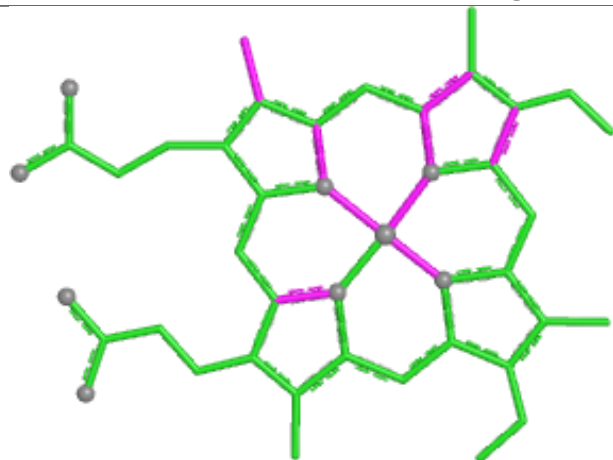




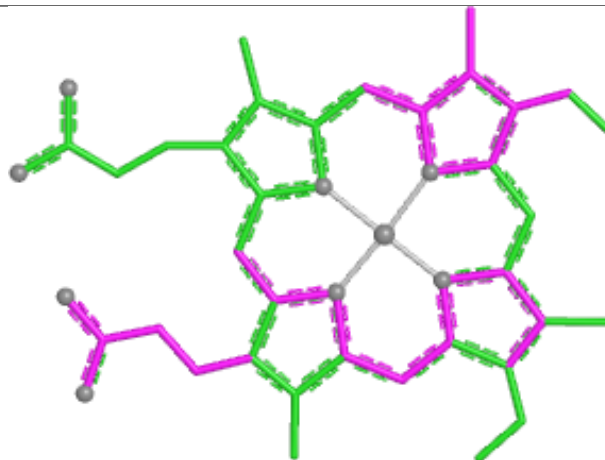




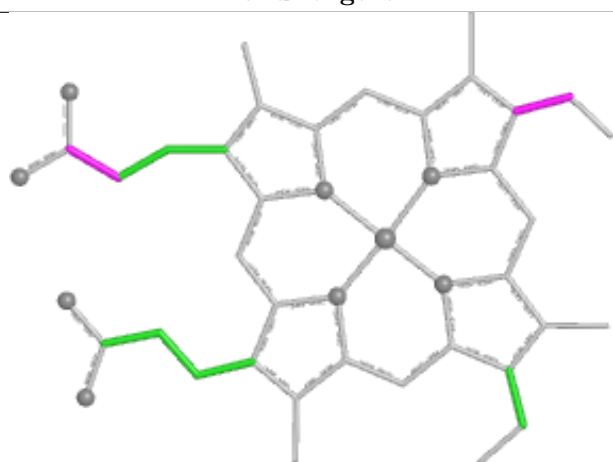
Ligand HEM A 502



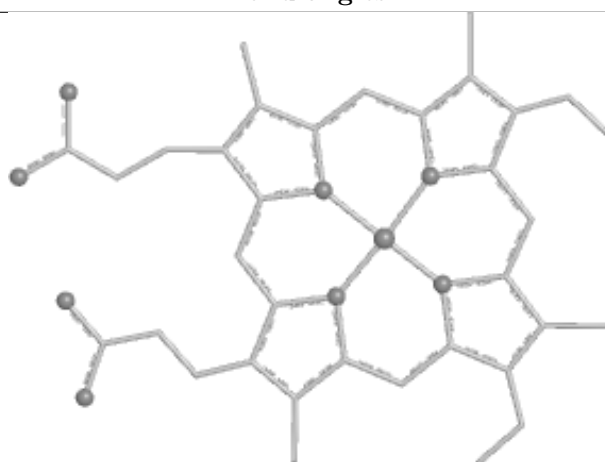
Bond lengths



Bond angles

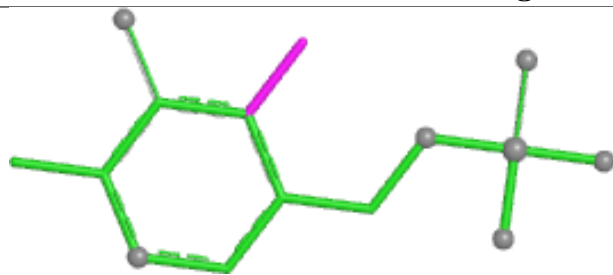


Torsions

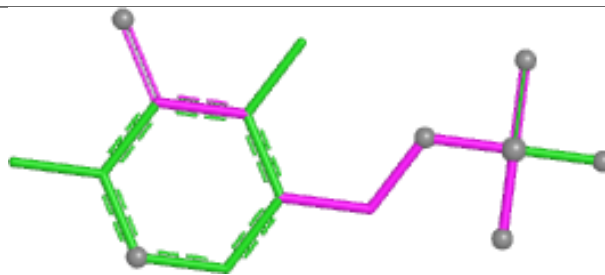


Rings

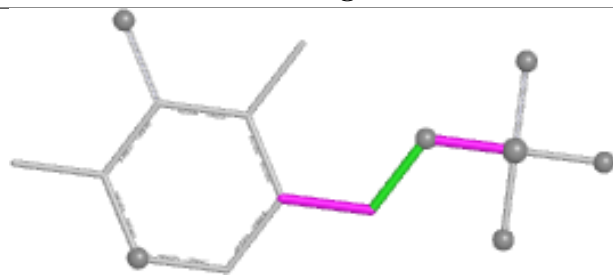
Ligand PLP A 501



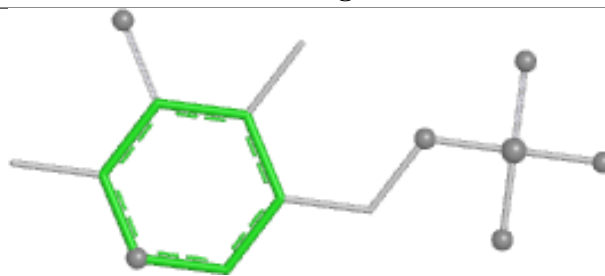
Bond lengths



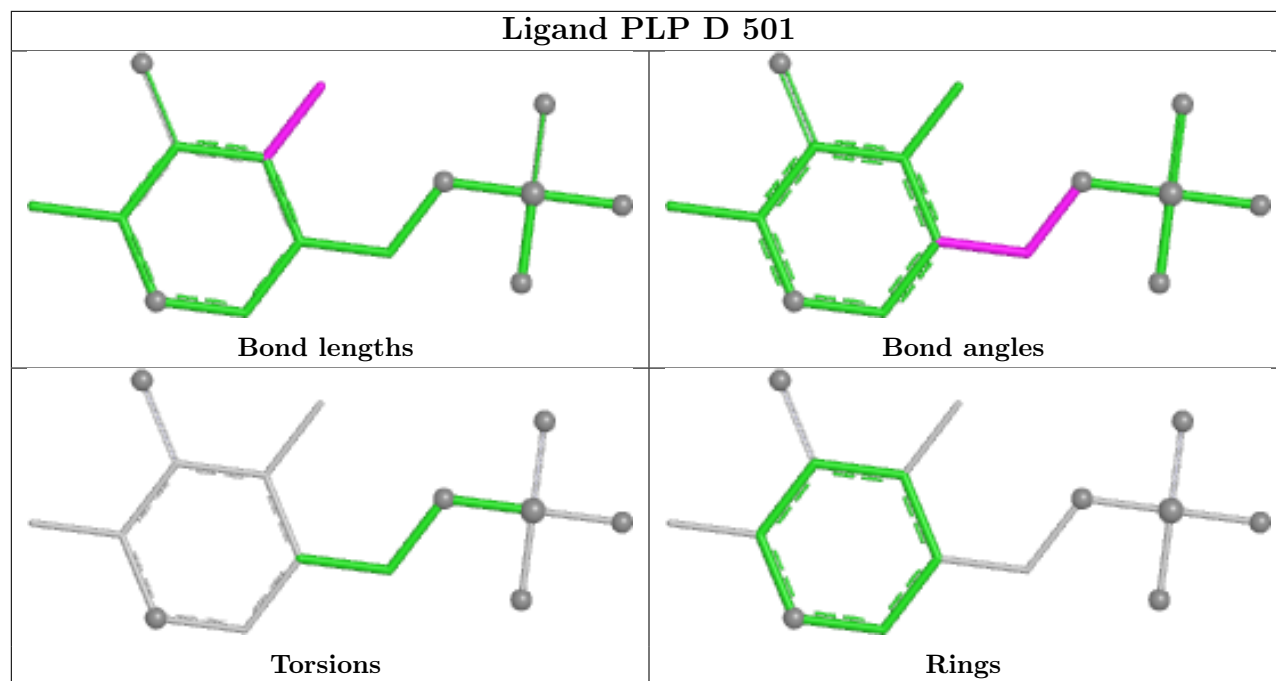
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	352/363 (96%)	0.26	18 (5%)	33	30	20, 34, 65, 94	0
1	B	352/363 (96%)	0.63	30 (8%)	16	13	23, 42, 78, 107	0
1	C	358/363 (98%)	0.40	23 (6%)	25	22	21, 36, 74, 116	0
1	D	353/363 (97%)	0.69	32 (9%)	15	12	26, 44, 92, 128	0
1	E	351/363 (96%)	0.69	27 (7%)	19	16	25, 46, 85, 128	0
1	F	352/363 (96%)	0.54	23 (6%)	25	21	22, 41, 77, 131	0
All	All	2118/2178 (97%)	0.53	153 (7%)	21	18	20, 41, 80, 131	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	397	LEU	6.5
1	B	197	PHE	5.9
1	C	195	ALA	5.8
1	F	197	PHE	5.8
1	C	194	ASN	5.3
1	C	299	THR	5.2
1	E	59	PRO	4.5
1	D	195	ALA	4.5
1	D	392	LEU	4.5
1	C	44	MET	4.2
1	A	289	GLU	4.0
1	D	299	THR	4.0
1	B	208	TRP	4.0
1	D	208	TRP	4.0
1	A	201	GLU	3.9
