



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2021 – 12:46 PM EDT

PDB ID : 6UDM
Title : Structure of Human Cytochrome P450 1A1 with Duocarmycin Prodrug (S)
ICT-2726
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2019-09-19
Resolution : 3.08 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

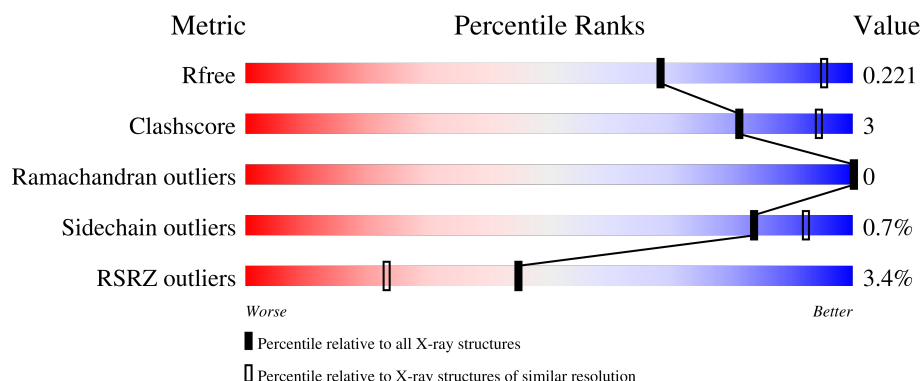
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

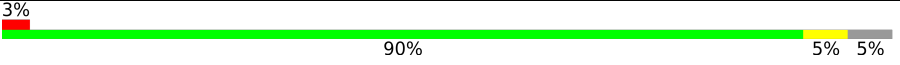
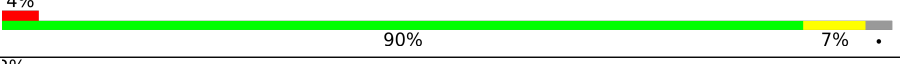
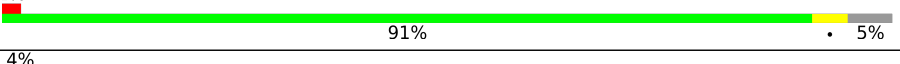

The reported resolution of this entry is 3.08 Å.

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}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	491	 3% 90% 5% 5%
1	B	491	 4% 90% 7% 5%
1	C	491	 2% 91% 5% 5%
1	D	491	 4% 89% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q4P	B	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30602 atoms, of which 15258 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	467	Total	C	H	N	O	S	0	0	0
			7485	2399	3744	650	671	21			
1	B	476	Total	C	H	N	O	S	0	0	0
			7620	2440	3808	663	688	21			
1	C	468	Total	C	H	N	O	S	0	0	0
			7496	2404	3746	652	673	21			
1	D	465	Total	C	H	N	O	S	0	0	0
			7449	2388	3726	647	667	21			

There are 52 discrepancies between the modelled and reference sequences:

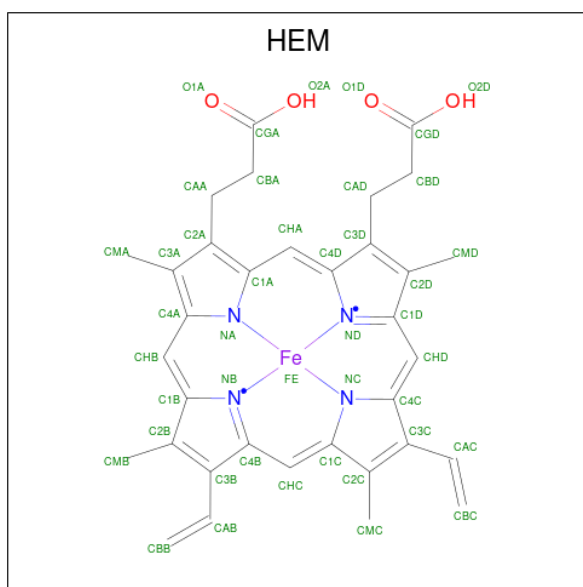
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	expression tag	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

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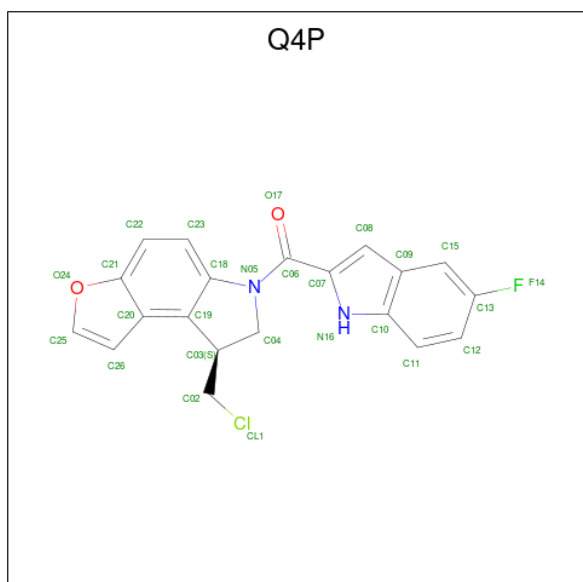
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	expression tag	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



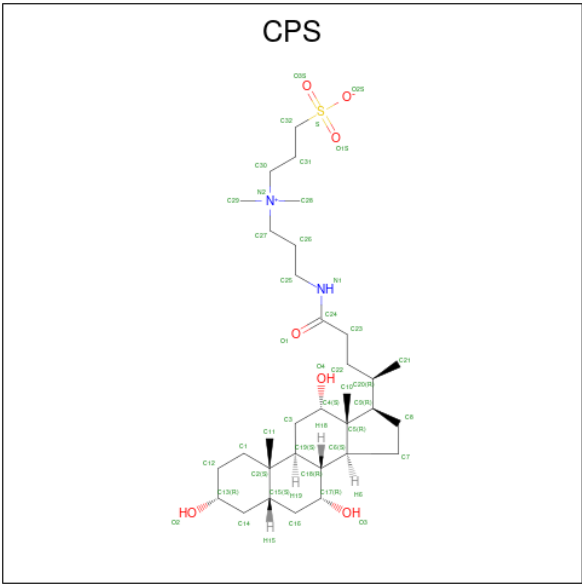
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 3 is [(8S)-8-(chloromethyl)-7,8-dihydro-6H-furo[3,2-e]indol-6-yl](5-fluoro-1H-indol-2-yl)methanone (three-letter code: Q4P) (formula: C₂₀H₁₄ClFN₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			40	20	1	1	14	2	2		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			40	20	1	1	14	2	2		
3	C	1	Total	C	Cl	F	H	N	O	0	0
			40	20	1	1	14	2	2		
3	D	1	Total	C	Cl	F	H	N	O	0	0
			40	20	1	1	14	2	2		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).

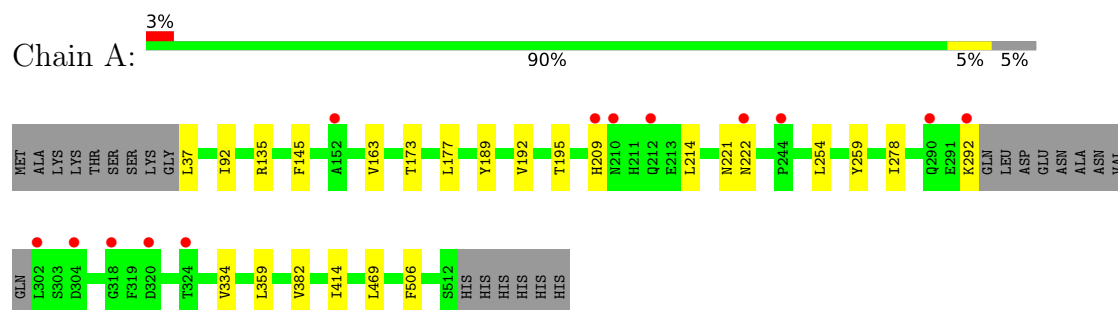


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S		0	0
			100	32	58	2	7	1			

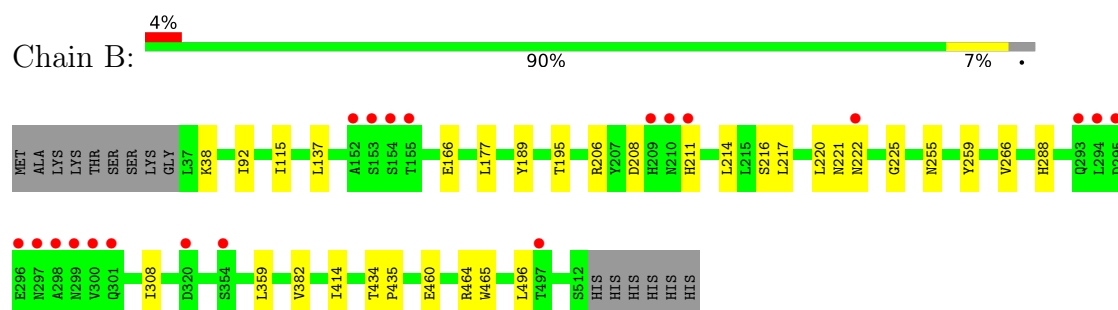
3 Residue-property plots [i](#)

