



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:45 am BST

PDB ID : 6DWN
Title : Structure of Human Cytochrome P450 1A1 with Erlotinib
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2018-06-26
Resolution : 3.00 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 : 2.11
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) : 2.11

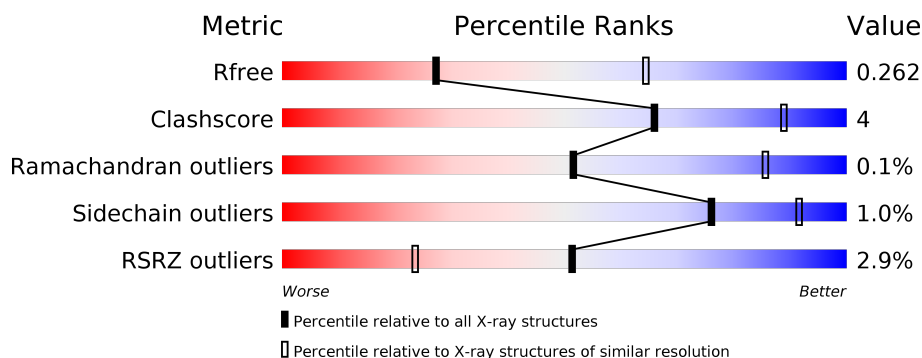
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	491	<div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	C	491	<div> <div>5%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	D	491	<div> <div>3%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30308 atoms, of which 15121 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	476	Total	C	H	N	O	S	0	0	0
			7619	2440	3807	663	688	21			
1	B	465	Total	C	H	N	O	S	0	0	0
			7437	2384	3718	647	667	21			
1	C	462	Total	C	H	N	O	S	0	0	0
			7395	2371	3697	643	663	21			
1	D	453	Total	C	H	N	O	S	0	0	0
			7251	2325	3628	629	648	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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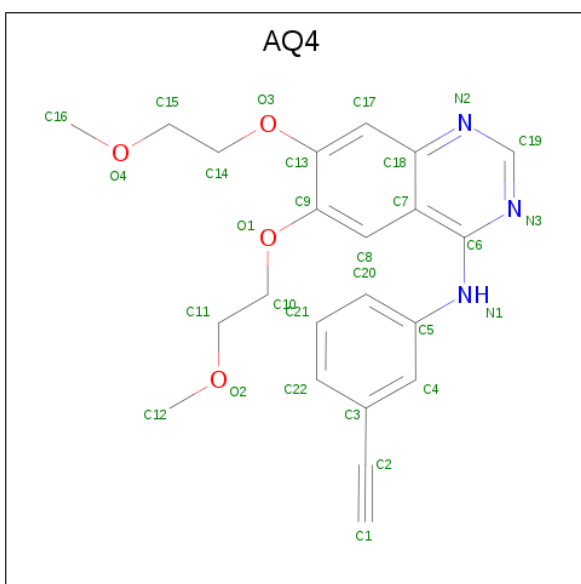
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	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: $C_{34}H_{32}FeN_4O_4$).



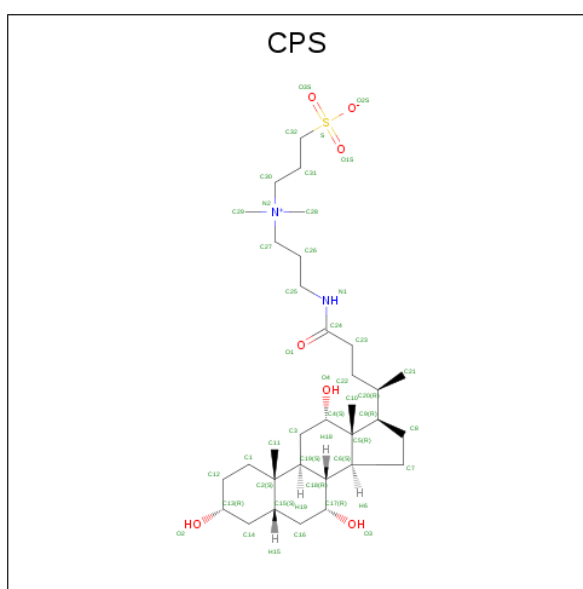
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 3 is [6,7-BIS(2-METHOXY-ETHOXY)QUINAZOLINE-4-YL]-(3-ETHYNYLPHE
NYL)AMINE (three-letter code: AQ4) (formula: C₂₂H₂₃N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			52	22	23	3	4		
3	B	1	Total	C	H	N	O	0	0
			52	22	23	3	4		
3	C	1	Total	C	H	N	O	0	0
			36	18	13	3	2		
3	D	1	Total	C	H	N	O	0	0
			33	17	11	3	2		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O		0	0
			65	23	39	3			
4	B	1	Total	C	H	N	O	0	0
			72	25	42	1	4		

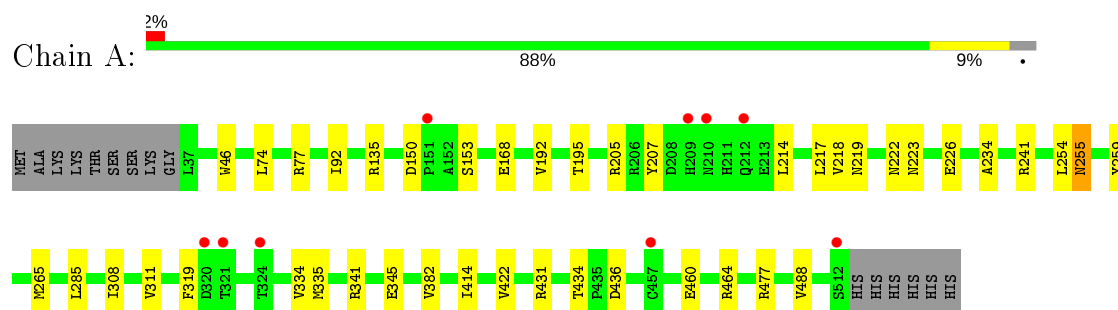
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total 3 3	0	0
5	B	1	Total 1 1	0	0

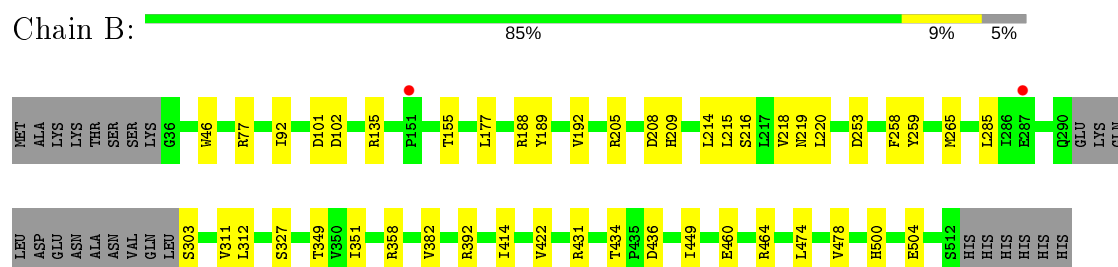
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

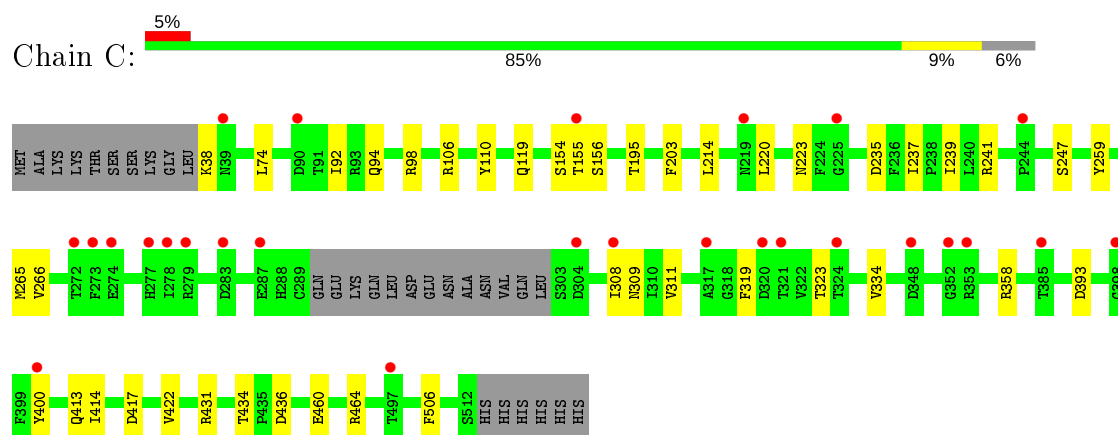
• Molecule 1: Cytochrome P450 1A1



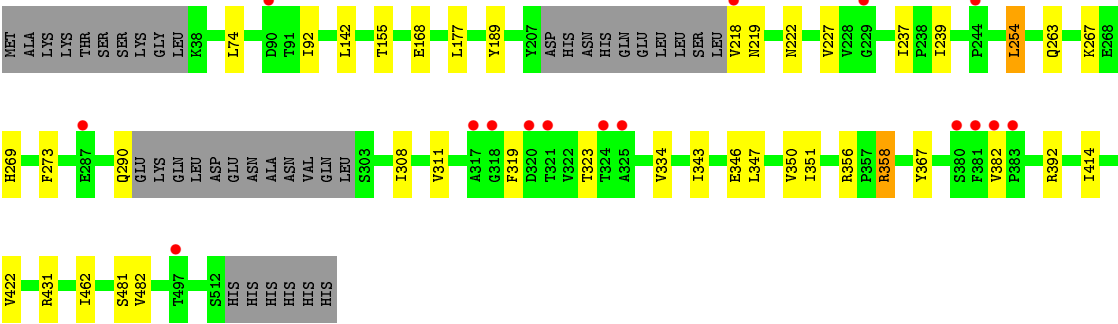
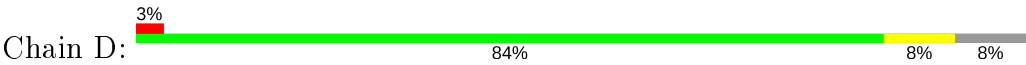
• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.86Å 195.08Å 238.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.98 – 3.00 38.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.98-3.00) 93.0 (38.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.241 , 0.261 0.241 , 0.262	Depositor DCC
R_{free} test set	1997 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30308	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: AQ4, CPS, 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	0.27	0/3907	0.44	0/5295
1	B	0.26	0/3813	0.43	0/5166
1	C	0.25	0/3792	0.41	0/5138
1	D	0.26	0/3714	0.42	0/5030
All	All	0.26	0/15226	0.43	0/20629