1	B	299	THR	3.9
1	A	392	LEU	3.9
1	F	195	ALA	3.8
1	E	44	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	193	THR	3.7
1	F	71	ALA	3.7
1	D	221	ASP	3.7
1	B	399	GLU	3.7
1	B	72	LYS	3.6
1	A	197	PHE	3.6
1	E	190	ARG	3.5
1	E	195	ALA	3.5
1	E	290	PRO	3.5
1	D	194	ASN	3.4
1	D	192	PRO	3.4
1	B	56	LEU	3.4
1	C	290	PRO	3.4
1	A	68	THR	3.4
1	D	308	TYR	3.3
1	E	208	TRP	3.3
1	E	63	SER	3.3
1	E	147	SER	3.2
1	A	198	ASP	3.2
1	C	198	ASP	3.2
1	D	301	TYR	3.2
1	D	197	PHE	3.1
1	B	392	LEU	3.1
1	C	193	THR	3.1
1	E	302	GLU	3.1
1	C	309	ASP	3.1
1	B	196	ARG	3.1
1	D	44	MET	3.0
1	F	72	LYS	3.0
1	D	193	THR	3.0
1	E	99	PHE	3.0
1	B	289	GLU	2.9
1	A	290	PRO	2.9
1	A	398	LYS	2.9
1	A	193	THR	2.9
1	C	398	LYS	2.9
1	B	397	LEU	2.9
1	F	298	GLN	2.8
1	B	398	LYS	2.8
1	C	197	PHE	2.8
1	E	197	PHE	2.8
1	F	392	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	196	ARG	2.8
1	F	296	THR	2.8
1	F	299	THR	2.8
1	C	247	LYS	2.7
1	A	172	LYS	2.7
1	E	172	LYS	2.7
1	F	283	GLU	2.7
1	D	395	GLY	2.7
1	C	172	LYS	2.7
1	C	173	MET	2.7
1	E	56	LEU	2.7
1	A	208	TRP	2.7
1	C	289	GLU	2.7
1	D	318	THR	2.7
1	D	196	ARG	2.6
1	B	193	THR	2.6
1	B	290	PRO	2.6
1	A	299	THR	2.6
1	B	171	GLU	2.6
1	D	204	VAL	2.6
1	D	290	PRO	2.6
1	D	172	LYS	2.6
1	E	192	PRO	2.5
1	B	147	SER	2.5