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

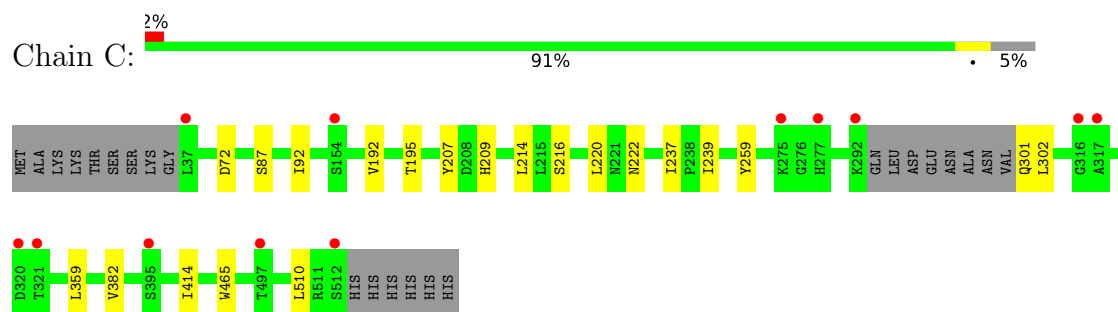
• Molecule 1: Cytochrome P450 1A1



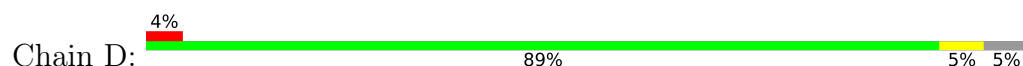
• Molecule 1: Cytochrome P450 1A1

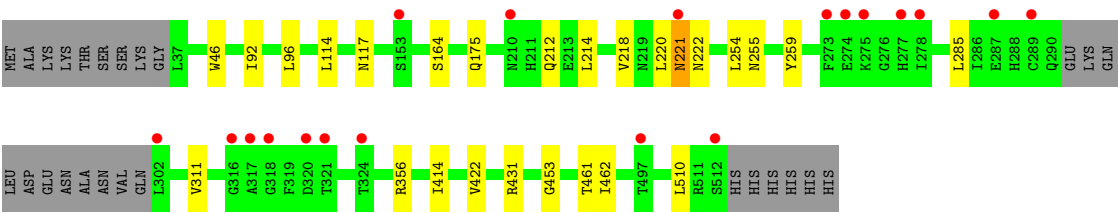


• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	241.28Å 241.28Å 125.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.64 – 3.08 39.64 – 3.07	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.64-3.08) 95.3 (39.64-3.07)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.209 , 0.221 0.209 , 0.221	Depositor DCC
R_{free} test set	2000 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30602	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: CPS, Q4P, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3835	0.44	0/5195
1	B	0.33	0/3907	0.45	0/5295
1	C	0.30	0/3844	0.43	0/5207
1	D	0.34	0/3817	0.45	0/5172
All	All	0.32	0/15403	0.44	0/20869

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3741	3744	3742	15	0
1	B	3812	3808	3806	16	0
1	C	3750	3746	3750	14	0
1	D	3723	3726	3724	17	0
2	A	43	30	30	6	0
2	B	43	30	30	5	0
2	C	43	30	30	5	0
2	D	43	30	30	4	0
3	A	26	14	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	14	0	1	0
3	C	26	14	0	2	0
3	D	26	14	0	0	0
4	A	42	58	58	2	0
All	All	15344	15258	15200	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 3.

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:C:92:ILE:HD12	1:C:414:ILE:HD11	1.63	0.79
1:A:92:ILE:HD12	1:A:414:ILE:HD11	1.72	0.71
1:B:222:ASN:OD1	3:B:602:Q4P:CL1	2.47	0.70
1:A:195:THR:HG21	1:A:214:LEU:HD11	1.76	0.68
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.76	0.67
1:B:217:LEU:O	1:B:221:ASN:HB3	1.96	0.66
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.79	0.65
4:A:603:CPS:H10B	4:A:603:CPS:H21A	1.80	0.64
1:A:173:THR:HG1	1:A:209:HIS:CE1	2.16	0.63
1:B:195:THR:HG21	1:B:214:LEU:HD11	1.79	0.63
1:C:195:THR:HG21	1:C:214:LEU:HD11	1.82	0.61
1:D:212:GLN:O	1:D:212:GLN:HG3	2.01	0.61
1:B:359:LEU:HD21	1:B:465:TRP:CE3	2.37	0.60
1:D:114:LEU:O	1:D:255:ASN:ND2	2.35	0.59
1:D:461:THR:HG23	1:D:462:ILE:HD12	1.85	0.59
1:C:192:VAL:HG11	1:C:209:HIS:HA	1.86	0.58
1:A:221:ASN:O	1:A:254:LEU:HD22	2.03	0.57
2:B:601:HEM:HMC1	2:B:601:HEM:HBC2	1.87	0.56
1:D:422:VAL:O	1:D:431:ARG:NH2	2.38	0.56
1:C:207:TYR:HB2	1:C:214:LEU:HD22	1.86	0.55
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.88	0.55
1:D:220:LEU:HD23	1:D:220:LEU:O	2.07	0.55
2:D:601:HEM:HMC1	2:D:601:HEM:HBC2	1.89	0.54
1:B:137:LEU:HD21	1:B:288:HIS:CD2	2.42	0.54
2:D:601:HEM:HMB2	2:D:601:HEM:HBB2	1.89	0.54
2:C:601:HEM:HMC1	2:C:601:HEM:HBC2	1.91	0.53
1:D:285:LEU:HD12	1:D:311:VAL:HG23	1.91	0.53
1:C:72:ASP:HB3	1:C:87:SER:O	2.08	0.52
1:C:92:ILE:CD1	1:C:414:ILE:HD11	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.92	0.52
1:A:334:VAL:HG21	1:A:506:PHE:CE2	2.45	0.52
1:C:239:ILE:HD13	1:D:46:TRP:CE2	2.45	0.52
1:C:216:SER:HA	1:C:220:LEU:HB2	1.93	0.51
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.92	0.51
1:A:222:ASN:OD1	3:A:602:Q4P:CL1	2.65	0.51
1:C:237:ILE:HG22	1:C:239:ILE:HG22	1.91	0.51
1:C:359:LEU:HD21	1:C:465:TRP:CE3	2.46	0.51
1:B:460:GLU:OE2	1:B:464:ARG:NH1	2.44	0.50
1:B:266:VAL:HG21	1:B:308:ILE:CG2	2.42	0.49
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.41	0.49
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.42	0.49
1:C:222:ASN:ND2	3:C:602:Q4P:CL1	2.79	0.48
1:A:177:LEU:HD11	1:A:189:TYR:CZ	2.48	0.48
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.93	0.48
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.43	0.48
1:B:216:SER:O	1:B:221:ASN:HB2	2.14	0.47
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.43	0.47
1:B:177:LEU:HD11	1:B:189:TYR:CZ	2.49	0.47
1:B:208:ASP:OD1	1:B:211:HIS:ND1	2.48	0.47
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.45	0.46
1:D:92:ILE:CD1	1:D:414:ILE:HD11	2.44	0.46
2:C:601:HEM:HBC2	2:C:601:HEM:CMC	2.45	0.46
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	1.96	0.46
1:B:115:ILE:HA	1:B:255:ASN:OD1	2.16	0.45
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.47	0.45
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.46	0.45
1:A:145:PHE:HZ	1:A:278:ILE:HG22	1.82	0.44
1:A:359:LEU:CD1	1:A:469:LEU:HD11	2.48	0.44
1:D:221:ASN:O	1:D:254:LEU:HD13	2.18	0.44
1:B:225:GLY:HA2	1:B:496:LEU:HB3	2.01	0.43
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	2.00	0.43
1:D:175:GLN:OE1	1:D:510:LEU:HD21	2.19	0.43
4:A:603:CPS:H21A	4:A:603:CPS:H4	2.01	0.42
1:B:434:THR:HB	1:B:435:PRO:CD	2.49	0.42
1:A:92:ILE:CD1	1:A:414:ILE:HD11	2.47	0.42
1:D:510:LEU:HD12	1:D:510:LEU:H	1.85	0.42
1:C:510:LEU:N	1:C:510:LEU:HD22	2.35	0.42
1:D:117:ASN:O	1:D:117:ASN:ND2	2.52	0.42
1:A:163:VAL:HG11	1:A:469:LEU:HB3	2.02	0.41
1:D:218:VAL:O	1:D:222:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:SER:O	1:C:220:LEU:HB3	2.20	0.41
1:D:96:LEU:O	1:D:453:GLY:HA3	2.20	0.41
1:D:285:LEU:CD1	1:D:311:VAL:HG23	2.49	0.41
3:C:602:Q4P:O17	3:C:602:Q4P:C23	2.65	0.41
1:B:166:GLU:OE2	1:B:206:ARG:HD2	2.20	0.41
1:D:356:ARG:HE	1:D:356:ARG:HB2	1.65	0.41
1:A:135:ARG:NH1	2:A:601:HEM:O1D	2.54	0.40
1:A:192:VAL:HG11	1:A:209:HIS:HA	2.03	0.40
1:A:37:LEU:N	1:A:37:LEU:HD12	2.35	0.40
1:C:382:VAL:HG21	2:C:601:HEM:HMB1	2.03	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	463/491 (94%)	452 (98%)	11 (2%)	0	100	100
1	B	474/491 (96%)	458 (97%)	16 (3%)	0	100	100
1	C	464/491 (94%)	452 (97%)	12 (3%)	0	100	100
1	D	461/491 (94%)	447 (97%)	14 (3%)	0	100	100
All	All	1862/1964 (95%)	1809 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/439 (95%)	416 (100%)	2 (0%)	88	94
1	B	426/439 (97%)	423 (99%)	3 (1%)	84	92
1	C	419/439 (95%)	416 (99%)	3 (1%)	84	92
1	D	416/439 (95%)	412 (99%)	4 (1%)	76	89
All	All	1679/1756 (96%)	1667 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	TYR
1	A	292	LYS
1	B	38	LYS
1	B	220	LEU
1	B	259	TYR
1	C	259	TYR
1	C	301	GLN
1	C	302	LEU
1	D	164	SER
1	D	214	LEU
1	D	221	ASN
1	D	259	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	B	222	ASN
1	C	301	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	HEM	B	601	-	27,50,50	1.88	4 (14%)	17,82,82	1.44	2 (11%)
3	Q4P	D	602	-	23,30,30	2.43	8 (34%)	26,45,45	2.35	11 (42%)
2	HEM	A	601	1	27,50,50	1.87	4 (14%)	17,82,82	1.42	2 (11%)
3	Q4P	B	602	-	23,30,30	2.35	7 (30%)	26,45,45	2.61	11 (42%)
4	CPS	A	603	-	45,45,45	1.13	2 (4%)	69,70,70	2.10	24 (34%)
3	Q4P	C	602	-	23,30,30	2.92	12 (52%)	26,45,45	3.09	12 (46%)
2	HEM	D	601	-	27,50,50	1.86	4 (14%)	17,82,82	1.45	2 (11%)
2	HEM	C	601	-	27,50,50	1.87	5 (18%)	17,82,82	1.46	2 (11%)
3	Q4P	A	602	-	23,30,30	2.27	8 (34%)	26,45,45	2.42	11 (42%)