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	3812	3807	3806	28	0
1	B	3719	3718	3716	27	0
1	C	3698	3697	3694	22	0
1	D	3623	3628	3625	22	0
2	A	43	30	30	5	0
2	B	43	30	30	5	0
2	C	43	30	30	5	0
2	D	43	30	30	4	0
3	A	29	23	23	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	23	23	2	0
3	C	23	13	11	2	0
3	D	22	11	9	2	0
4	A	26	39	37	1	0
4	B	30	42	40	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
All	All	15187	15121	15104	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (120) 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:188:ARG:NH2	1:B:504:GLU:OE2	2.08	0.85
1:A:255:ASN:ND2	3:A:602:AQ4:O4	2.16	0.78
1:C:434:THR:OG1	1:C:436:ASP:OD1	2.04	0.76
1:D:155:THR:OG1	1:D:358:ARG:NH2	2.20	0.74
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.71	0.72
3:A:602:AQ4:N3	3:A:602:AQ4:H21	2.06	0.71
3:B:602:AQ4:H21	3:B:602:AQ4:N3	2.06	0.70
1:A:422:VAL:O	1:A:431:ARG:NH2	2.25	0.70
1:D:168:GLU:OE2	1:D:356:ARG:NH1	2.27	0.68
1:B:192:VAL:HG11	1:B:209:HIS:HA	1.74	0.67
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.78	0.66
1:A:195:THR:HG21	1:A:214:LEU:HD11	1.79	0.63
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.82	0.62
1:D:142:LEU:HD22	1:D:462:ILE:CD1	2.30	0.62
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.82	0.61
1:A:254:LEU:HD23	3:A:602:AQ4:H17	1.80	0.61
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.83	0.61
4:A:603:CPS:H10B	4:A:603:CPS:H21A	1.83	0.60
1:C:422:VAL:O	1:C:431:ARG:NH2	2.35	0.60
1:C:237:ILE:HG22	1:C:239:ILE:HG22	1.83	0.60
1:A:205:ARG:NH2	1:A:207:TYR:OH	2.36	0.58
1:B:102:ASP:OD1	1:B:392:ARG:NH1	2.36	0.58
1:B:208:ASP:OD1	1:B:209:HIS:N	2.36	0.58
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.85	0.58
1:D:334:VAL:HG21	1:D:482:VAL:HB	1.85	0.57
1:A:205:ARG:NH1	1:A:265:MET:SD	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ASP:OD2	1:C:400:TYR:OH	2.16	0.57
1:B:258:PHE:HD2	1:B:312:LEU:HD11	1.70	0.56
1:C:156:SER:OG	1:C:358:ARG:NH2	2.33	0.56
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	1.87	0.56
1:C:413:GLN:NE2	1:C:417:ASP:OD2	2.39	0.56
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.89	0.55
1:D:263:GLN:HB3	1:D:267:LYS:NZ	2.22	0.55
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.89	0.55
3:A:602:AQ4:C20	3:A:602:AQ4:N3	2.71	0.54
1:B:349:THR:HG23	1:D:350:VAL:HG22	1.90	0.54
1:C:319:PHE:O	1:C:323:THR:OG1	2.17	0.53
1:D:422:VAL:O	1:D:431:ARG:NH2	2.41	0.53
1:A:319:PHE:CZ	3:A:602:AQ4:H8	2.44	0.53
1:B:351:ILE:HG22	1:B:351:ILE:O	2.09	0.53
1:B:460:GLU:OE1	1:B:464:ARG:NH1	2.42	0.52
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.90	0.52
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.90	0.52
1:D:177:LEU:HD11	1:D:189:TYR:CZ	2.45	0.52
1:B:214:LEU:O	1:B:218:VAL:N	2.43	0.51
1:B:434:THR:OG1	1:B:436:ASP:OD1	2.17	0.51
1:D:237:ILE:HG22	1:D:239:ILE:HG22	1.91	0.51
1:C:92:ILE:HD12	1:C:414:ILE:HD11	1.91	0.51
1:A:168:GLU:OE1	1:A:477:ARG:NH1	2.43	0.51
3:D:602:AQ4:H21	3:D:602:AQ4:N3	2.26	0.51
1:A:434:THR:OG1	1:A:436:ASP:OD1	2.20	0.50
1:B:155:THR:O	1:B:358:ARG:NH2	2.45	0.50
3:B:602:AQ4:C20	3:B:602:AQ4:N3	2.71	0.50
1:A:335:MET:HE3	1:A:488:VAL:HG11	1.94	0.50
1:A:308:ILE:O	1:A:311:VAL:HG22	2.11	0.50
1:D:308:ILE:O	1:D:311:VAL:HG22	2.11	0.50
1:B:422:VAL:O	1:B:431:ARG:NH2	2.45	0.50
1:B:285:LEU:HD12	1:B:311:VAL:HG13	1.93	0.49
3:D:602:AQ4:C20	3:D:602:AQ4:N3	2.74	0.49
1:C:119:GLN:O	1:C:309:ASN:ND2	2.46	0.49
1:C:308:ILE:O	1:C:311:VAL:HG22	2.12	0.49
1:D:92:ILE:CD1	1:D:414:ILE:HD11	2.39	0.49
1:B:214:LEU:O	1:B:218:VAL:HG22	2.13	0.48
1:B:474:LEU:O	1:B:478:VAL:HG22	2.13	0.48
1:D:346:GLU:OE1	1:D:367:TYR:HB3	2.14	0.48
1:B:351:ILE:CG2	1:B:351:ILE:O	2.62	0.47
1:D:218:VAL:HG23	1:D:219:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ILE:O	1:D:347:LEU:HD13	2.14	0.47
1:A:192:VAL:HG13	1:A:214:LEU:CD2	2.44	0.47
1:B:215:LEU:O	1:B:220:LEU:N	2.47	0.47
1:C:110:TYR:HB3	1:C:241:ARG:NH1	2.30	0.47
1:B:205:ARG:HE	1:B:265:MET:HE1	1.80	0.47
1:A:460:GLU:OE2	1:A:464:ARG:NH1	2.48	0.46
1:C:223:ASN:ND2	1:C:247:SER:O	2.48	0.46
1:D:347:LEU:O	1:D:351:ILE:O	2.34	0.46
1:A:341:ARG:O	1:A:345:GLU:N	2.41	0.45
3:C:602:AQ4:N3	3:C:602:AQ4:C20	2.79	0.45
1:A:92:ILE:HD12	1:A:414:ILE:HD11	1.98	0.45
1:D:222:ASN:ND2	1:D:254:LEU:HD23	2.33	0.44
1:A:192:VAL:HG13	1:A:214:LEU:HD21	2.00	0.44
1:D:334:VAL:HG23	1:D:481:SER:HA	1.99	0.44
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.47	0.44
1:C:106:ARG:NH2	2:C:601:HEM:O2D	2.47	0.44
1:A:195:THR:CG2	1:A:214:LEU:HD11	2.47	0.44
1:A:234:ALA:O	1:A:241:ARG:NH1	2.51	0.44
1:A:135:ARG:NH1	2:A:601:HEM:O1D	2.51	0.44
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.48	0.44
1:C:334:VAL:HG21	1:C:506:PHE:CE2	2.53	0.44
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	2.01	0.43
1:B:216:SER:HA	1:B:220:LEU:HB3	1.99	0.43
1:B:135:ARG:NH1	2:B:601:HEM:O1D	2.51	0.43
1:C:195:THR:HG21	1:C:214:LEU:HD11	1.99	0.43
1:C:94:GLN:OE1	1:C:98:ARG:NH2	2.46	0.43
1:A:150:ASP:O	1:A:153:SER:O	2.36	0.43
1:A:74:LEU:HD12	1:A:74:LEU:C	2.38	0.43
1:B:177:LEU:HD11	1:B:189:TYR:CZ	2.53	0.43
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.49	0.43
1:C:460:GLU:OE2	1:C:464:ARG:NH1	2.52	0.43
2:C:601:HEM:CMB	2:C:601:HEM:HBB2	2.48	0.43
1:D:269:HIS:O	1:D:273:PHE:N	2.51	0.43
1:A:223:ASN:HB2	1:A:226:GLU:OE1	2.20	0.42
1:B:218:VAL:HG23	1:B:219:ASN:N	2.33	0.42
1:B:327:SER:OG	1:B:500:HIS:NE2	2.44	0.42
1:C:266:VAL:HG21	1:C:308:ILE:HG21	2.02	0.42
3:C:602:AQ4:N3	3:C:602:AQ4:H21	2.35	0.42
1:A:254:LEU:HG	3:A:602:AQ4:H14	2.02	0.41
1:A:285:LEU:HD12	1:A:311:VAL:HG13	2.03	0.41
1:C:154:SER:OG	1:C:155:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ASP:HA	1:C:241:ARG:HH22	1.86	0.41
1:C:203:PHE:HB3	1:C:265:MET:HE2	2.02	0.41
1:A:222:ASN:HD21	3:A:602:AQ4:H15	1.86	0.41
1:D:382:VAL:HG11	2:D:601:HEM:HMA2	2.03	0.41
2:C:601:HEM:CMC	2:C:601:HEM:HBC2	2.47	0.40
1:A:218:VAL:HG23	1:A:219:ASN:N	2.37	0.40
1:A:46:TRP:O	1:A:77:ARG:NH2	2.54	0.40
1:B:285:LEU:CD1	1:B:311:VAL:HG13	2.51	0.40
1:D:74:LEU:HD12	1:D:74:LEU:C	2.42	0.40
1:B:46:TRP:O	1:B:77:ARG:NH2	2.54	0.40
1:C:74:LEU:HD12	1:C:74:LEU:C	2.41	0.40
1:D:319:PHE:O	1:D:323:THR:OG1	2.23	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	474/491 (96%)	463 (98%)	11 (2%)	0	100	100
1	B	461/491 (94%)	449 (97%)	11 (2%)	1 (0%)	47	82
1	C	458/491 (93%)	447 (98%)	11 (2%)	0	100	100
1	D	447/491 (91%)	437 (98%)	10 (2%)	0	100	100
All	All	1840/1964 (94%)	1796 (98%)	43 (2%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449	ILE

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	426/439 (97%)	422 (99%)	4 (1%)	78	92
1	B	415/439 (94%)	411 (99%)	4 (1%)	76	91
1	C	413/439 (94%)	410 (99%)	3 (1%)	84	94
1	D	404/439 (92%)	399 (99%)	5 (1%)	71	90
All	All	1658/1756 (94%)	1642 (99%)	16 (1%)	76	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	LEU
1	A	255	ASN
1	A	259	TYR
1	A	334	VAL
1	B	101	ASP
1	B	253	ASP
1	B	259	TYR
1	B	303	SER
1	C	38	LYS
1	C	220	LEU
1	C	259	TYR
1	D	227	VAL
1	D	254	LEU
1	D	290	GLN
1	D	358	ARG
1	D	392	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	255	ASN
1	B	344	GLN