1	D	173	MET	2.5
1	C	260	THR	2.5
1	E	320	VAL	2.5
1	F	66	HIS	2.5
1	F	147	SER	2.5
1	B	200	PRO	2.4
1	B	172	LYS	2.4
1	D	203	HIS	2.4
1	C	208	TRP	2.4
1	B	70	PRO	2.4
1	C	192	PRO	2.4
1	F	387	SER	2.4
1	D	391	MET	2.4
1	B	191	THR	2.4
1	E	101	LEU	2.4
1	D	145	PRO	2.3
1	D	200	PRO	2.3
1	A	192	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLY	2.3
1	A	397	LEU	2.3
1	D	219	ILE	2.3
1	B	44	MET	2.3
1	F	172	LYS	2.3
1	B	204	VAL	2.3
1	B	170	PRO	2.3
1	D	331	ALA	2.3
1	E	226	ALA	2.3
1	E	132	ARG	2.3
1	F	196	ARG	2.3
1	B	284	GLY	2.3
1	F	133	ASP	2.3
1	A	247	LYS	2.3
1	F	290	PRO	2.3
1	F	300	THR	2.3
1	B	300	THR	2.2
1	F	193	THR	2.2
1	A	393	GLN	2.2
1	C	284	GLY	2.2
1	F	74	PRO	2.2
1	B	192	PRO	2.2
1	E	191	THR	2.2
1	C	57	GLY	2.2
1	E	323	TRP	2.2
1	E	358	VAL	2.2
1	F	139	GLY	2.2
1	B	71	ALA	2.1
1	C	298	GLN	2.1
1	B	293	LEU	2.1
1	C	300	THR	2.1
1	E	299	THR	2.1
1	D	188	ILE	2.1
1	E	182	ARG	2.1
1	B	169	MET	2.1
1	D	393	GLN	2.1
1	D	201	GLU	2.1
1	E	201	GLU	2.1
1	F	297	GLU	2.1
1	E	362	GLN	2.1
1	D	137	LYS	2.1
1	B	202	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	310	PHE	2.1
1	F	295	GLN	2.1
1	A	363	GLU	2.0
1	D	289	GLU	2.0
1	E	248	LEU	2.0
1	B	173	MET	2.0
1	D	199	SER	2.0
1	D	217	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