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	HEM	B	601	-	-	0/6/54/54	-
3	Q4P	D	602	-	-	2/7/28/28	0/5/5/5
2	HEM	A	601	1	-	0/6/54/54	-
3	Q4P	B	602	-	-	2/7/28/28	0/5/5/5
4	CPS	A	603	-	-	7/25/90/90	1/4/4/4
3	Q4P	C	602	-	-	2/7/28/28	0/5/5/5
2	HEM	D	601	-	-	0/6/54/54	-
2	HEM	C	601	-	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Q4P	A	602	-	-	2/7/28/28	0/5/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	Q4P	C06-N05	6.46	1.47	1.36
3	B	602	Q4P	C06-N05	5.98	1.46	1.36
3	A	602	Q4P	C06-N05	5.84	1.46	1.36
3	C	602	Q4P	C10-N16	-5.78	1.20	1.38
3	C	602	Q4P	C07-C06	-5.55	1.41	1.50
4	A	603	CPS	C32-S	5.35	1.85	1.77
3	D	602	Q4P	C18-C19	5.12	1.43	1.37
3	A	602	Q4P	C18-C19	5.01	1.43	1.37
3	C	602	Q4P	C11-C10	-4.99	1.33	1.41
3	B	602	Q4P	C18-C19	4.97	1.42	1.37
2	B	601	HEM	C3B-C2B	-4.34	1.34	1.40
3	B	602	Q4P	C04-N05	4.28	1.54	1.47
2	B	601	HEM	C3C-C2C	-4.27	1.34	1.40
2	C	601	HEM	C3C-C2C	-4.21	1.34	1.40
2	A	601	HEM	C3B-C2B	-4.20	1.34	1.40
2	D	601	HEM	C3B-C2B	-4.18	1.34	1.40
2	C	601	HEM	C3B-C2B	-4.16	1.34	1.40
2	A	601	HEM	C3C-C2C	-4.15	1.34	1.40
2	D	601	HEM	C3C-C2C	-4.13	1.34	1.40
3	C	602	Q4P	C19-C20	-4.11	1.36	1.43
3	D	602	Q4P	C04-N05	4.07	1.53	1.47
3	C	602	Q4P	C19-C03	-4.06	1.47	1.52
3	A	602	Q4P	C04-N05	3.99	1.53	1.47
3	D	602	Q4P	C18-N05	3.84	1.47	1.39
3	C	602	Q4P	C12-C13	-3.71	1.29	1.37
2	C	601	HEM	C3C-CAC	3.67	1.55	1.47
2	A	601	HEM	C3C-CAC	3.66	1.55	1.47
2	D	601	HEM	C3C-CAC	3.65	1.55	1.47
2	B	601	HEM	C3C-CAC	3.61	1.55	1.47
2	A	601	HEM	C3B-CAB	3.59	1.55	1.47
2	D	601	HEM	C3B-CAB	3.59	1.55	1.47
2	C	601	HEM	C3B-CAB	3.59	1.55	1.47
2	B	601	HEM	C3B-CAB	3.53	1.55	1.47
3	A	602	Q4P	C18-N05	3.48	1.46	1.39
3	B	602	Q4P	C18-N05	3.27	1.46	1.39
3	C	602	Q4P	C06-N05	-3.14	1.31	1.36
3	C	602	Q4P	C20-C21	-3.10	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	Q4P	C04-C03	2.95	1.60	1.53
3	C	602	Q4P	C18-C19	-2.85	1.34	1.37
3	D	602	Q4P	C23-C18	2.68	1.44	1.39
3	A	602	Q4P	C23-C18	2.54	1.43	1.39
3	B	602	Q4P	C23-C18	2.49	1.43	1.39
3	D	602	Q4P	C04-C03	2.34	1.59	1.53
3	C	602	Q4P	C08-C07	-2.28	1.35	1.39
3	C	602	Q4P	C02-C03	-2.25	1.47	1.52
4	A	603	CPS	C30-N2	2.09	1.56	1.52
3	A	602	Q4P	C22-C23	2.09	1.41	1.36
3	D	602	Q4P	C22-C23	2.07	1.41	1.36
3	D	602	Q4P	F14-C13	2.05	1.41	1.36
3	C	602	Q4P	C22-C23	-2.03	1.32	1.36
3	A	602	Q4P	F14-C13	2.02	1.41	1.36
3	B	602	Q4P	F14-C13	2.02	1.41	1.36
2	C	601	HEM	CAA-C2A	2.02	1.55	1.52
3	A	602	Q4P	C04-C03	2.01	1.58	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	Q4P	C07-C06-N05	8.55	129.03	118.39
3	B	602	Q4P	C07-C06-N05	7.28	127.44	118.39
3	A	602	Q4P	C07-C06-N05	5.89	125.72	118.39
3	C	602	Q4P	O17-C06-N05	-5.84	113.96	121.69
4	A	603	CPS	C5-C9-C20	-5.69	112.70	119.50
3	D	602	Q4P	C07-C06-N05	5.50	125.23	118.39
4	A	603	CPS	C25-N1-C24	-5.36	112.88	122.84
3	C	602	Q4P	C26-C20-C21	-5.18	101.94	109.97
3	A	602	Q4P	C23-C18-C19	-4.71	116.51	122.22
3	C	602	Q4P	C23-C18-C19	-4.65	116.58	122.22
3	D	602	Q4P	C23-C18-C19	-4.65	116.58	122.22
3	C	602	Q4P	C07-N16-C10	4.55	113.94	104.45
3	B	602	Q4P	C23-C18-C19	-4.48	116.79	122.22
3	B	602	Q4P	C26-C20-C21	-4.40	103.14	109.97
3	D	602	Q4P	C26-C20-C21	-4.32	103.27	109.97
3	A	602	Q4P	C26-C20-C21	-4.26	103.36	109.97
4	A	603	CPS	C22-C23-C24	-4.13	103.80	113.04
4	A	603	CPS	C19-C18-C6	-4.13	104.05	109.71
4	A	603	CPS	O1S-S-C32	-4.08	102.00	106.92
3	B	602	Q4P	O17-C06-N05	-3.77	116.70	121.69
4	A	603	CPS	C31-C32-S	-3.73	107.53	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	Q4P	C19-C18-N05	3.69	114.75	109.72
4	A	603	CPS	C19-C2-C15	3.58	113.61	108.58
3	B	602	Q4P	C07-N16-C10	3.50	111.74	104.45
3	A	602	Q4P	C07-N16-C10	3.43	111.61	104.45
3	D	602	Q4P	C07-N16-C10	3.43	111.60	104.45
4	A	603	CPS	C14-C15-C2	-3.34	109.11	112.66
3	B	602	Q4P	C19-C18-N05	3.30	114.21	109.72
4	A	603	CPS	O3S-S-C32	-3.23	103.03	106.92
3	B	602	Q4P	C12-C13-C15	3.23	126.79	123.23
3	A	602	Q4P	O17-C06-N05	-3.22	117.43	121.69
3	C	602	Q4P	F14-C13-C12	-3.18	113.14	118.54
3	A	602	Q4P	C12-C13-C15	3.10	126.64	123.23
3	D	602	Q4P	C12-C13-C15	3.05	126.59	123.23
4	A	603	CPS	C15-C14-C13	-3.04	108.29	112.76
4	A	603	CPS	C23-C24-N1	-3.03	111.32	116.42
3	C	602	Q4P	C15-C09-C10	-3.01	115.67	119.87
3	D	602	Q4P	C19-C18-N05	3.01	113.82	109.72
3	A	602	Q4P	C19-C18-N05	2.95	113.74	109.72
3	C	602	Q4P	C22-C23-C18	2.92	125.65	119.95
4	A	603	CPS	C31-C30-N2	-2.90	109.24	115.38
4	A	603	CPS	C5-C6-C18	-2.88	111.05	114.74
3	D	602	Q4P	O17-C06-N05	-2.80	117.98	121.69
4	A	603	CPS	C19-C3-C4	-2.78	110.63	114.30
4	A	603	CPS	C3-C19-C2	-2.72	110.93	113.73
4	A	603	CPS	C23-C22-C20	-2.61	109.76	114.52
3	C	602	Q4P	C08-C07-C06	2.49	137.06	128.33
3	D	602	Q4P	C04-N05-C18	-2.47	106.36	109.21
3	A	602	Q4P	C04-N05-C18	-2.46	106.37	109.21
4	A	603	CPS	C21-C20-C22	-2.46	106.50	110.36
4	A	603	CPS	C9-C5-C6	-2.44	97.63	100.09
4	A	603	CPS	C26-C25-N1	-2.41	105.33	112.21
2	B	601	HEM	CBD-CAD-C3D	-2.40	108.06	112.48
3	A	602	Q4P	C07-C08-C09	2.39	109.54	106.55
3	D	602	Q4P	C07-C08-C09	2.37	109.51	106.55
2	C	601	HEM	CBD-CAD-C3D	-2.32	108.20	112.48
3	B	602	Q4P	C22-C23-C18	2.31	124.46	119.95
3	C	602	Q4P	C11-C12-C13	-2.31	116.09	118.74
2	B	601	HEM	CAA-CBA-CGA	-2.29	108.83	112.67
3	C	602	Q4P	C12-C13-C15	2.29	125.75	123.23
4	A	603	CPS	O2S-S-C32	-2.23	102.15	105.77
3	D	602	Q4P	C22-C23-C18	2.23	124.30	119.95
3	B	602	Q4P	C11-C12-C13	-2.23	116.19	118.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	Q4P	C22-C23-C18	2.18	124.21	119.95
3	B	602	Q4P	C04-N05-C18	-2.18	106.70	109.21
2	A	601	HEM	CBD-CAD-C3D	-2.16	108.50	112.48
4	A	603	CPS	C3-C4-C5	-2.15	109.04	111.24
3	D	602	Q4P	C11-C12-C13	-2.14	116.29	118.74
2	D	601	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
4	A	603	CPS	C16-C15-C2	-2.10	110.43	112.66
4	A	603	CPS	O1-C24-C23	2.09	125.83	122.02
3	B	602	Q4P	C07-C08-C09	2.08	109.15	106.55
3	A	602	Q4P	C11-C12-C13	-2.08	116.36	118.74
2	C	601	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
2	D	601	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
2	A	601	HEM	CMD-C2D-C1D	-2.03	125.35	128.46
4	A	603	CPS	O4-C4-C5	-2.02	107.62	111.03