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Mol	Chain	Res	Type
1	C	416	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	601	-	27,50,50	1.89	5 (18%)	17,82,82	1.33	2 (11%)
4	CPS	B	603	-	33,33,45	0.66	0	52,52,70	1.91	17 (32%)
3	AQ4	C	602	-	25,25,31	1.17	2 (8%)	34,34,40	1.37	6 (17%)
3	AQ4	A	602	-	31,31,31	1.25	3 (9%)	40,40,40	1.16	5 (12%)
3	AQ4	B	602	-	31,31,31	1.19	2 (6%)	40,40,40	1.09	4 (10%)
3	AQ4	D	602	-	24,24,31	1.26	2 (8%)	33,33,40	1.33	4 (12%)
2	HEM	A	601	1	27,50,50	1.84	5 (18%)	17,82,82	1.48	3 (17%)
2	HEM	C	601	-	27,50,50	1.85	4 (14%)	17,82,82	1.35	1 (5%)
2	HEM	B	601	-	27,50,50	1.94	5 (18%)	17,82,82	1.34	3 (17%)
4	CPS	A	603	-	29,29,45	1.01	1 (3%)	47,47,70	2.02	15 (31%)

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	D	601	-	-	0/6/54/54	-
4	CPS	B	603	-	-	3/11/76/90	0/4/4/4
3	AQ4	C	602	-	-	4/9/9/16	0/3/3/3
3	AQ4	A	602	-	-	7/16/16/16	0/3/3/3
3	AQ4	B	602	-	-	5/16/16/16	0/3/3/3
3	AQ4	D	602	-	-	3/8/8/16	0/3/3/3
2	HEM	A	601	1	-	0/6/54/54	-
2	HEM	C	601	-	-	0/6/54/54	-
2	HEM	B	601	-	-	2/6/54/54	-
4	CPS	A	603	-	-	0/6/71/90	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-C2B	-4.43	1.34	1.40
2	B	601	HEM	C3C-C2C	-4.17	1.34	1.40
2	C	601	HEM	C3C-C2C	-4.03	1.34	1.40
2	A	601	HEM	C3B-C2B	-4.03	1.34	1.40
2	D	601	HEM	C3C-C2C	-4.02	1.34	1.40
2	D	601	HEM	C3B-C2B	-3.95	1.34	1.40
2	C	601	HEM	C3B-C2B	-3.88	1.35	1.40
3	D	602	AQ4	C6-N1	3.83	1.42	1.36
3	A	602	AQ4	C6-N1	3.79	1.42	1.36
2	D	601	HEM	C3C-CAC	3.77	1.55	1.47
2	C	601	HEM	C3C-CAC	3.77	1.55	1.47
3	B	602	AQ4	C6-N1	3.76	1.41	1.36
2	A	601	HEM	C3C-C2C	-3.76	1.35	1.40
2	D	601	HEM	C3B-CAB	3.73	1.55	1.47
2	C	601	HEM	C3B-CAB	3.71	1.55	1.47
2	B	601	HEM	C3C-CAC	3.71	1.55	1.47
2	A	601	HEM	C3C-CAC	3.69	1.55	1.47
2	B	601	HEM	C3B-CAB	3.65	1.55	1.47
2	A	601	HEM	C3B-CAB	3.56	1.55	1.47
3	C	602	AQ4	C6-N1	3.27	1.41	1.36
3	B	602	AQ4	C5-N1	2.63	1.46	1.40
2	A	601	HEM	CAA-C2A	2.37	1.55	1.52
3	A	602	AQ4	C5-N1	2.27	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	AQ4	C19-N3	2.25	1.38	1.33
4	A	603	CPS	C5-C9	2.16	1.59	1.55
3	D	602	AQ4	C19-N3	2.15	1.37	1.33
3	C	602	AQ4	C19-N3	2.10	1.37	1.33
2	B	601	HEM	CAA-C2A	2.09	1.55	1.52
2	D	601	HEM	CAA-C2A	2.03	1.55	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	CPS	C5-C9-C20	-6.14	112.16	119.50
4	B	603	CPS	C5-C9-C20	-5.88	112.47	119.50
4	A	603	CPS	C19-C18-C6	-4.70	103.26	109.71
4	A	603	CPS	C5-C6-C18	-4.00	109.63	114.74
4	B	603	CPS	C22-C23-C24	-3.88	104.38	113.04
4	A	603	CPS	C2-C19-C18	-3.82	107.71	111.82
3	D	602	AQ4	C10-O1-C9	-3.72	111.92	117.53
4	B	603	CPS	C23-C24-N1	-3.71	111.13	116.29
4	B	603	CPS	C15-C14-C13	-3.28	107.94	112.76
4	B	603	CPS	C5-C6-C18	-3.27	110.56	114.74
3	A	602	AQ4	C4-C3-C2	-3.25	115.92	120.09
4	B	603	CPS	C19-C18-C6	-3.22	105.29	109.71
3	C	602	AQ4	C14-O3-C13	-3.22	111.03	118.05
3	B	602	AQ4	C4-C3-C2	-3.11	116.10	120.09
4	A	603	CPS	C8-C7-C6	-3.05	99.08	105.13
3	C	602	AQ4	C4-C3-C2	-3.01	116.23	120.09
3	C	602	AQ4	C5-N1-C6	-3.01	120.43	128.26
4	B	603	CPS	C1-C12-C13	-2.95	106.68	110.47
3	D	602	AQ4	C4-C3-C2	-2.93	116.34	120.09
3	D	602	AQ4	C5-N1-C6	-2.89	120.73	128.26
4	A	603	CPS	C1-C12-C13	-2.78	106.90	110.47
4	B	603	CPS	C16-C15-C2	-2.77	109.72	112.66
4	B	603	CPS	C2-C19-C18	-2.62	109.00	111.82
4	B	603	CPS	C19-C2-C15	2.54	112.15	108.58
2	B	601	HEM	CMC-C2C-C3C	2.54	129.43	124.68
4	A	603	CPS	O4-C4-C5	-2.52	106.77	111.03
2	A	601	HEM	CMA-C3A-C4A	-2.52	124.59	128.46
4	A	603	CPS	C6-C5-C4	-2.52	105.06	107.40
4	A	603	CPS	C3-C19-C18	2.51	114.56	110.88
4	A	603	CPS	C15-C14-C13	-2.49	109.11	112.76
3	A	602	AQ4	C14-O3-C13	-2.41	111.79	117.69
3	C	602	AQ4	O3-C14-C15	-2.37	100.12	108.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	CPS	C19-C2-C15	2.35	111.88	108.58
2	C	601	HEM	CAA-CBA-CGA	-2.34	108.74	112.67
3	B	602	AQ4	O3-C14-C15	-2.34	100.79	108.72
3	A	602	AQ4	O3-C14-C15	-2.33	100.82	108.72
4	B	603	CPS	C3-C19-C2	-2.32	111.33	113.73
2	A	601	HEM	CMC-C2C-C3C	2.30	128.98	124.68
3	C	602	AQ4	C6-C7-C18	2.29	117.32	115.88
3	D	602	AQ4	C6-C7-C18	2.28	117.31	115.88
2	D	601	HEM	CMC-C2C-C3C	2.28	128.94	124.68
4	B	603	CPS	O1-C24-C23	2.28	126.18	122.02
2	B	601	HEM	CAA-CBA-CGA	-2.21	108.96	112.67
3	B	602	AQ4	C6-C7-C18	2.21	117.27	115.88
3	A	602	AQ4	C6-C7-C18	2.20	117.26	115.88
4	A	603	CPS	C16-C15-C2	-2.19	110.33	112.66
2	A	601	HEM	CMB-C2B-C3B	2.15	128.69	124.68
4	B	603	CPS	C9-C5-C6	-2.15	97.93	100.09
4	A	603	CPS	C21-C20-C22	-2.11	106.44	111.78
4	B	603	CPS	O4-C4-C5	-2.10	107.48	111.03
2	B	601	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
4	A	603	CPS	C21-C20-C9	-2.08	109.73	112.92
3	C	602	AQ4	C17-C13-C9	-2.07	118.67	120.69
2	D	601	HEM	CMB-C2B-C3B	2.05	128.51	124.68
4	B	603	CPS	C6-C5-C4	2.04	109.31	107.40
4	B	603	CPS	C23-C22-C20	-2.03	110.81	114.52
3	B	602	AQ4	C5-N1-C6	-2.03	122.98	128.26
4	A	603	CPS	C9-C5-C6	2.03	102.14	100.09
4	B	603	CPS	C14-C13-C12	-2.01	108.16	110.55
3	A	602	AQ4	C5-N1-C6	-2.01	123.03	128.26

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	AQ4	C1-C2-C3-C4
3	A	602	AQ4	C1-C2-C3-C22
3	A	602	AQ4	O1-C10-C11-O2
3	A	602	AQ4	O3-C14-C15-O4
3	D	602	AQ4	C13-C9-O1-C10
3	D	602	AQ4	C8-C9-O1-C10
3	C	602	AQ4	C17-C13-O3-C14
3	C	602	AQ4	C9-C13-O3-C14
3	B	602	AQ4	O1-C10-C11-O2