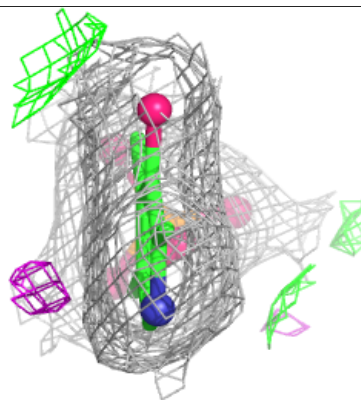
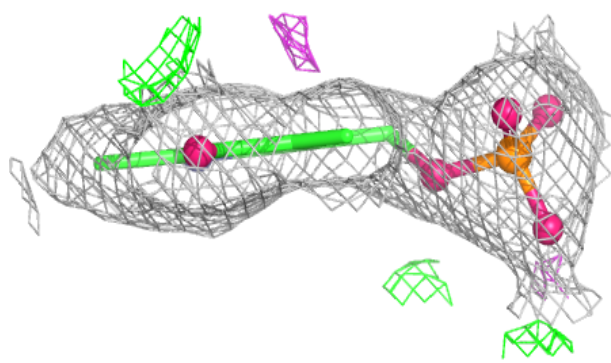
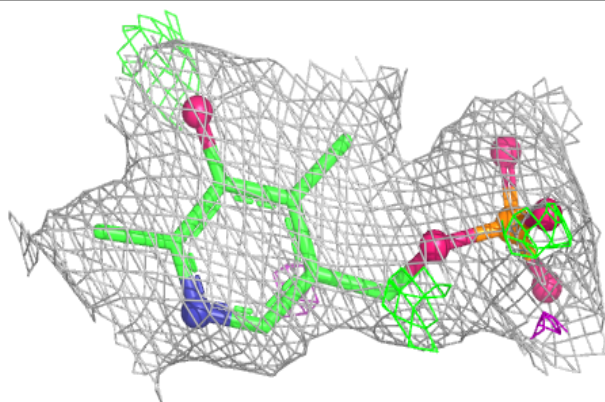
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	C	501	15/16	0.95	0.08	22,27,29,29	0
3	HEM	E	502	43/43	0.95	0.11	39,53,76,86	0
2	PLP	D	501	15/16	0.96	0.07	27,30,40,41	0
3	HEM	B	502	43/43	0.96	0.09	25,35,54,66	0
3	HEM	D	502	43/43	0.96	0.08	26,33,38,39	0
2	PLP	A	501	15/16	0.96	0.07	21,25,30,34	0
2	PLP	E	501	15/16	0.97	0.06	31,34,40,43	0
3	HEM	C	502	43/43	0.97	0.08	18,29,40,48	0
2	PLP	F	501	15/16	0.97	0.06	22,25,28,28	0
3	HEM	A	502	43/43	0.97	0.08	23,28,32,43	0
3	HEM	F	502	43/43	0.97	0.08	27,36,50,54	0
2	PLP	B	501	15/16	0.98	0.06	26,30,35,38	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.

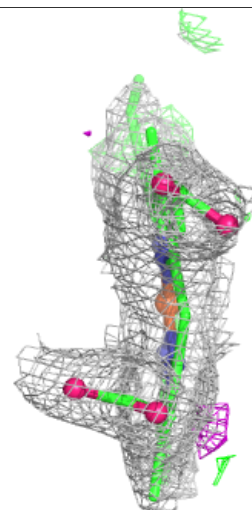
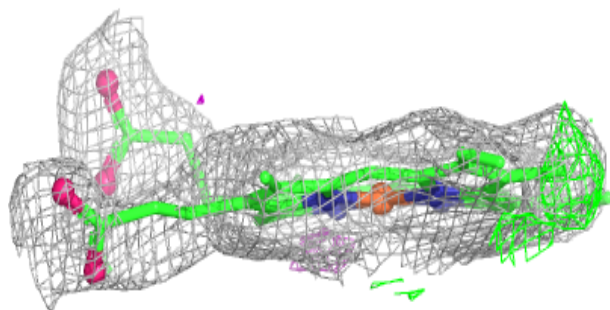
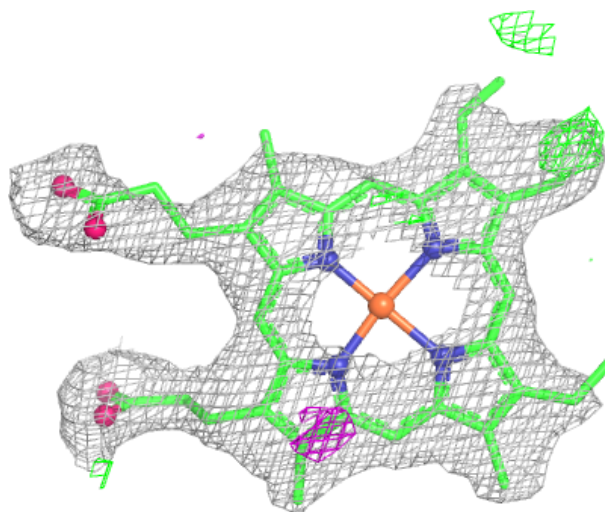
Electron density around PLP C 501:

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



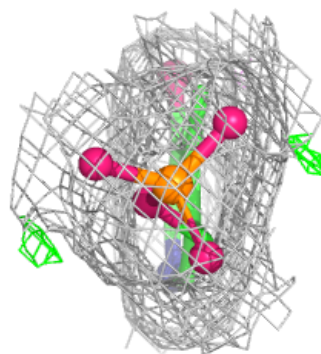
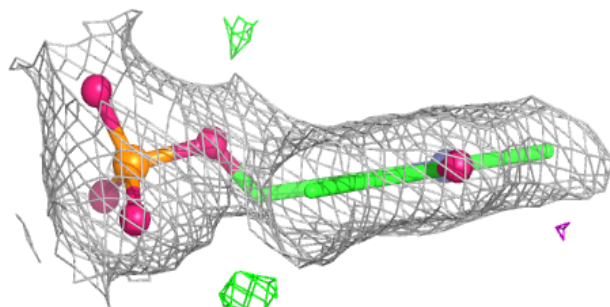
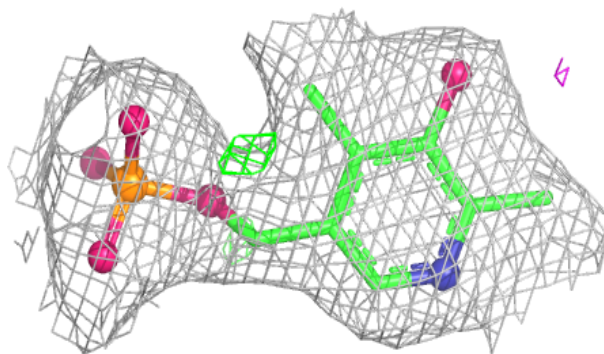
Electron density around HEM E 502:

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

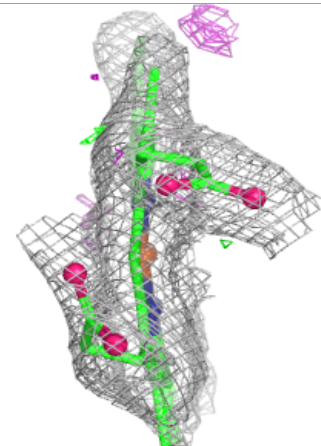
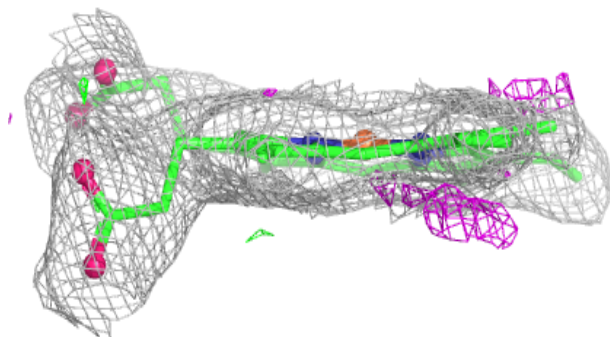
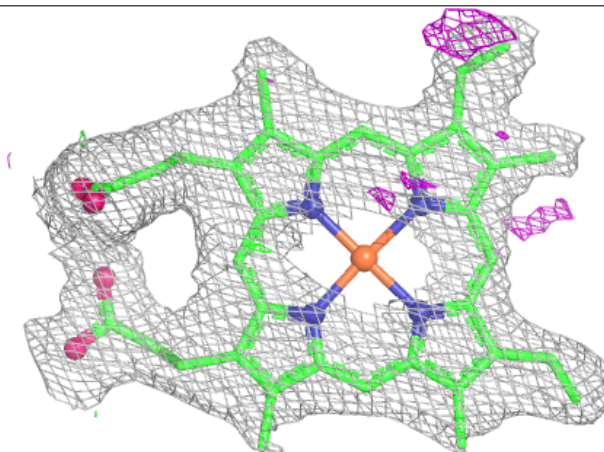


Electron density around PLP D 501:

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

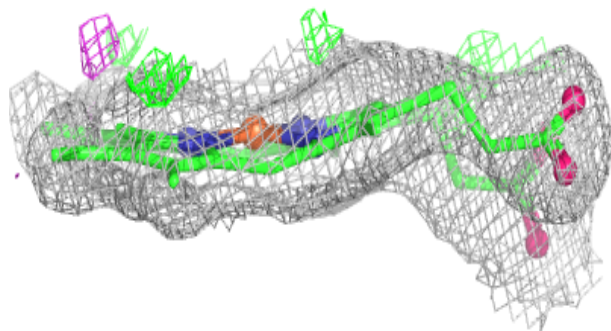
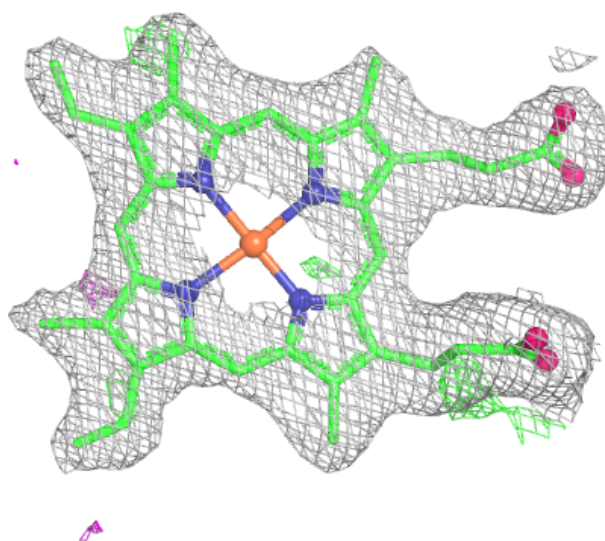
**Electron density around HEM B 502:**

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



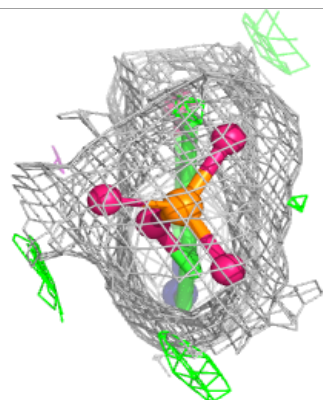
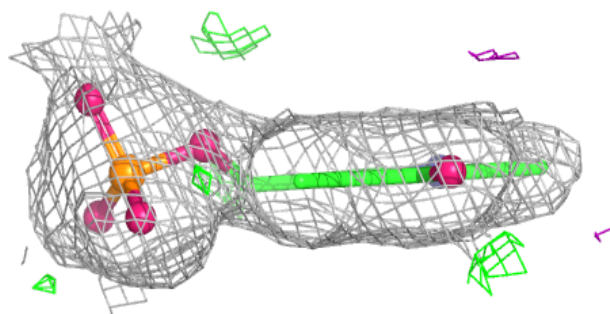
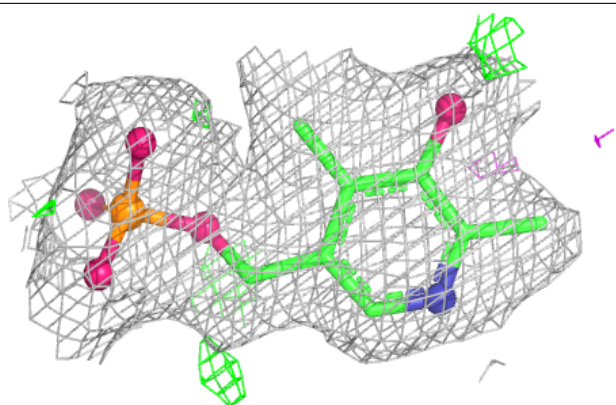
Electron density around HEM D 502:

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

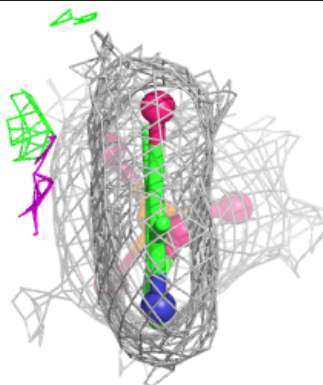
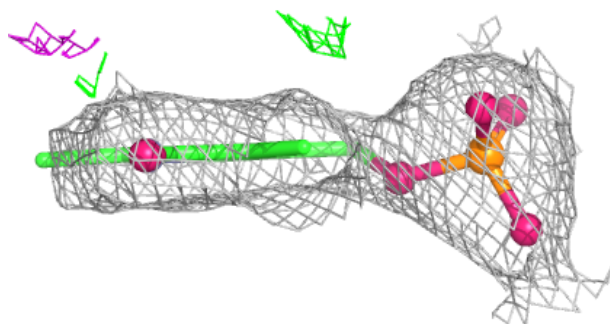
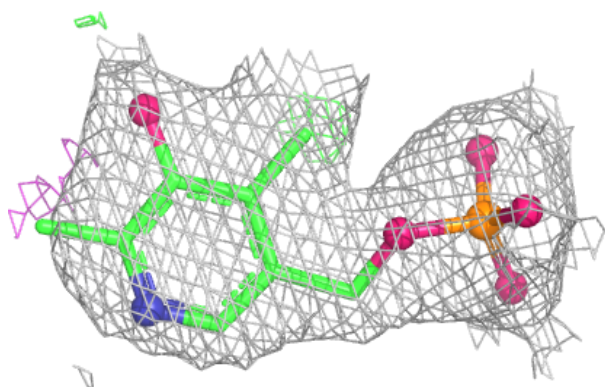