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	Q4P	CL1-C02-C03-C04
3	C	602	Q4P	CL1-C02-C03-C04
3	D	602	Q4P	CL1-C02-C03-C04
4	A	603	CPS	N1-C25-C26-C27
4	A	603	CPS	C9-C20-C22-C23
4	A	603	CPS	C21-C20-C22-C23
4	A	603	CPS	C20-C22-C23-C24
4	A	603	CPS	C22-C20-C9-C8
4	A	603	CPS	C25-C26-C27-N2
4	A	603	CPS	C31-C32-S-O3S
3	B	602	Q4P	CL1-C02-C03-C19
3	C	602	Q4P	CL1-C02-C03-C19
3	A	602	Q4P	C07-C06-N05-C04
3	A	602	Q4P	CL1-C02-C03-C19
3	D	602	Q4P	CL1-C02-C03-C19

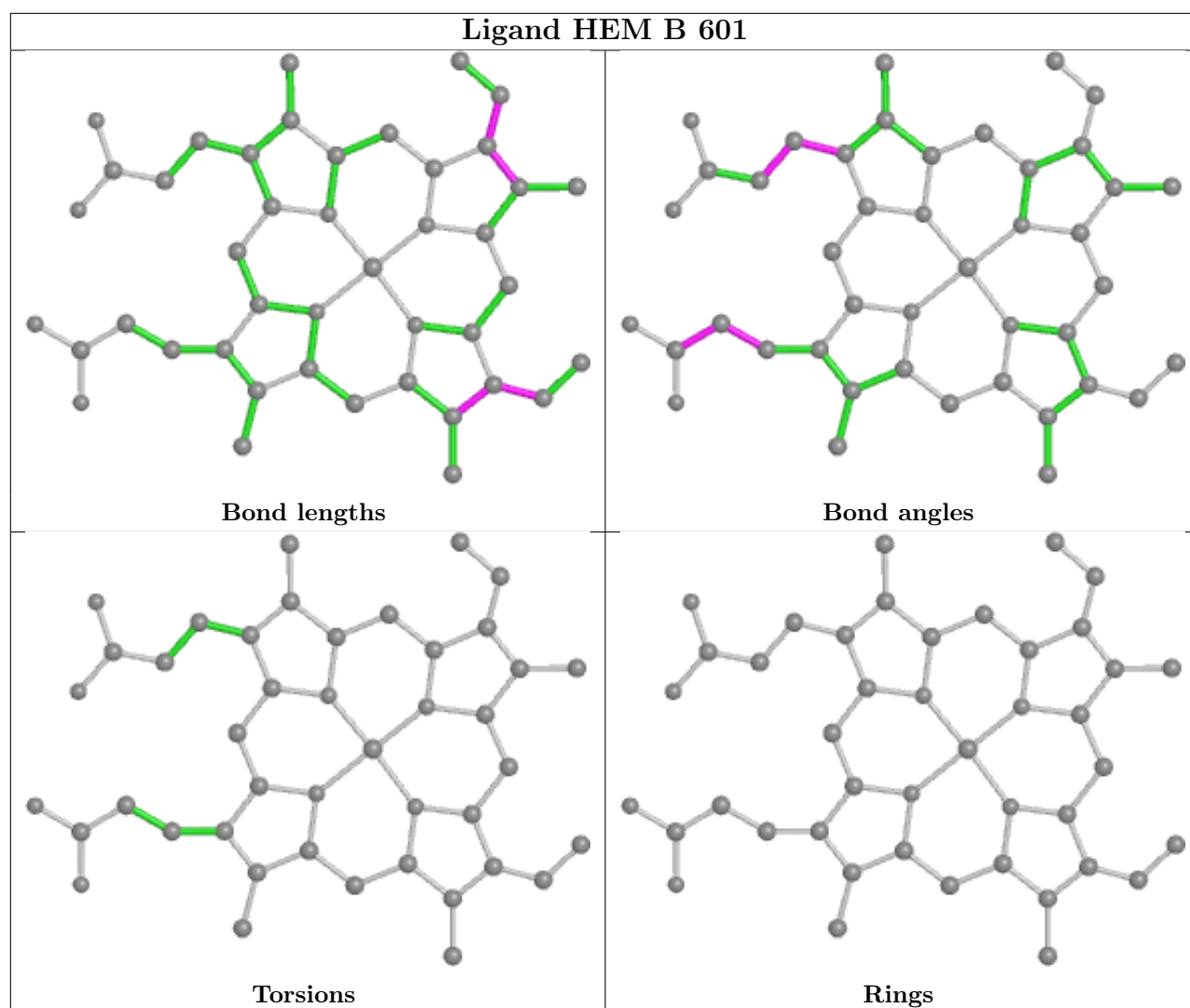
All (1) ring outliers are listed below:

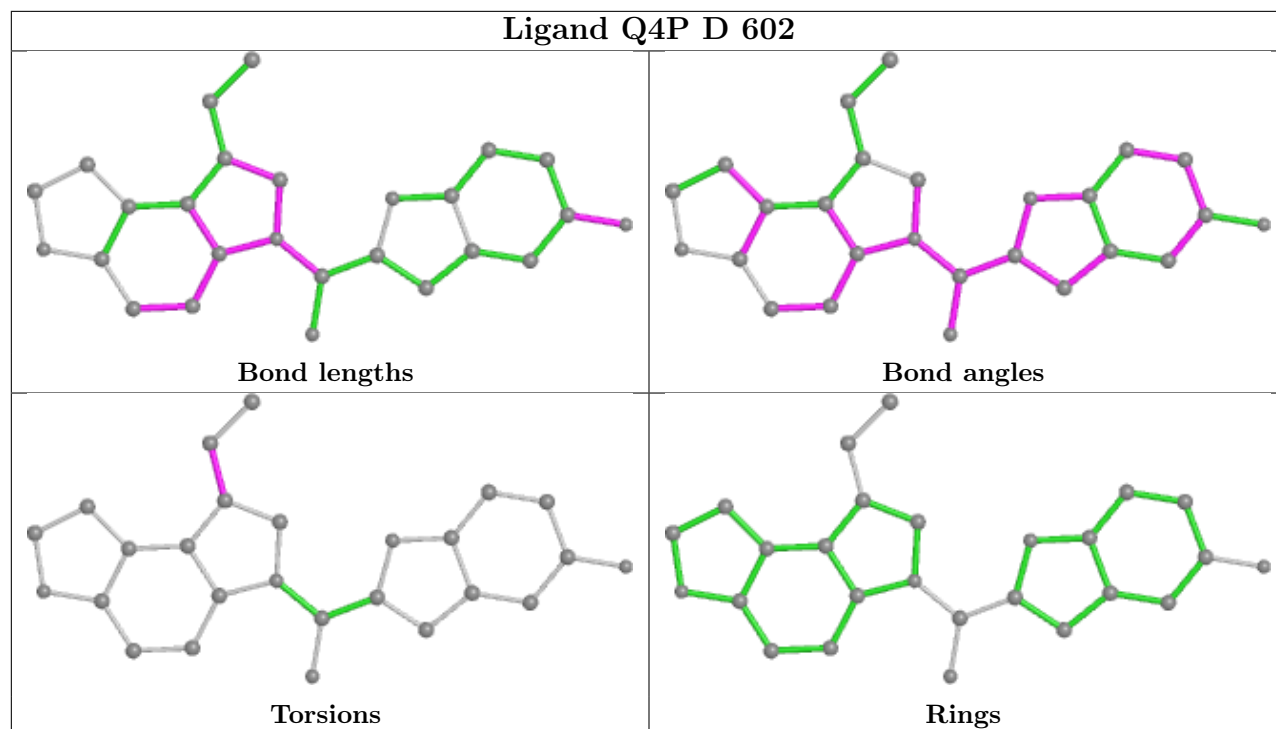
Mol	Chain	Res	Type	Atoms
4	A	603	CPS	C1-C12-C13-C14-C15-C2

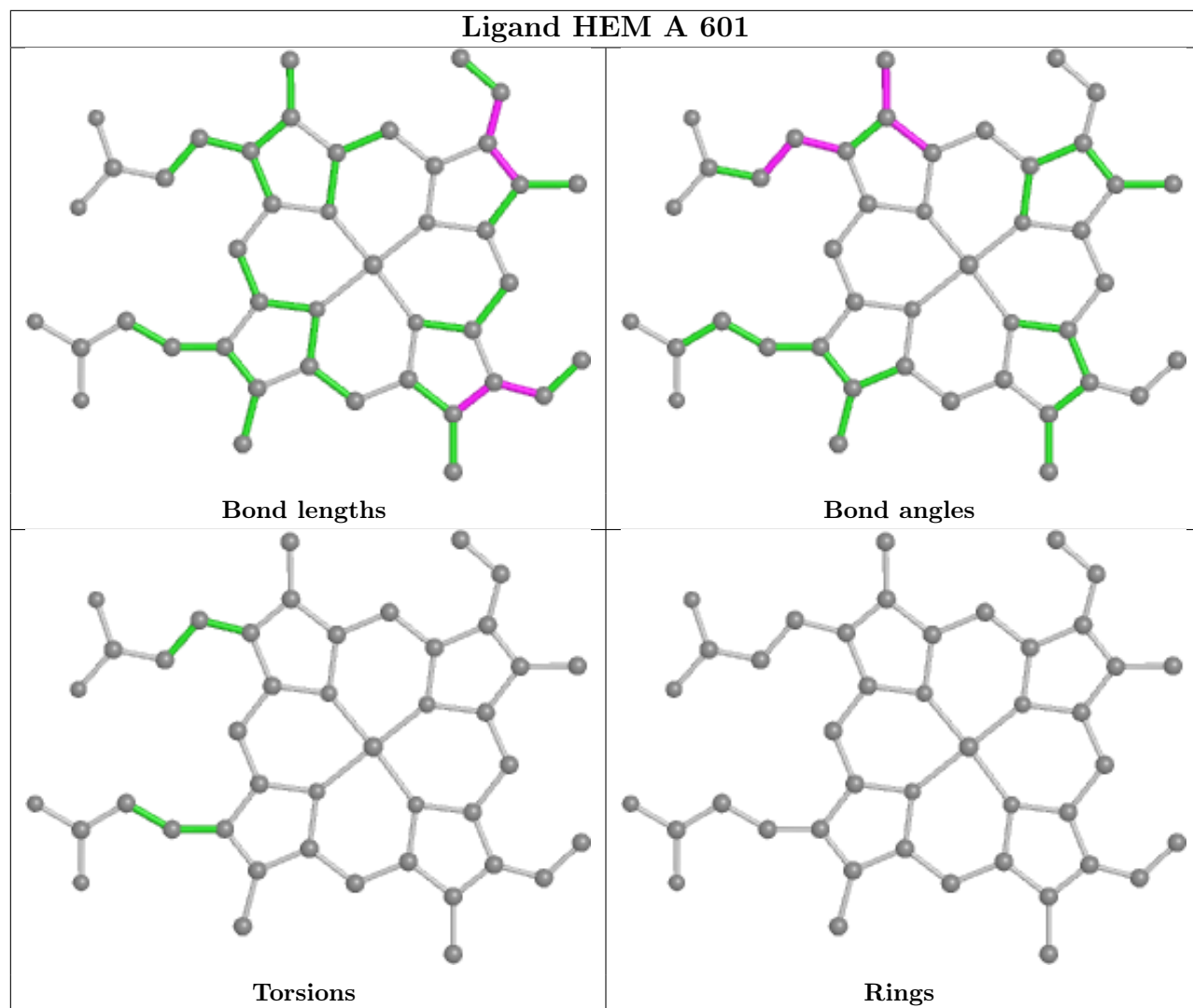
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	5	0
2	A	601	HEM	6	0
3	B	602	Q4P	1	0
4	A	603	CPS	2	0
3	C	602	Q4P	2	0
2	D	601	HEM	4	0
2	C	601	HEM	5	0
3	A	602	Q4P	1	0