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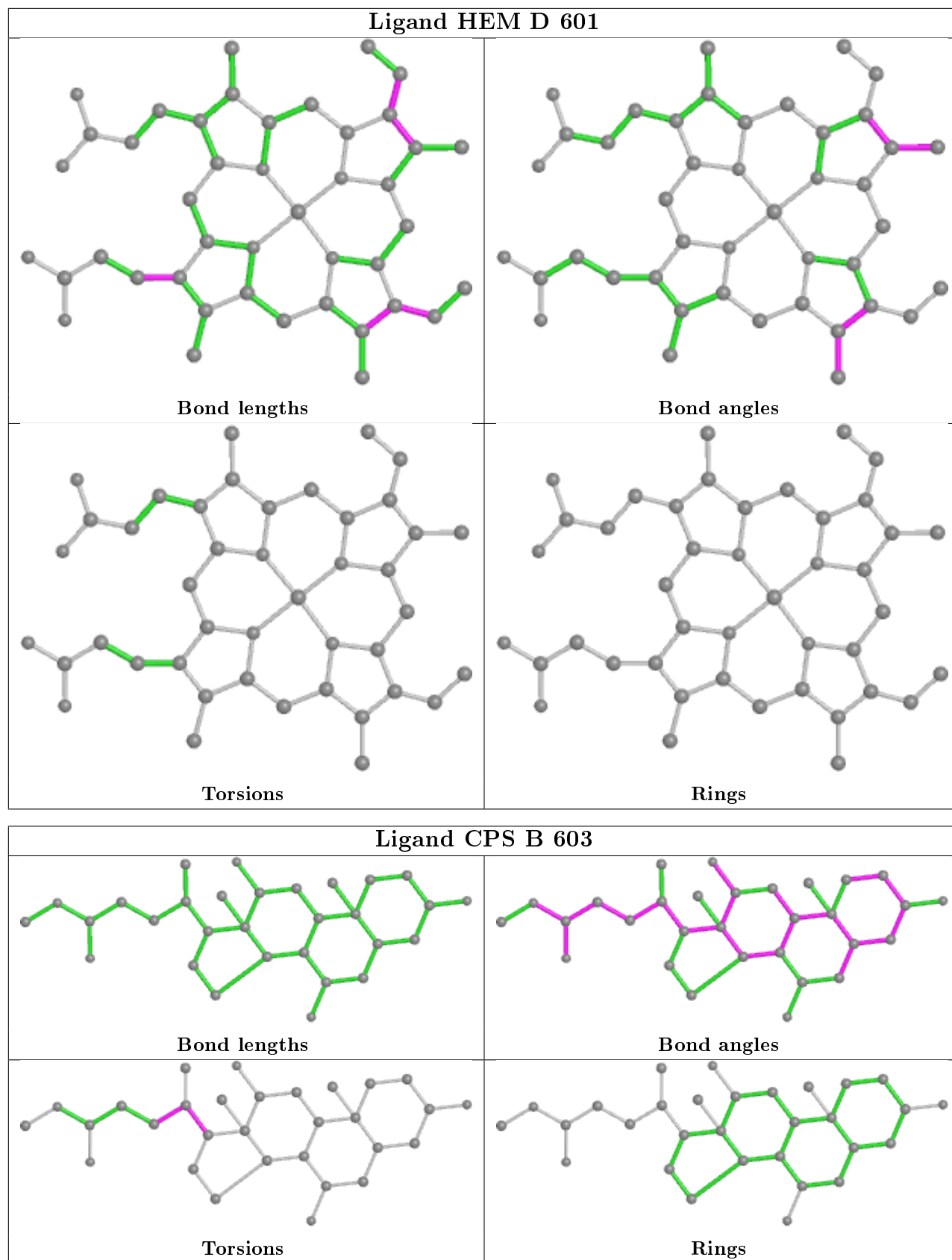
Mol	Chain	Res	Type	Atoms
4	B	603	CPS	C21-C20-C22-C23
4	B	603	CPS	C21-C20-C9-C5
3	B	602	AQ4	C10-C11-O2-C12
2	B	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C3A-C2A-CAA-CBA
3	A	602	AQ4	C10-C11-O2-C12
3	C	602	AQ4	C15-C14-O3-C13
4	B	603	CPS	C22-C20-C9-C5
3	C	602	AQ4	N3-C6-N1-C5
3	A	602	AQ4	C9-C13-O3-C14
3	B	602	AQ4	C14-C15-O4-C16
3	A	602	AQ4	C15-C14-O3-C13
3	B	602	AQ4	C1-C2-C3-C4
3	D	602	AQ4	C1-C2-C3-C4
3	B	602	AQ4	C15-C14-O3-C13

There are no ring outliers.

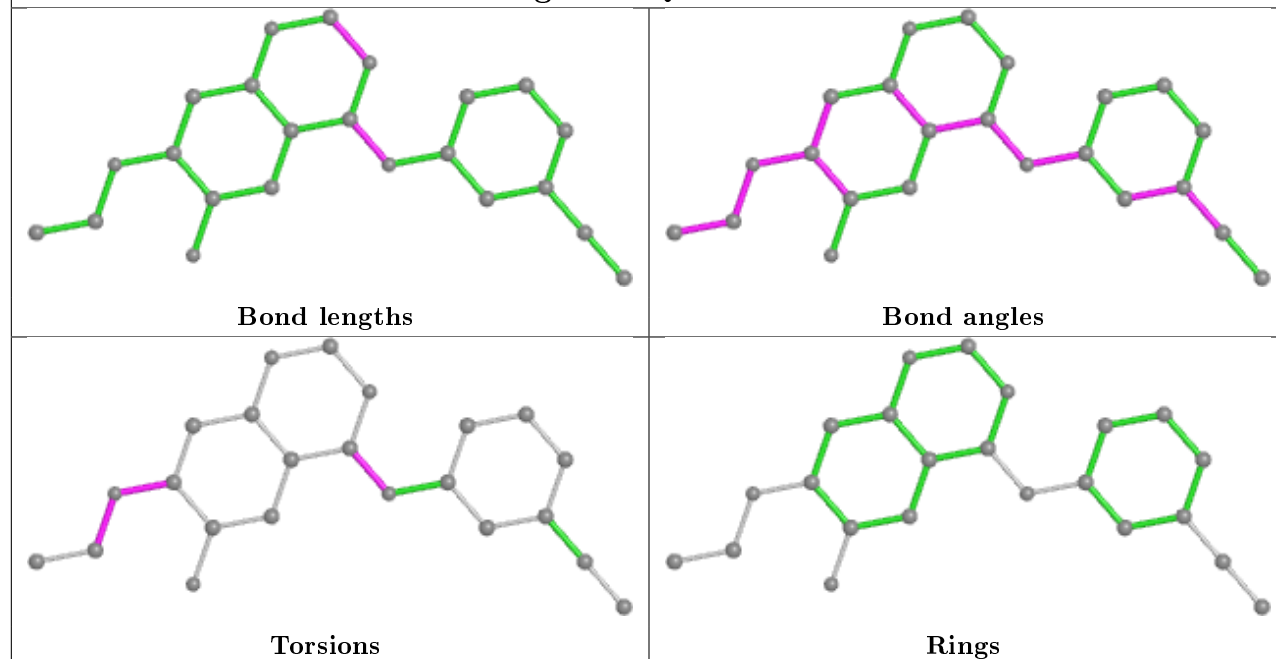
9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	4	0
3	C	602	AQ4	2	0
3	A	602	AQ4	7	0
3	B	602	AQ4	2	0
3	D	602	AQ4	2	0
2	A	601	HEM	5	0
2	C	601	HEM	5	0
2	B	601	HEM	5	0
4	A	603	CPS	1	0

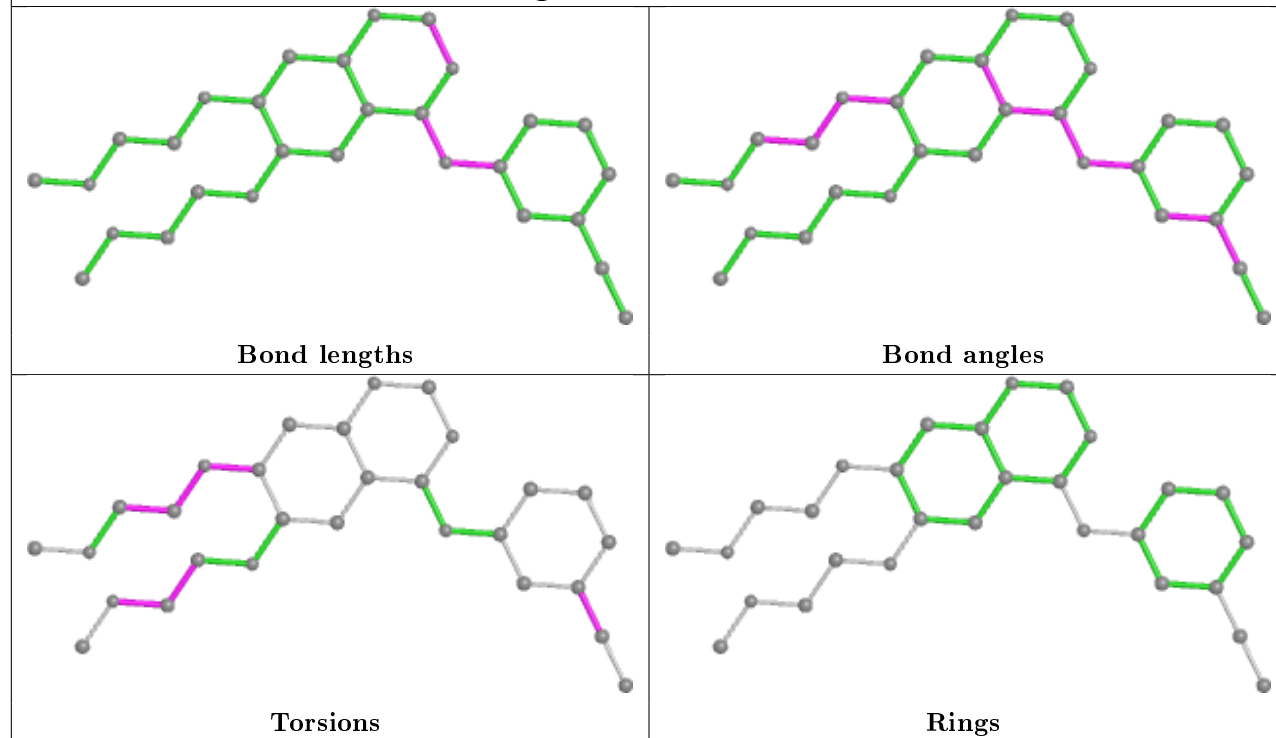
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