Electron density around PLP A 501:

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

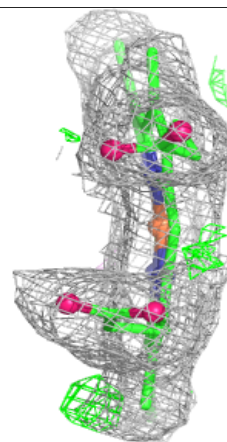
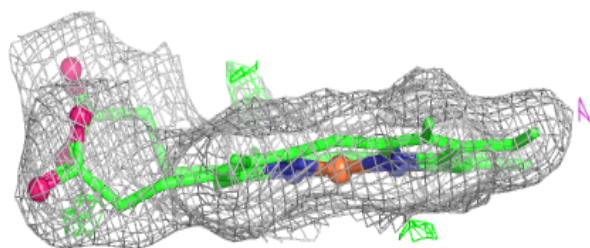
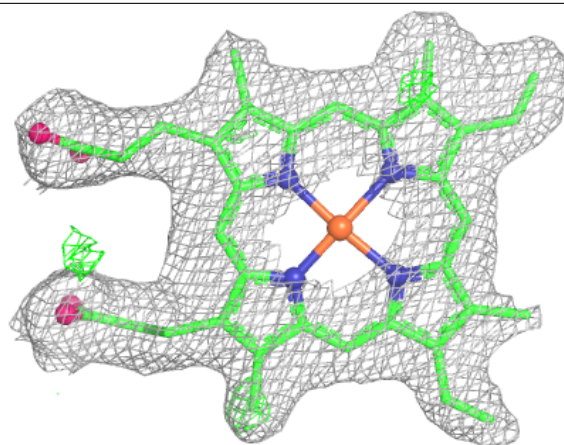
**Electron density around PLP E 501:**

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

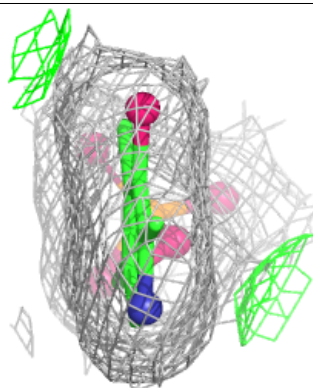
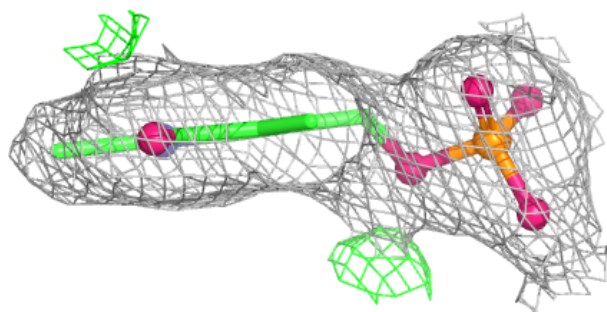
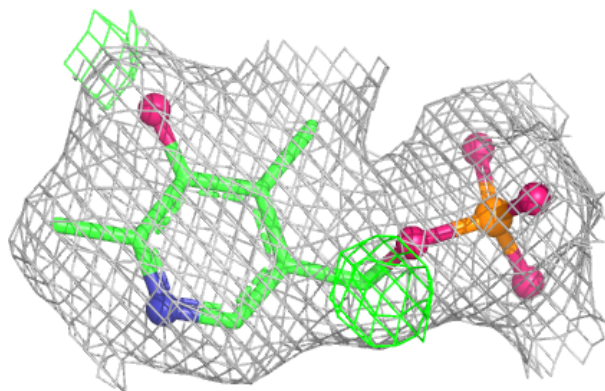


Electron density around HEM C 502:

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

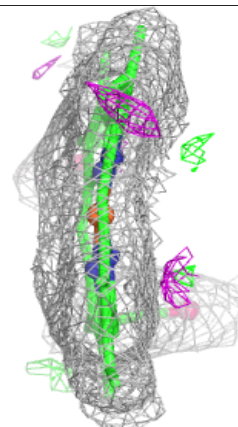
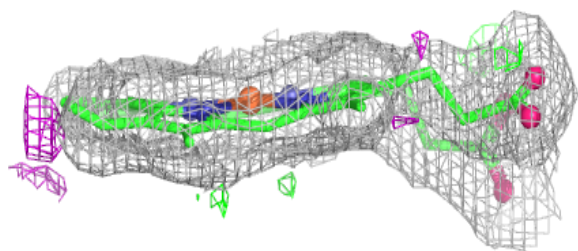
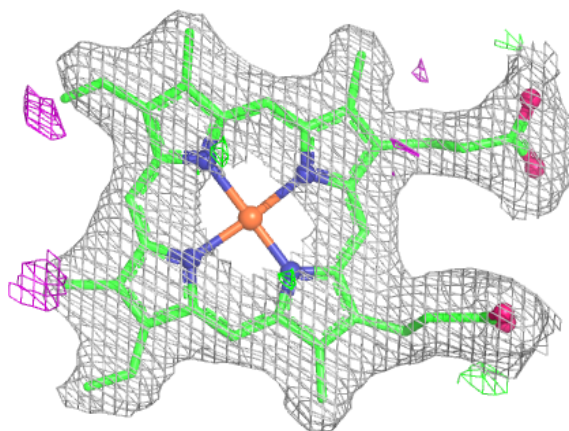
**Electron density around PLP F 501:**