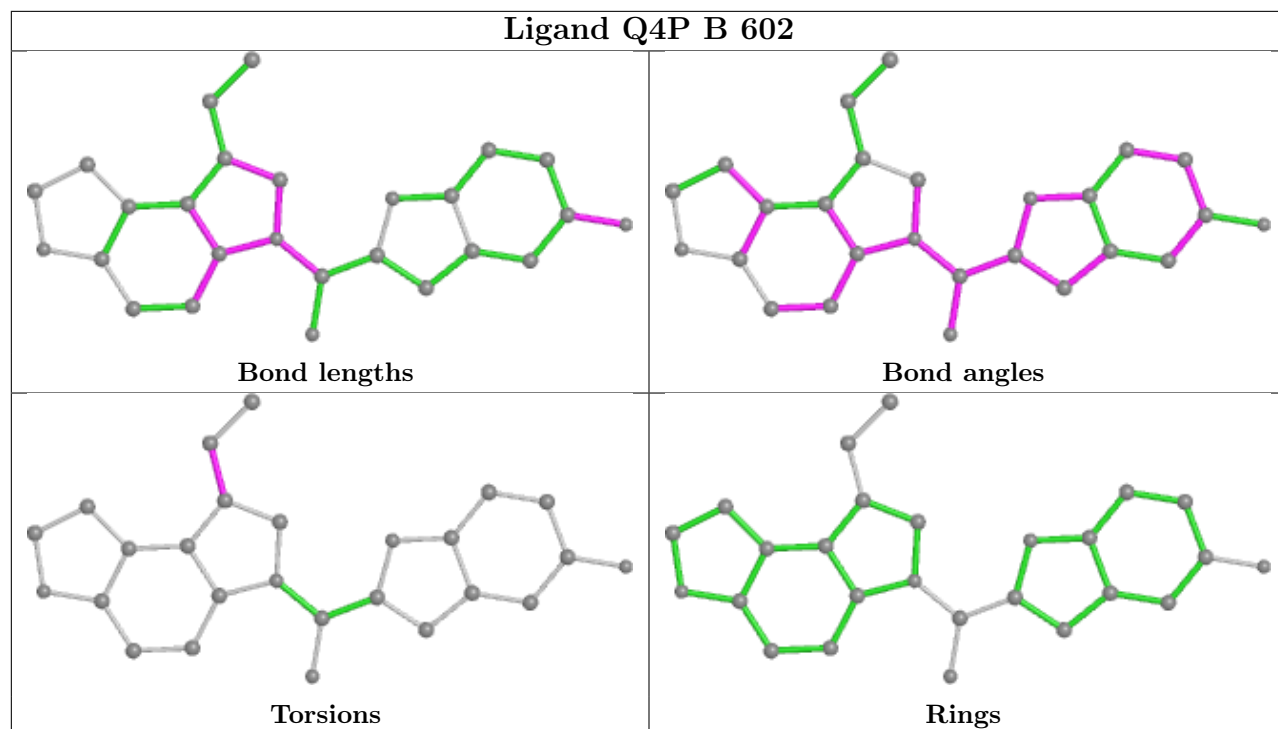
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