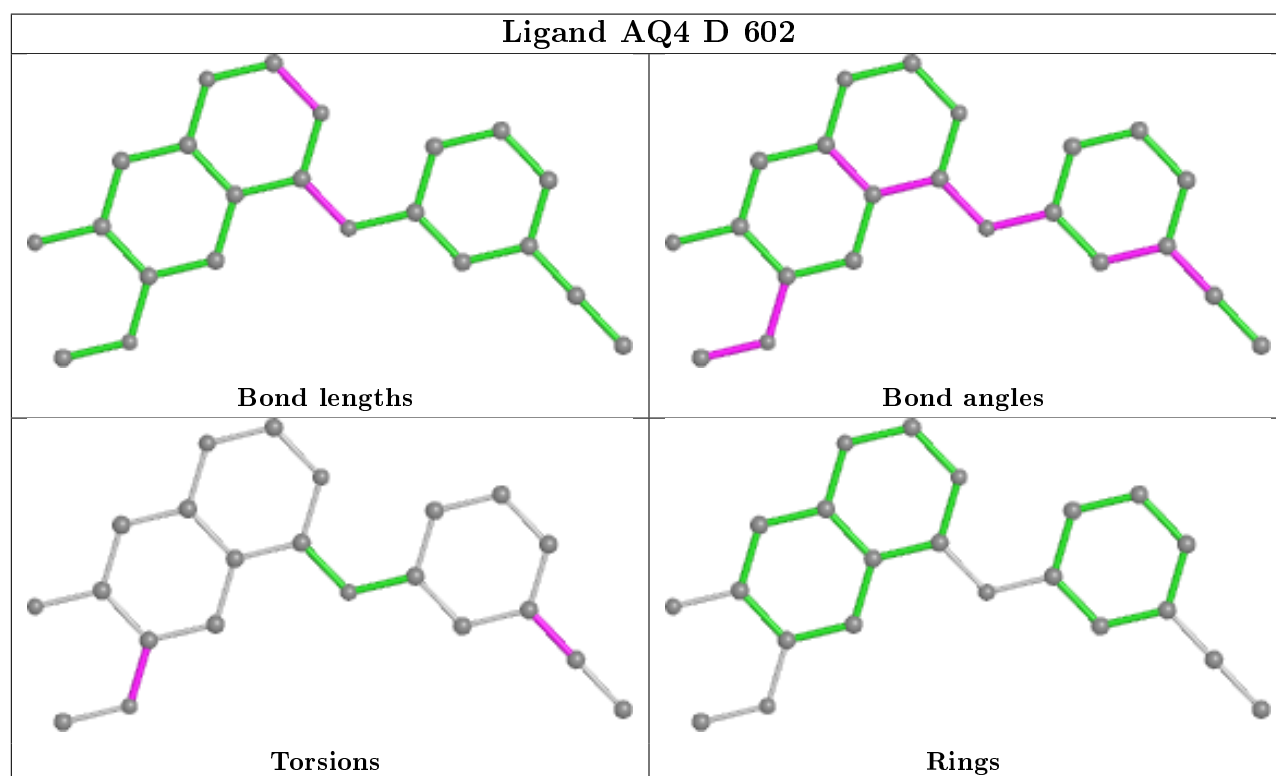
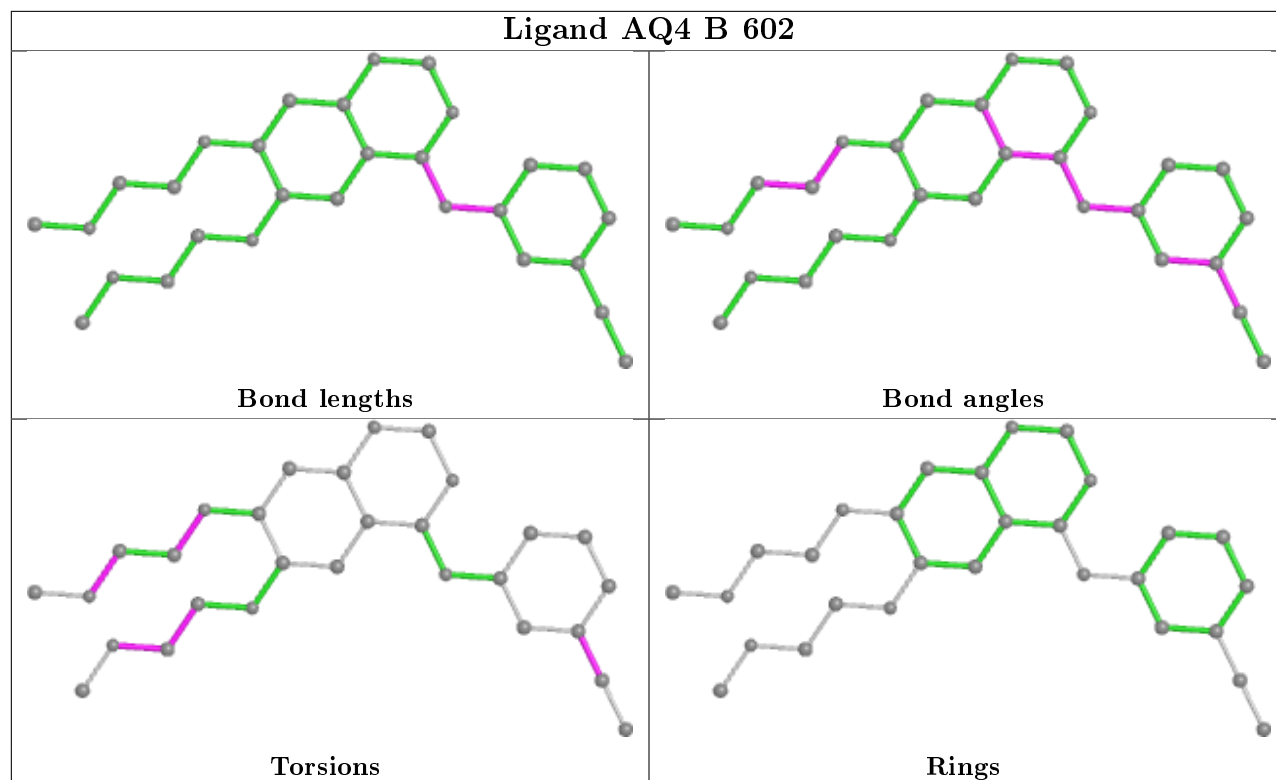