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



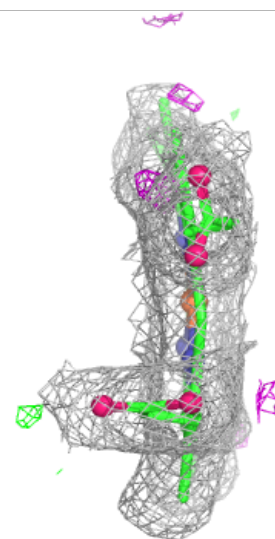
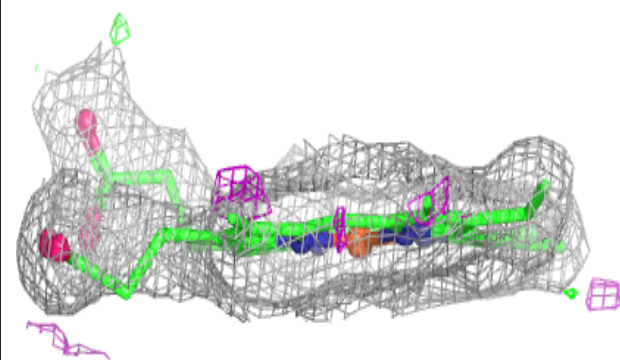
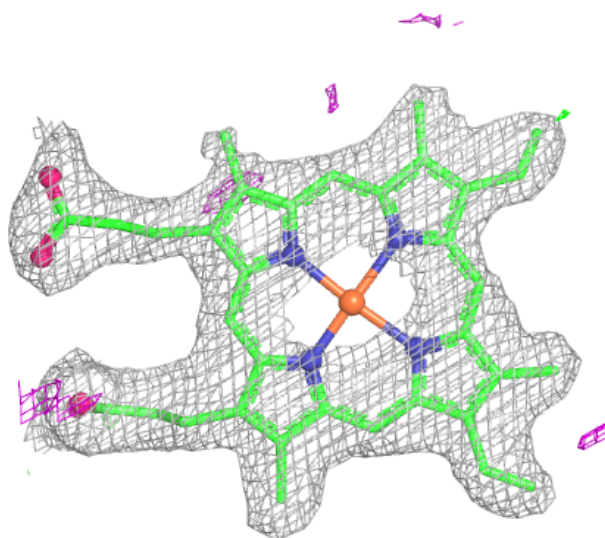
Electron density around HEM A 502:

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



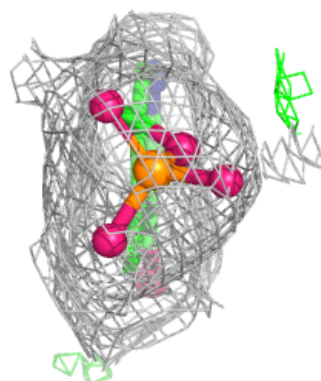
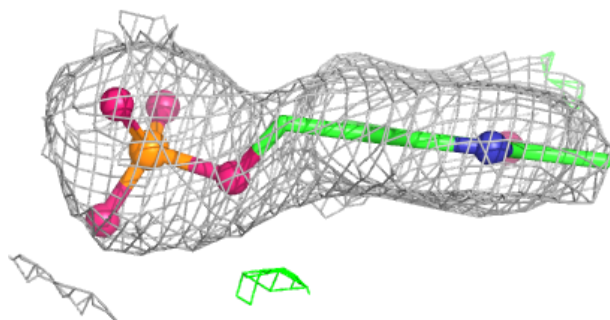
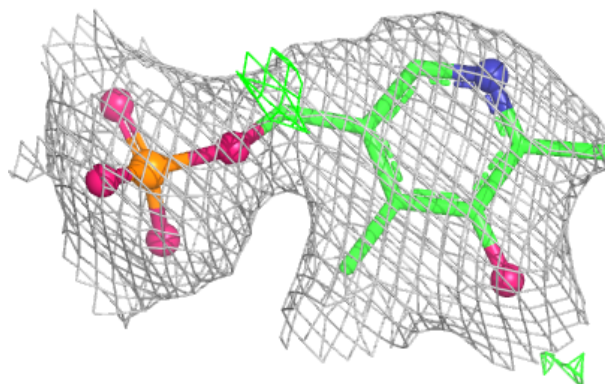
Electron density around HEM F 502:

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



Electron density around PLP B 501:

$2mF_o-DF_c$ (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.