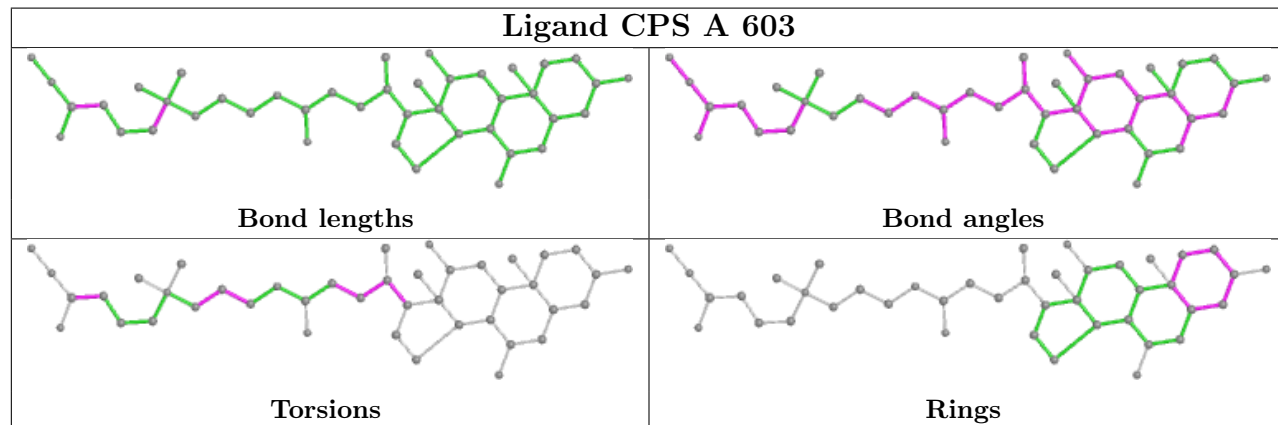


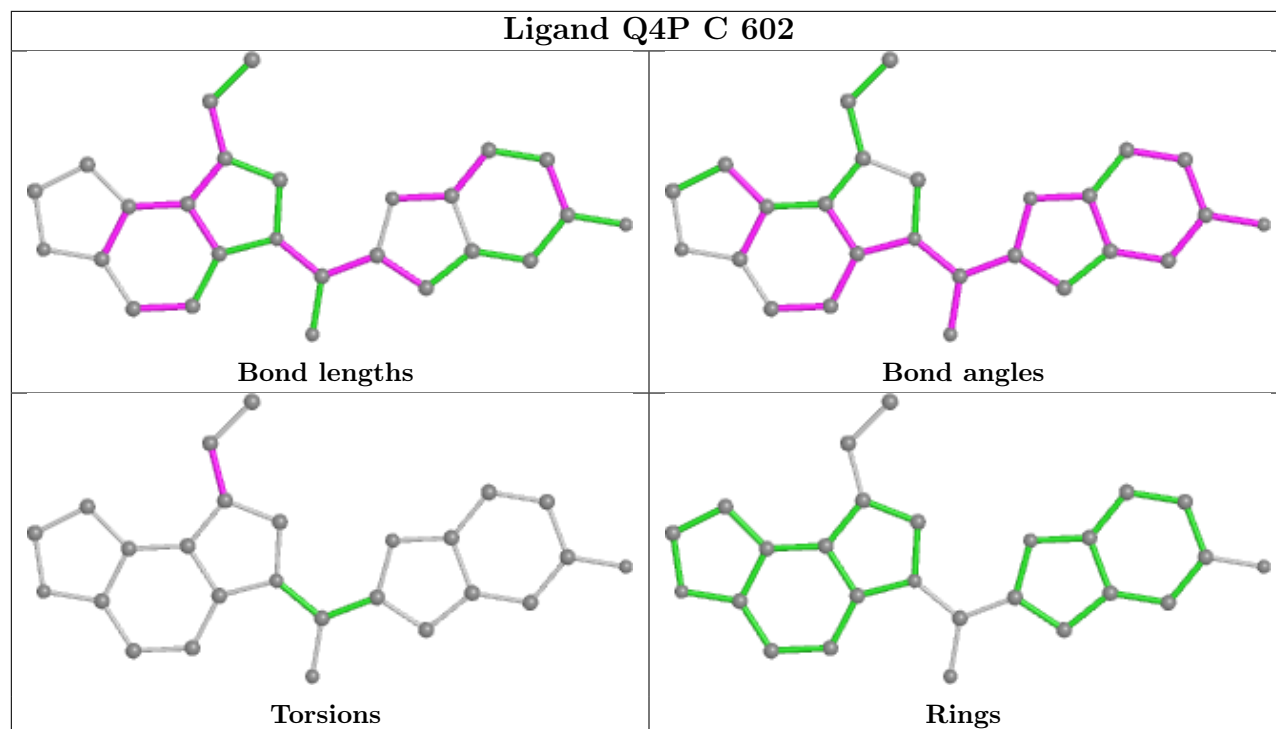


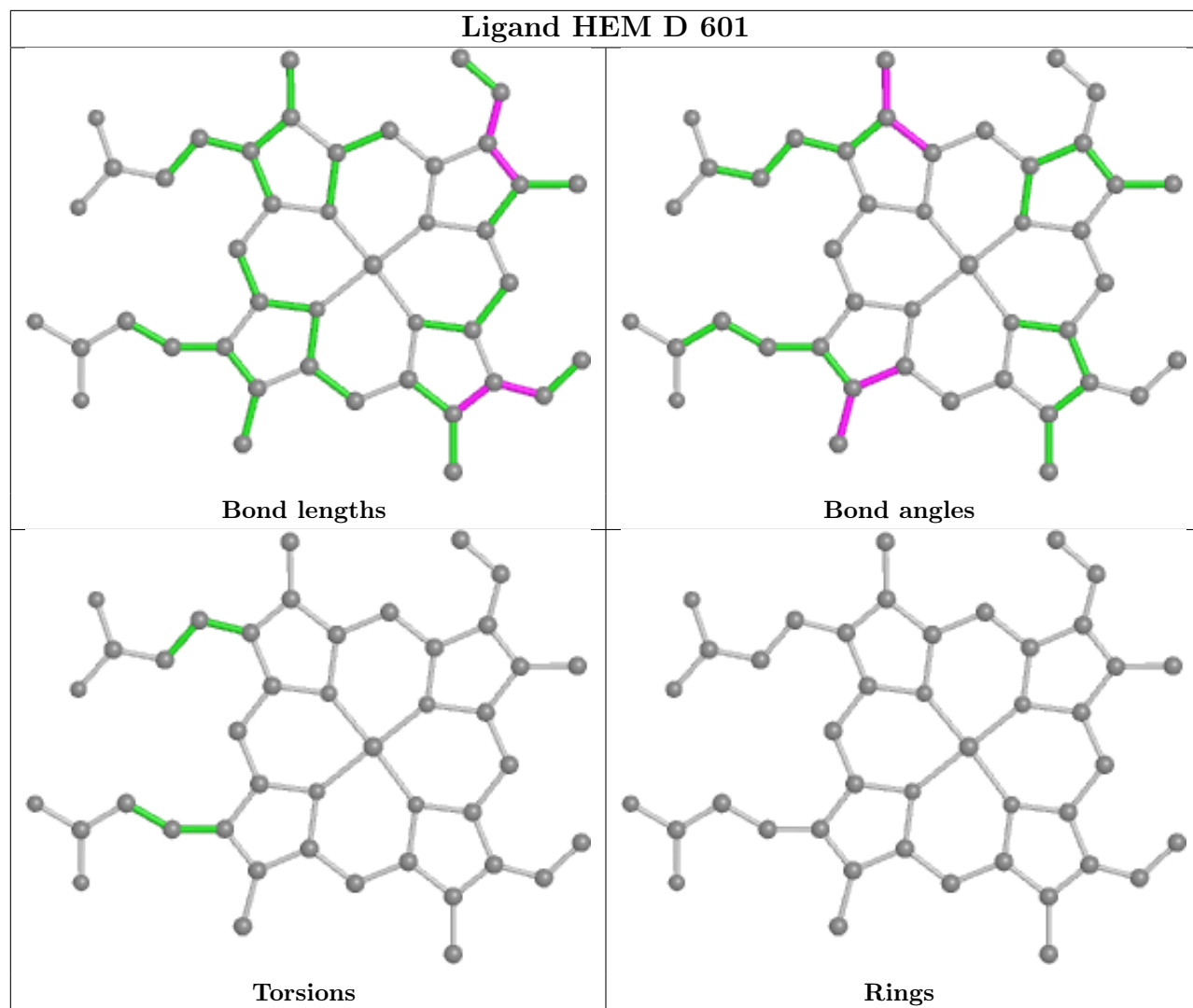
Ligand Q4P B 602

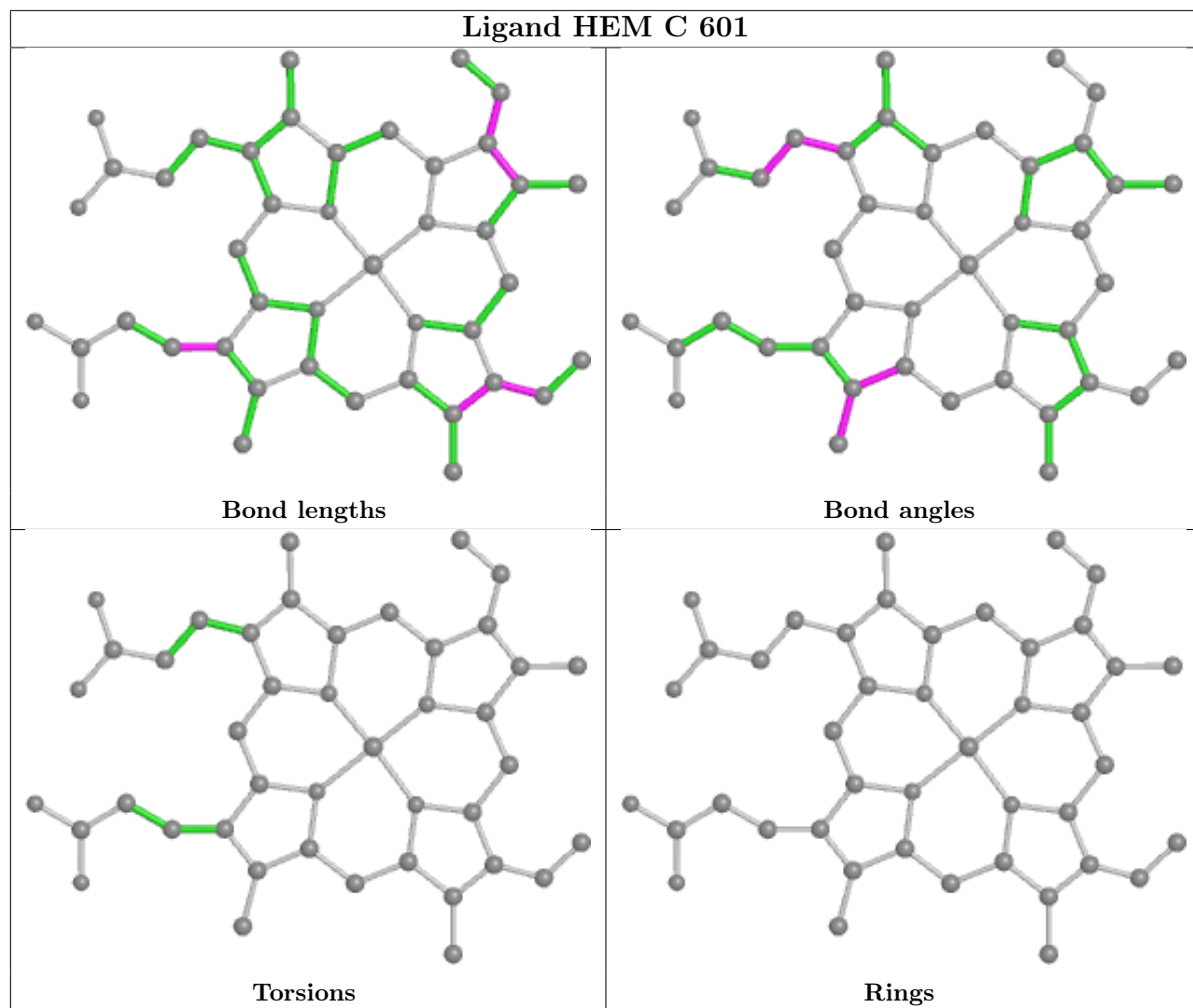


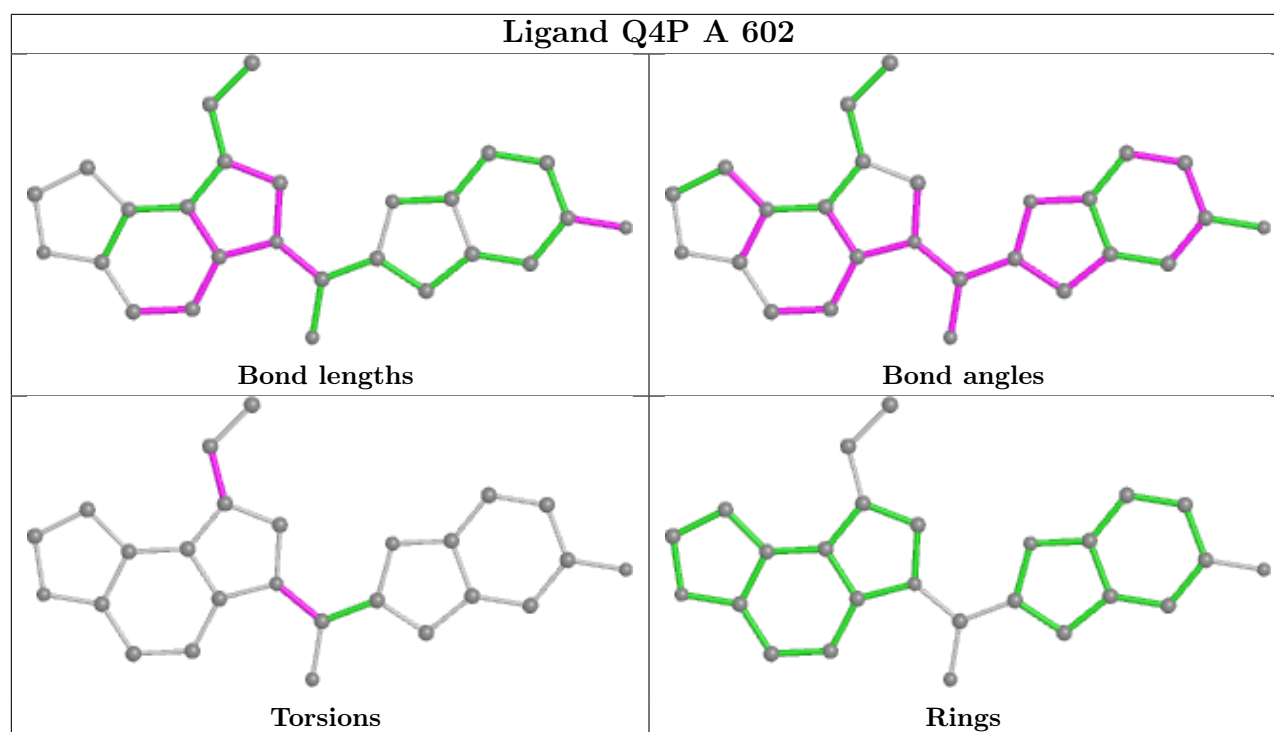
Ligand CPS A 603











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	467/491 (95%)	0.12	13 (2%)	53 28	56, 76, 107, 148	0
1	B	476/491 (96%)	0.14	20 (4%)	36 18	59, 74, 99, 136	0
1	C	468/491 (95%)	0.18	12 (2%)	56 31	50, 79, 96, 121	0
1	D	465/491 (94%)	0.28	19 (4%)	37 18	63, 87, 119, 142	0
All	All	1876/1964 (95%)	0.18	64 (3%)	45 23	50, 78, 109, 148	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	HIS	4.7
1	B	301	GLN	4.2
1	B	297	ASN	4.1
1	D	221	ASN	4.0
1	A	210	ASN	3.7
1	D	318	GLY	3.6
1	D	317	ALA	3.6
1	B	300	VAL	3.4
1	A	320	ASP	3.3
1	B	294	LEU	3.3
1	B	295	ASP	3.2
1	A	244	PRO	3.2
1	A	212	GLN	3.2
1	D	321	THR	3.2
1	D	302	LEU	3.2
1	B	210	ASN	3.2
1	C	321	THR	3.1
1	B	298	ALA	3.1
1	B	293	GLN	3.1
1	C	275	LYS	3.0
1	D	320	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	278	ILE	2.9
1	C	512	SER	2.9
1	D	316	GLY	2.9
1	B	354	SER	2.8
1	B	209	HIS	2.8
1	A	290	GLN	2.8
1	D	274	GLU	2.7
1	B	299	ASN	2.7
1	B	153	SER	2.7
1	C	292	LYS	2.7
1	D	324	THR	2.6
1	B	296	GLU	2.6
1	B	154	SER	2.5
1	A	152	ALA	2.5
1	A	222	ASN	2.5
1	C	277	HIS	2.5
1	D	287	GLU	2.5
1	D	273	PHE	2.4
1	D	275	LYS	2.4
1	A	292	LYS	2.3
1	C	317	ALA	2.3
1	A	304	ASP	2.3
1	A	324	THR	2.3
1	B	320	ASP	2.3
1	D	277	HIS	2.3
1	B	155	THR	2.2
1	C	316	GLY	2.2
1	D	153	SER	2.2
1	A	302	LEU	2.2
1	D	210	ASN	2.2