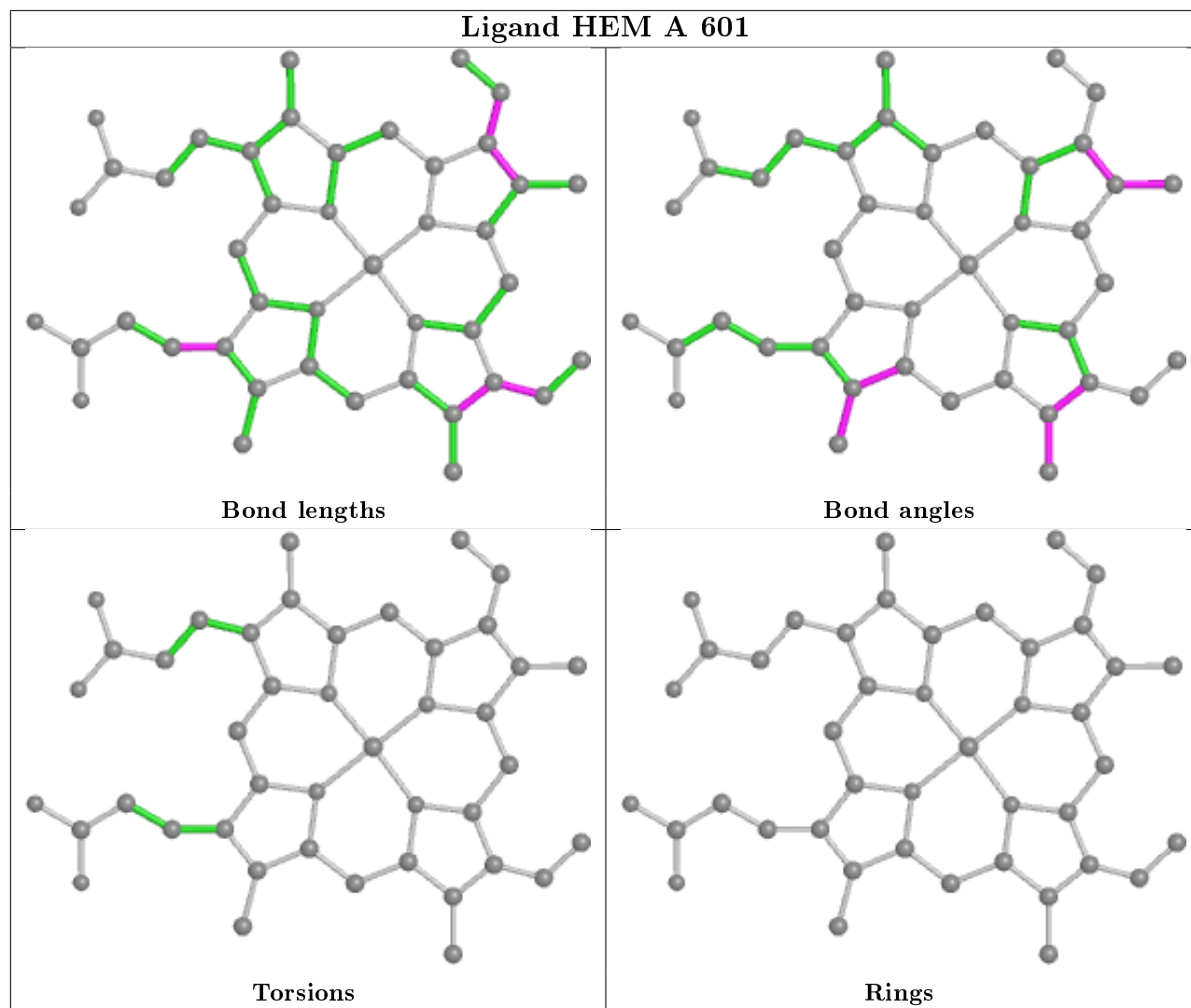
Ligand AQ4 C 602

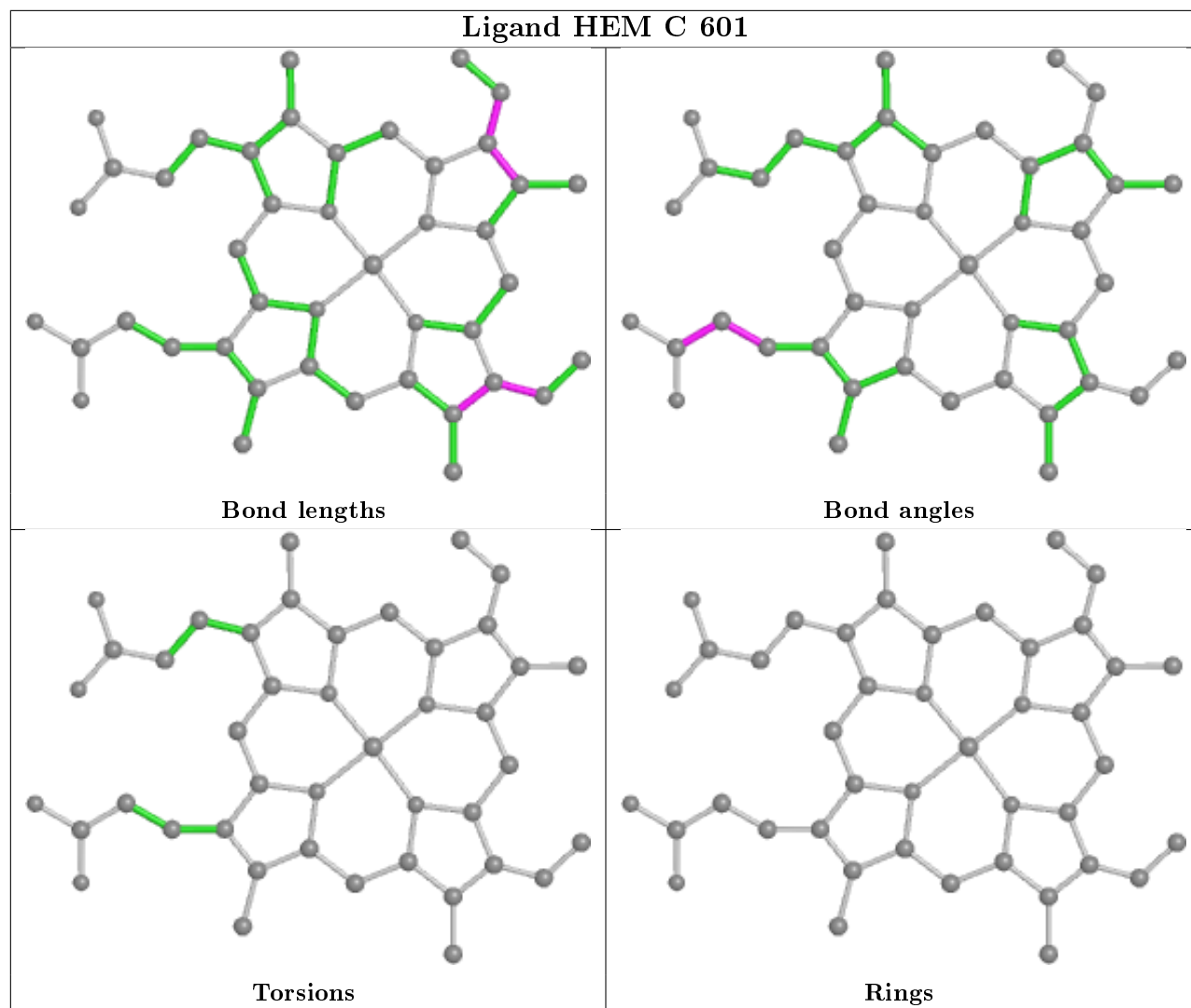


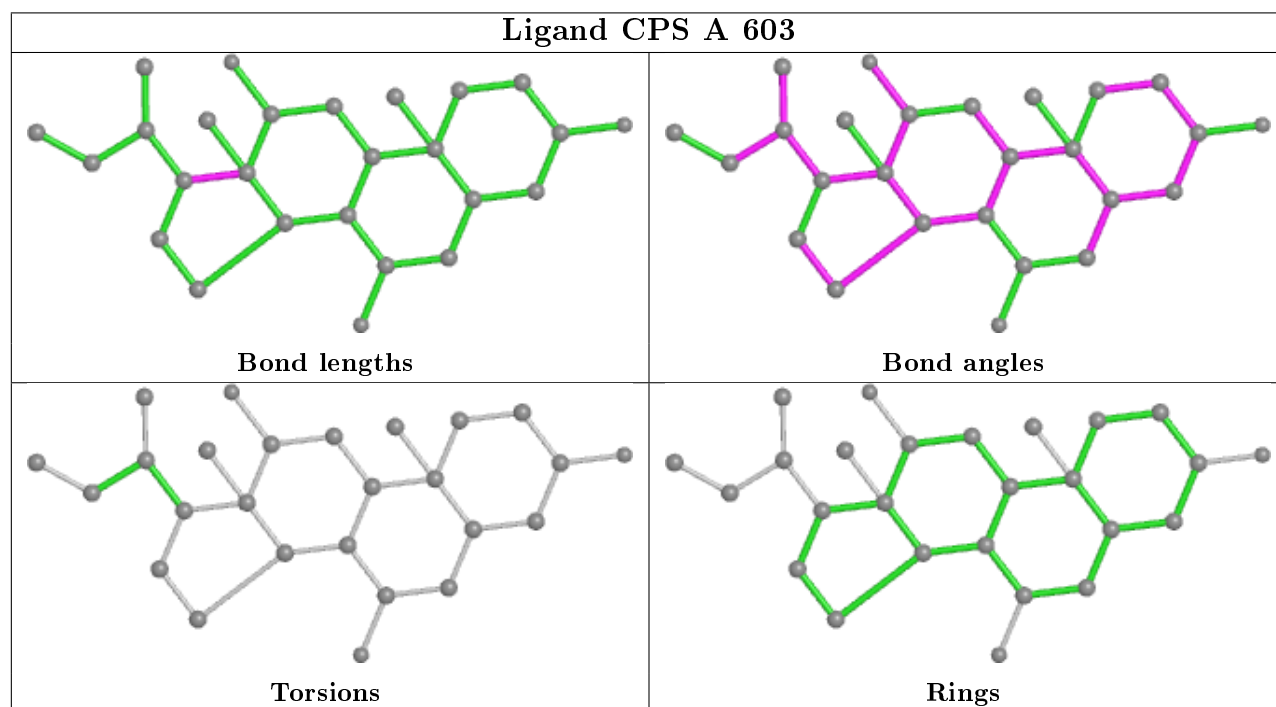
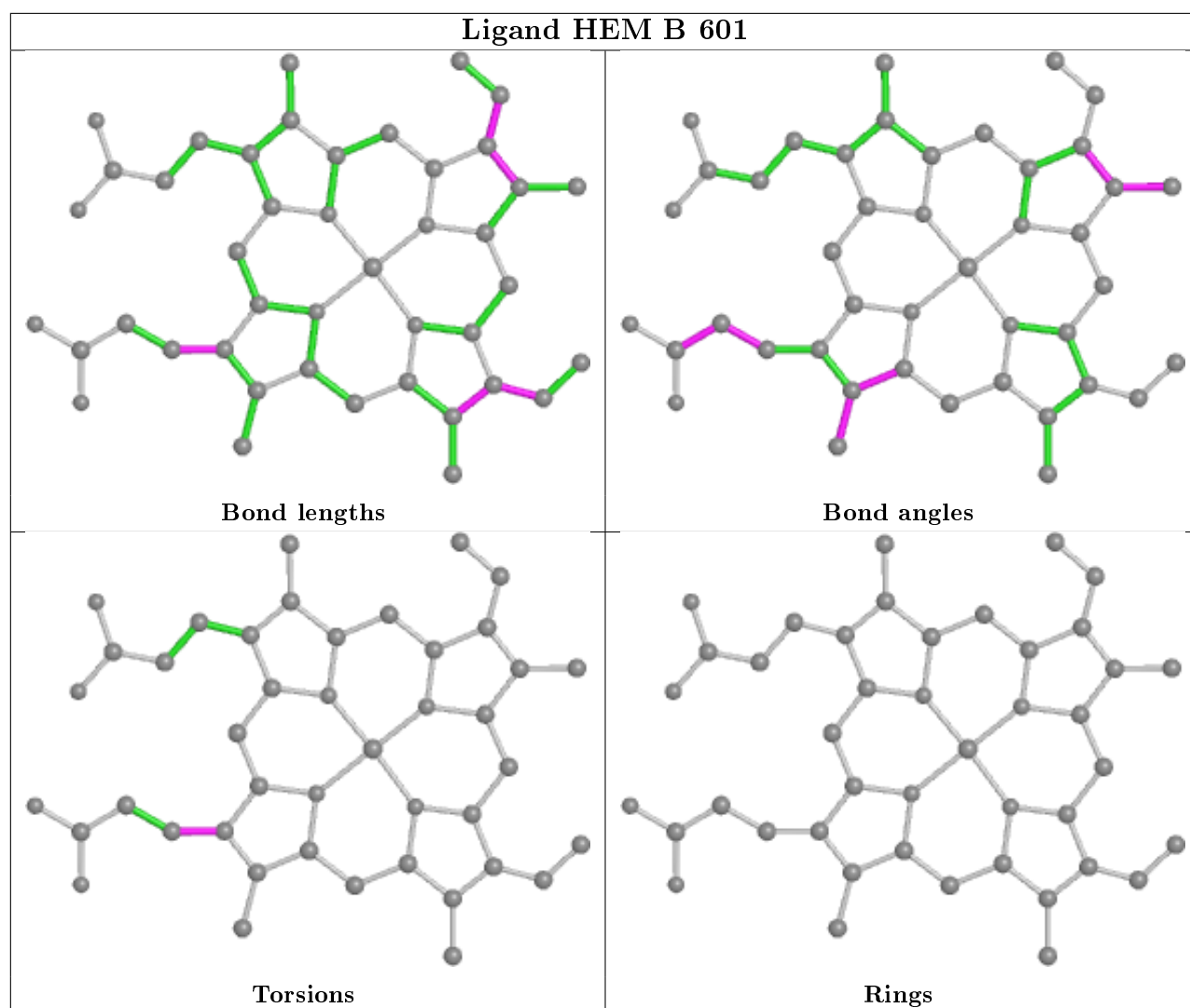
Ligand AQ4 A 602











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/491 (96%)	0.19	9 (1%) 66 37	47, 70, 107, 137	0
1	B	465/491 (94%)	0.17	2 (0%) 92 79	47, 75, 116, 143	0
1	C	462/491 (94%)	0.44	27 (5%) 23 7	82, 109, 129, 150	0
1	D	453/491 (92%)	0.41	16 (3%) 44 18	69, 98, 124, 141	0
All	All	1856/1964 (94%)	0.30	54 (2%) 51 23	47, 90, 124, 150	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	GLY	4.5
1	C	273	PHE	3.4
1	C	320	ASP	3.2
1	C	308	ILE	3.2
1	D	317	ALA	3.2
1	A	209	HIS	3.2
1	C	272	THR	3.1
1	C	39	ASN	3.0
1	C	155	THR	2.9
1	D	321	THR	2.9
1	D	324	THR	2.9
1	D	497	THR	2.8
1	D	318	GLY	2.8
1	A	151	PRO	2.8
1	C	90	ASP	2.8
1	D	320	ASP	2.6
1	C	225	GLY	2.6
1	D	325	ALA	2.6
1	D	382	VAL	2.5
1	D	244	PRO	2.5
1	A	210	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	274	GLU	2.5
1	D	380	SER	2.5
1	D	287	GLU	2.5
1	A	320	ASP	2.5
1	A	512	SER	2.5
1	D	90	ASP	2.5
1	C	277	HIS	2.3
1	C	283	ASP	2.3
1	B	151	PRO	2.3
1	A	321	THR	2.2
1	A	324	THR	2.2
1	C	287	GLU	2.2
1	C	385	THR	2.2
1	D	381	PHE	2.2
1	C	304	ASP	2.2
1	C	219	ASN	2.2
1	D	218	VAL	2.2
1	C	278	ILE	2.2
1	C	497	THR	2.2
1	C	400	TYR	2.1
1	C	352	GLY	2.1
1	D	229	GLY	2.1
1	C	321	THR	2.1
1	D	383	PRO	2.1
1	B	287	GLU	2.1
1	C	353	ARG	2.1
1	A	212	GLN	2.1
1	C	279	ARG	2.0
1	C	317	ALA	2.0
1	A	457	CYS	2.0
1	C	244	PRO	2.0
1	C	324	THR	2.0
1	C	348	ASP	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 carbohydrates in this entry.