1	B	152	ALA	2.2
1	D	289	CYS	2.2
1	D	512	SER	2.1
1	C	37	LEU	2.1
1	C	320	ASP	2.1
1	B	497	THR	2.1
1	C	154	SER	2.1
1	B	222	ASN	2.1
1	A	318	GLY	2.1
1	C	395	SER	2.1
1	B	211	HIS	2.0
1	D	497	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	497	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

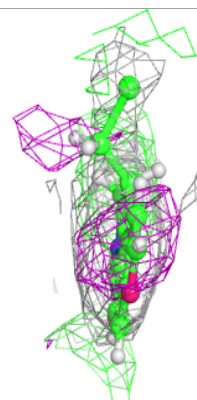
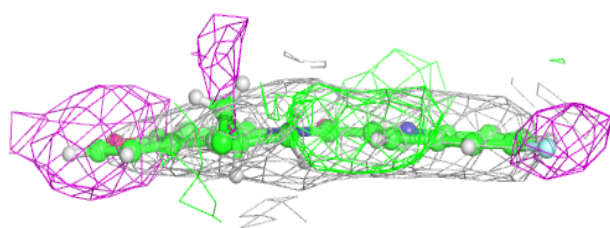
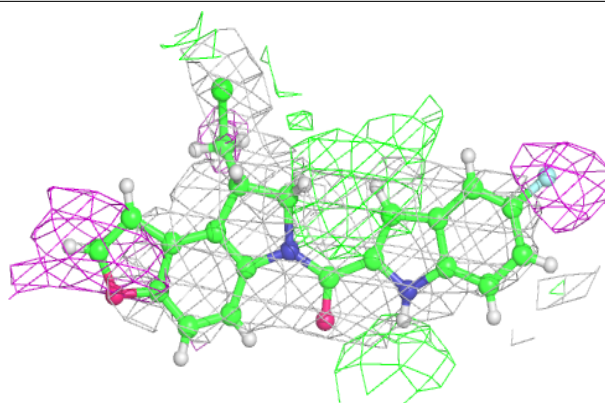
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	Q4P	B	602	26/26	0.79	0.41	69,75,85,96	0
3	Q4P	D	602	26/26	0.82	0.40	76,90,103,104	0
3	Q4P	C	602	26/26	0.84	0.34	68,78,85,100	0
3	Q4P	A	602	26/26	0.87	0.34	68,80,92,96	0
4	CPS	A	603	42/42	0.88	0.37	93,116,128,130	0
2	HEM	D	601	43/43	0.95	0.41	65,72,78,83	0
2	HEM	B	601	43/43	0.95	0.37	62,67,71,101	0
2	HEM	C	601	43/43	0.96	0.38	58,64,70,74	0
2	HEM	A	601	43/43	0.97	0.36	63,67,72,73	0

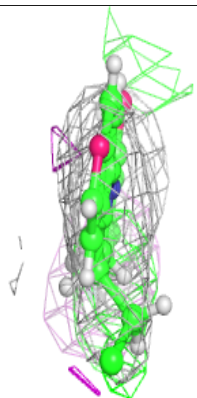
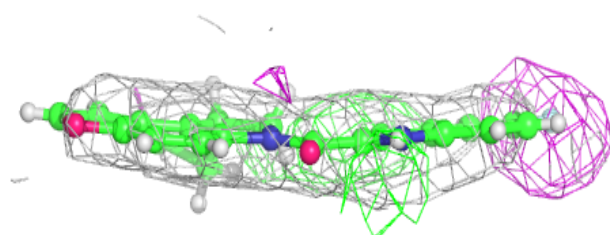
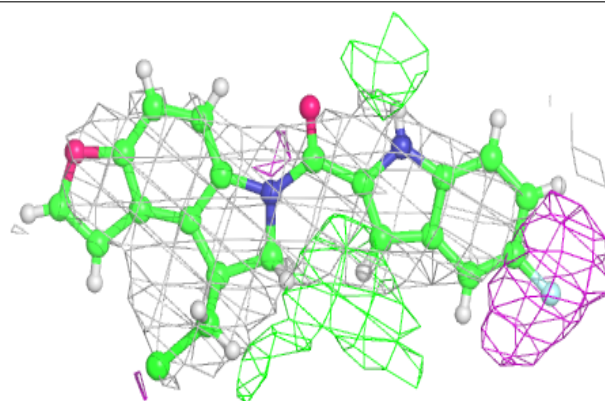
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q4P B 602:

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

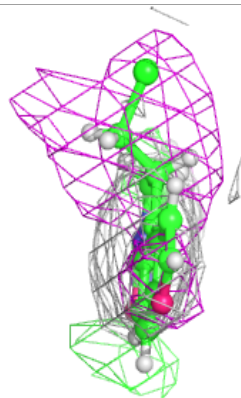
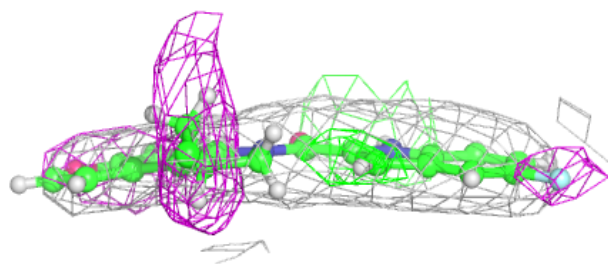
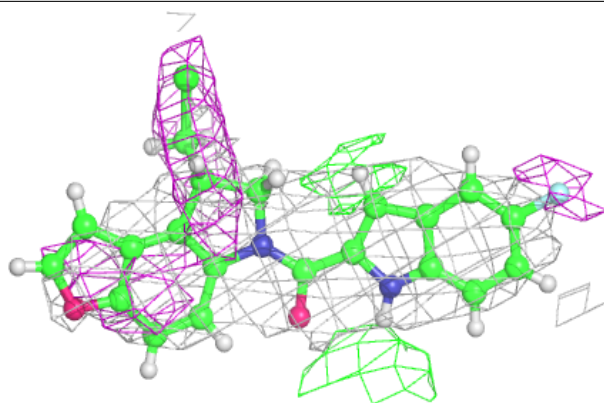
**Electron density around Q4P D 602:**

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

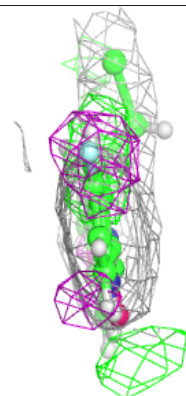
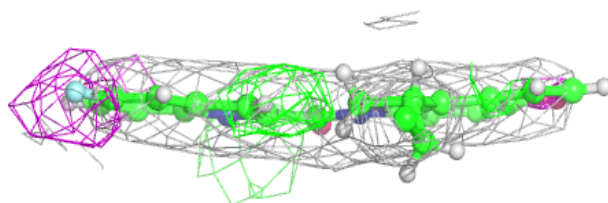
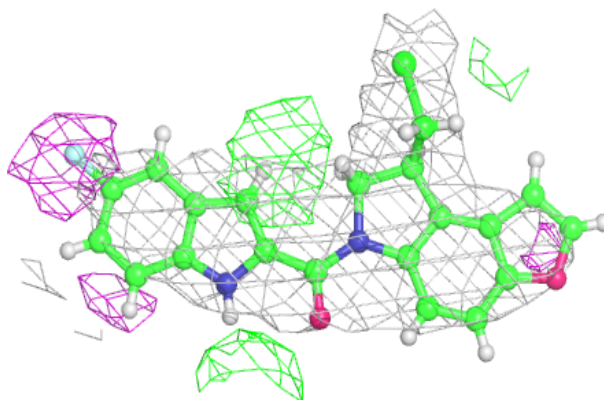


Electron density around Q4P C 602:

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

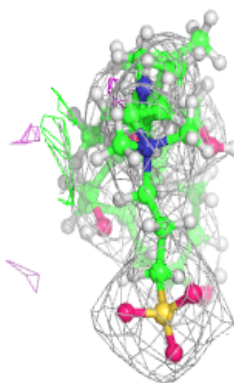
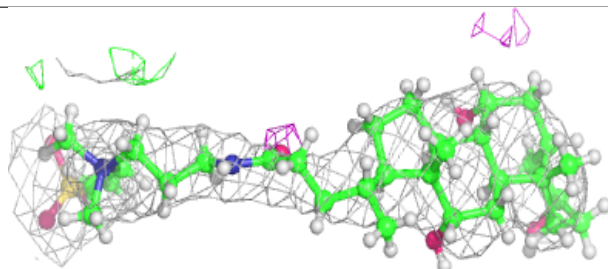
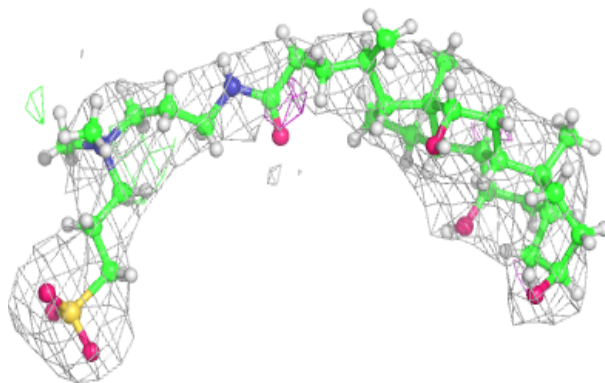
**Electron density around Q4P A 602:**

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

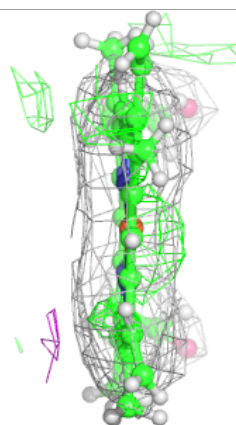
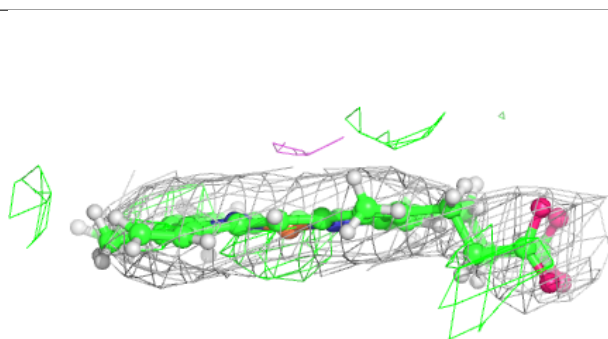
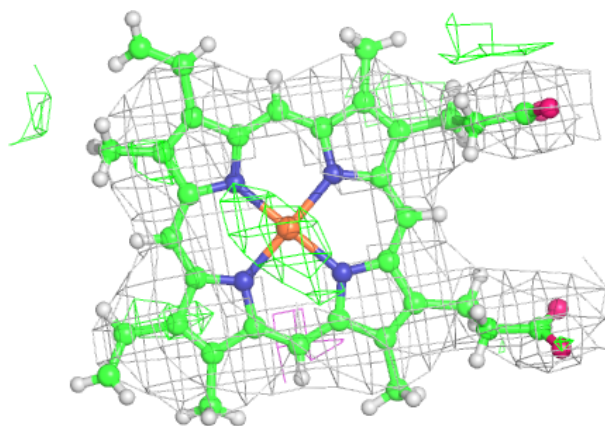


Electron density around CPS A 603:

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

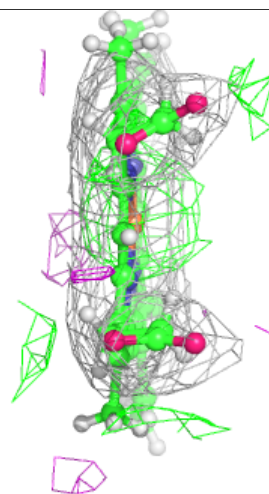
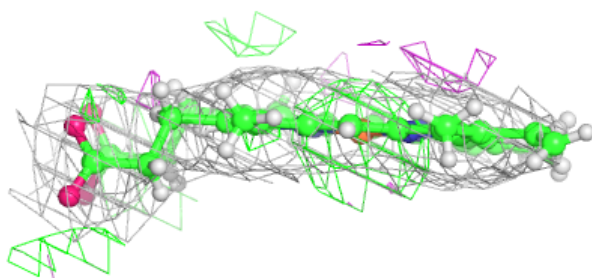
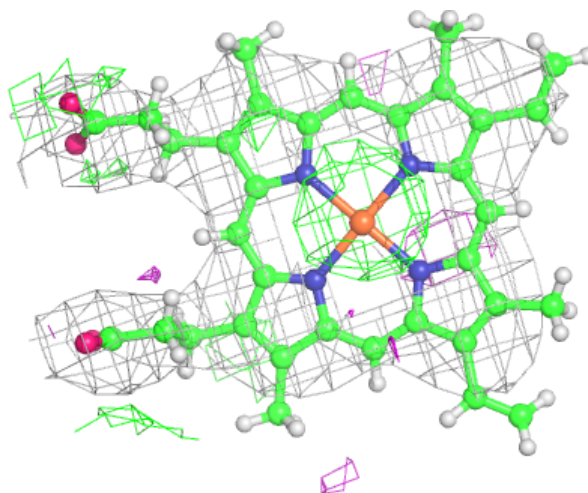
**Electron density around HEM D 601:**

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



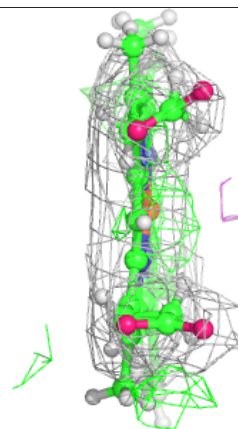
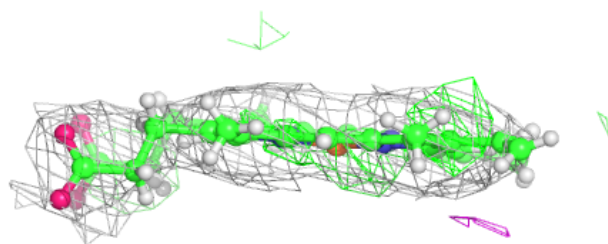
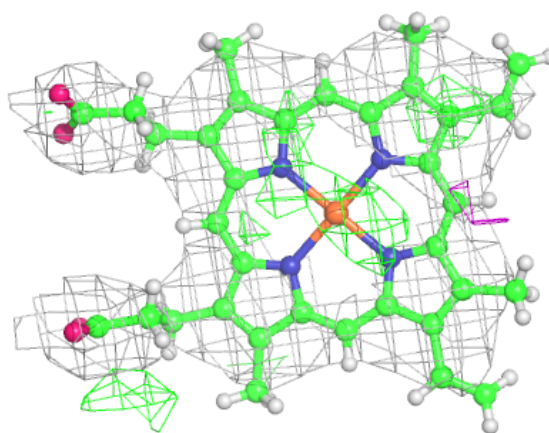
Electron density around HEM B 601:

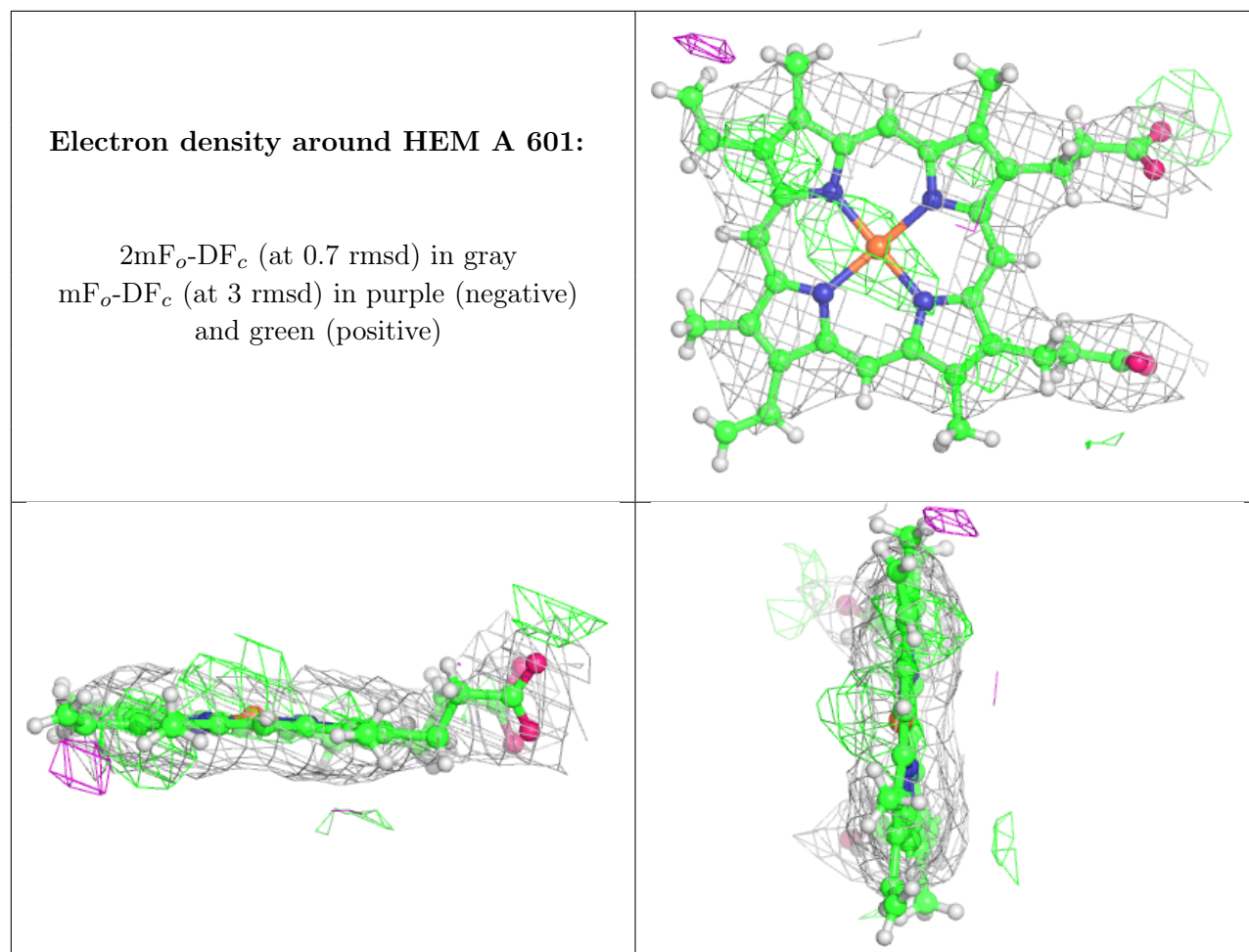
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 601:

$2mF_o-DF_c$ (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.