6.4 Ligands ⓘ

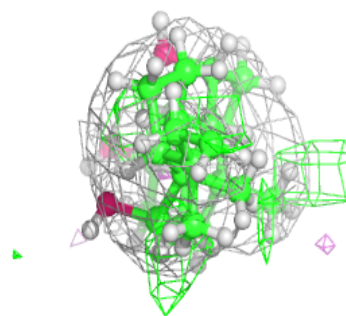
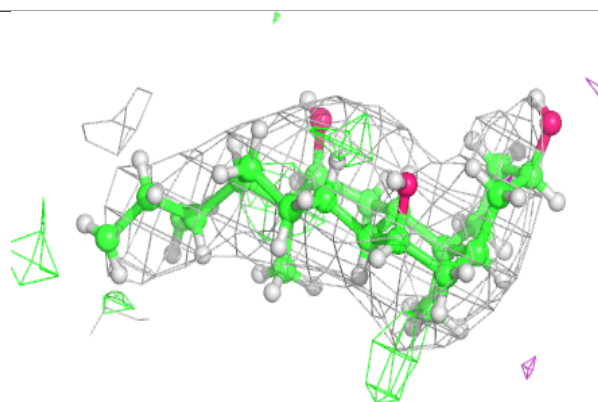
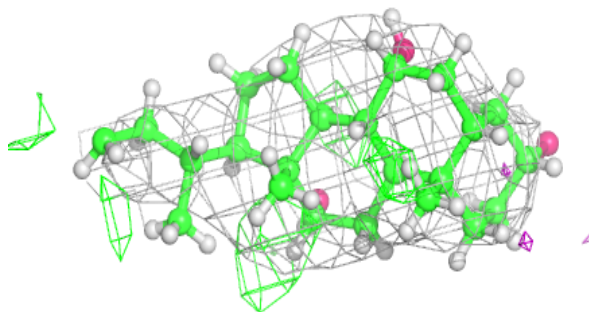
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CPS	A	603	26/42	0.82	0.36	72,93,110,115	0
4	CPS	B	603	30/42	0.83	0.46	92,119,131,148	0
2	HEM	A	601	43/43	0.85	0.39	43,52,67,162	0
2	HEM	B	601	43/43	0.85	0.43	54,77,90,240	0
3	AQ4	B	602	29/29	0.85	0.33	66,81,101,103	0
3	AQ4	A	602	29/29	0.88	0.35	47,66,92,102	0
3	AQ4	D	602	22/29	0.89	0.35	79,96,116,117	0
2	HEM	D	601	43/43	0.90	0.45	75,87,105,116	0
3	AQ4	C	602	23/29	0.92	0.37	89,105,127,132	0
2	HEM	C	601	43/43	0.94	0.45	84,100,121,125	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.

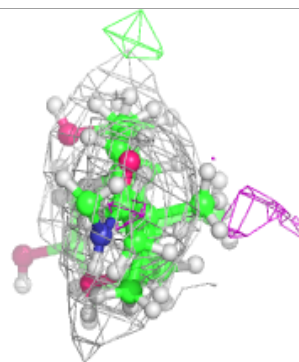
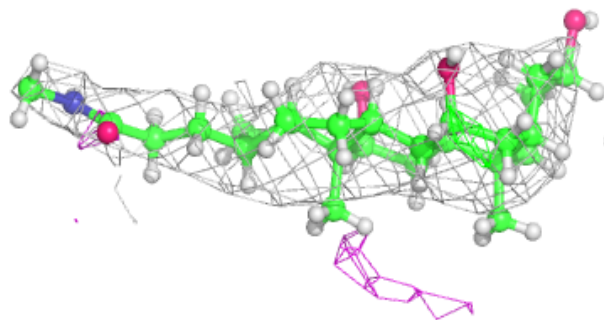
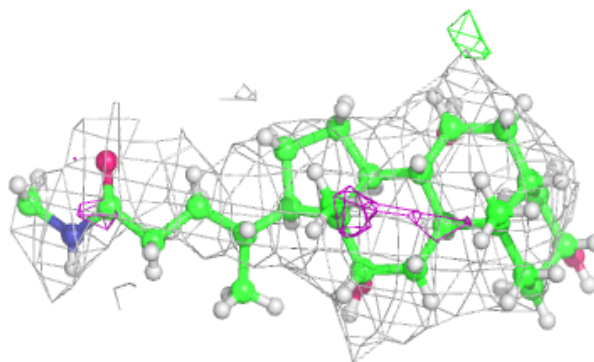
Electron density around CPS A 603:

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



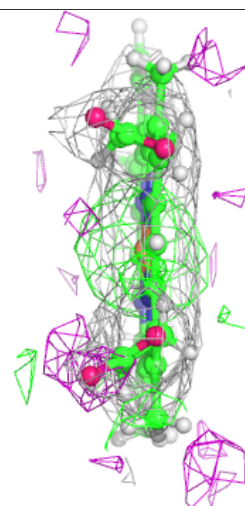
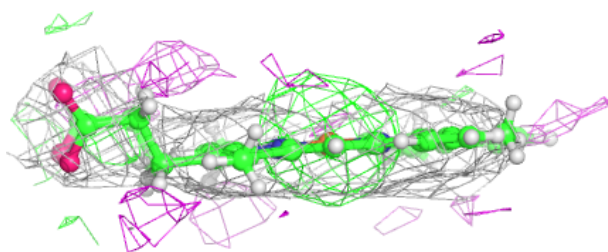
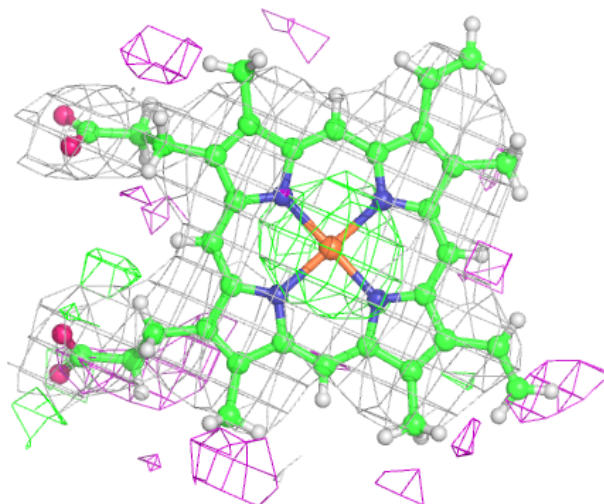
Electron density around CPS B 603:

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



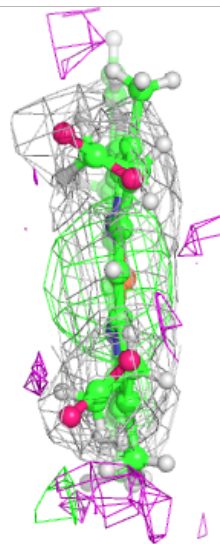
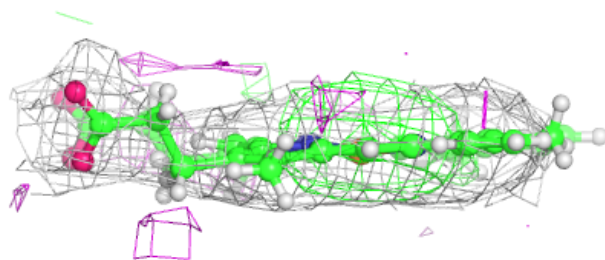
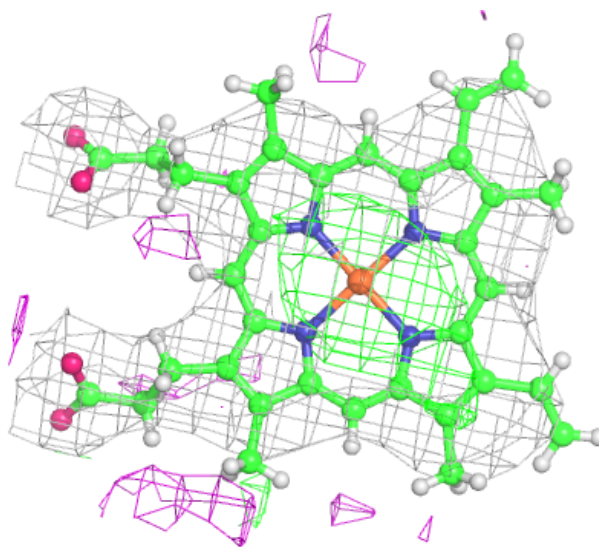
Electron density around HEM A 601:

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



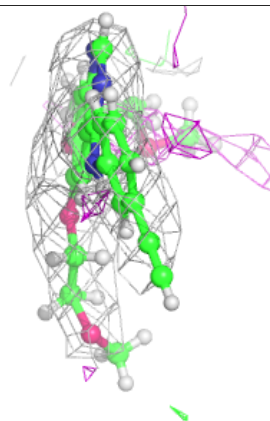
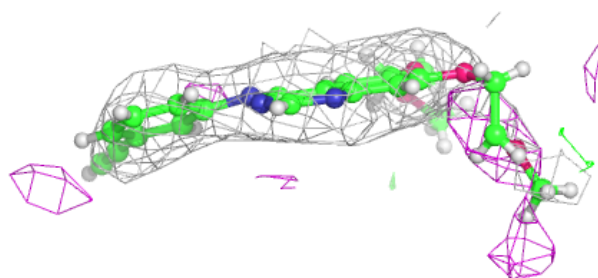
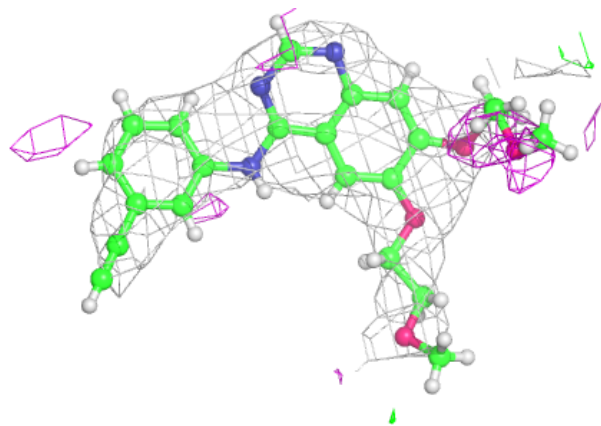
Electron density around HEM B 601:

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



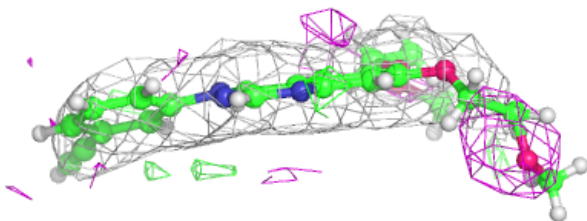
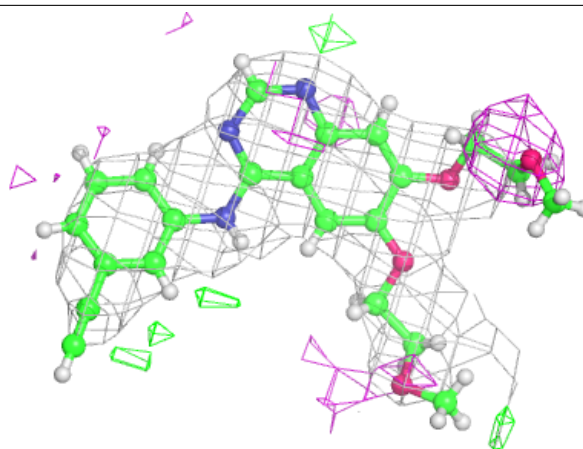
Electron density around AQ4 B 602:

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

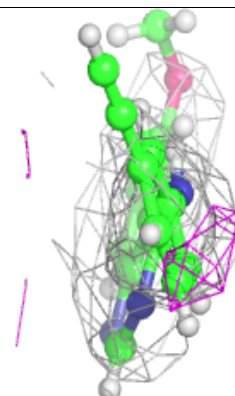
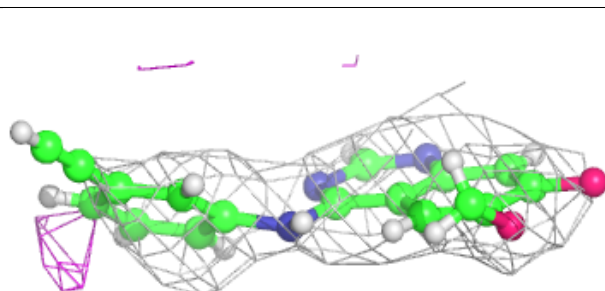
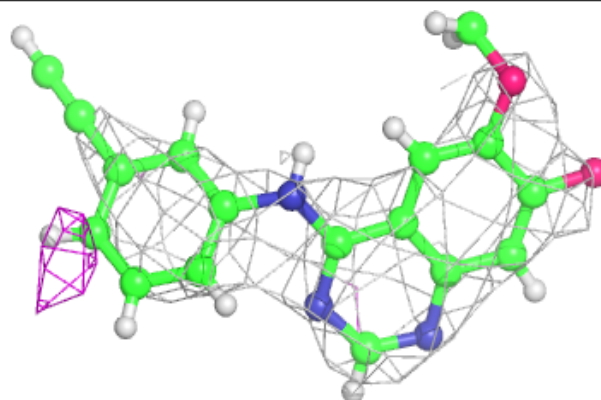


Electron density around AQ4 A 602:

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

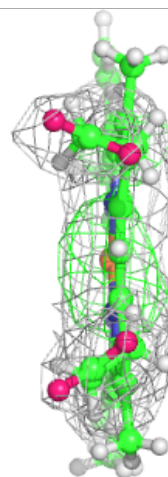
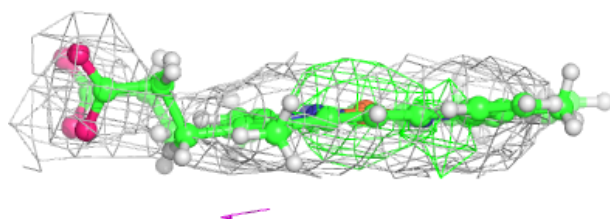
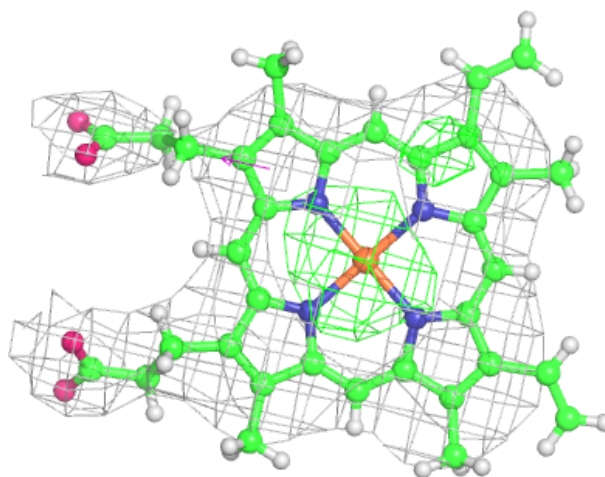
**Electron density around AQ4 D 602:**

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



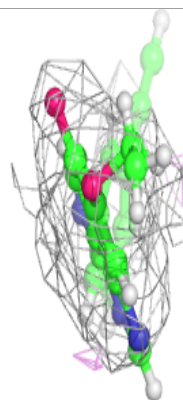
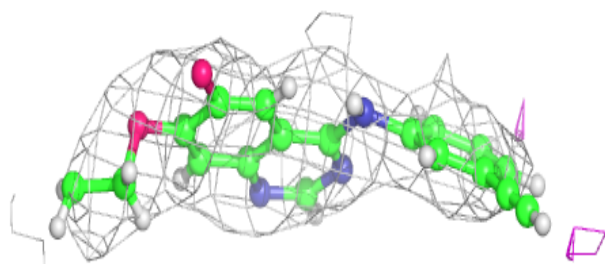
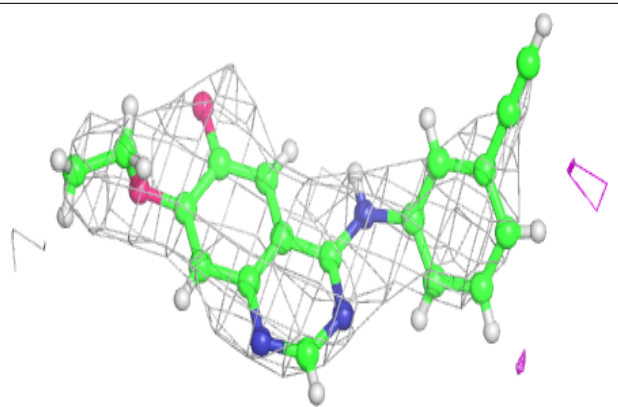
Electron density around HEM D 601:

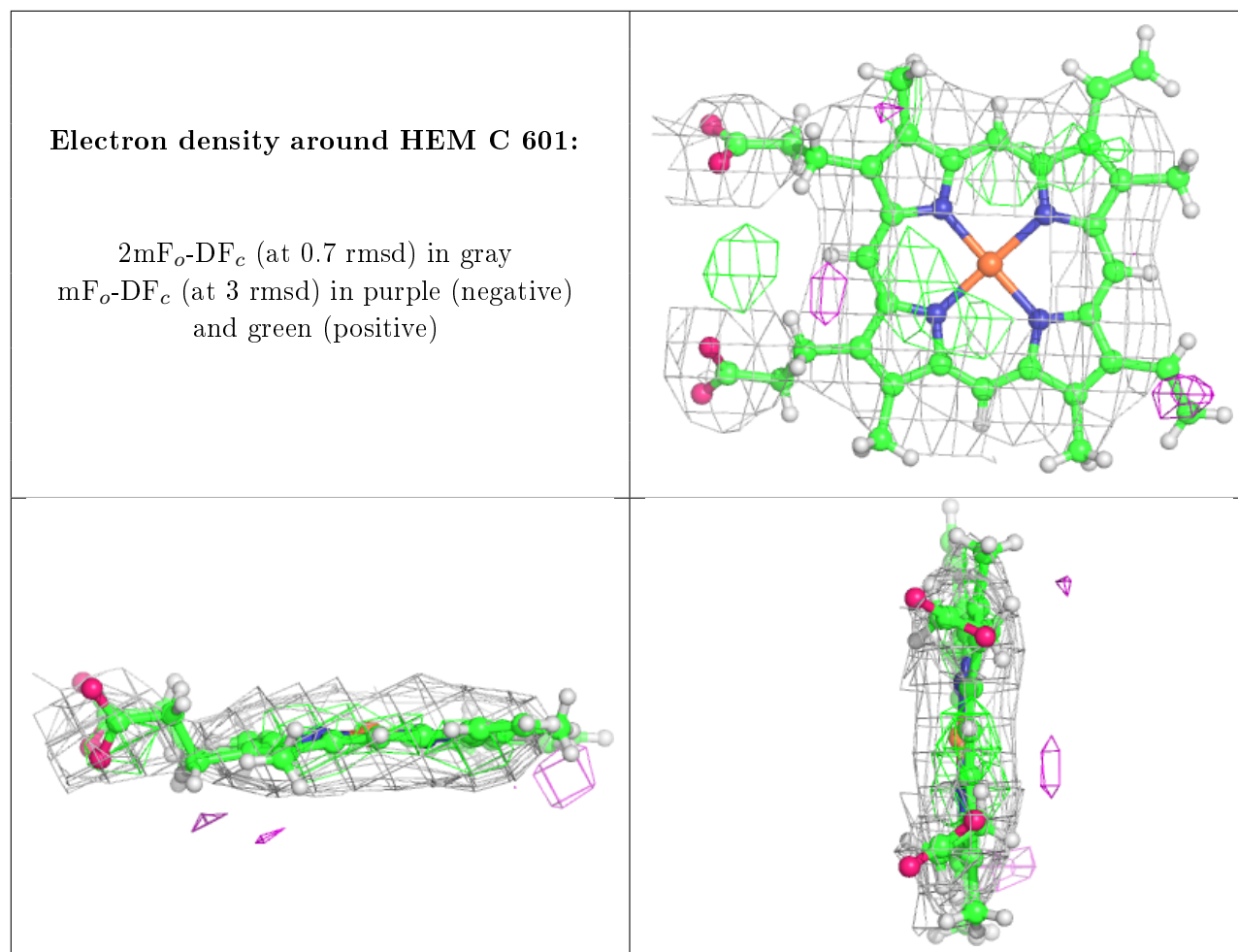
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AQ4 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.