



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:27 am BST

PDB ID : 5TFT
Title : Structure of cytochrome P450 2D6 (CYP2D6) BACE1 inhibitor complex
Authors : Hsu, M.H.; Johnson, E.F.
Deposited on : 2016-09-26
Resolution : 2.71 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

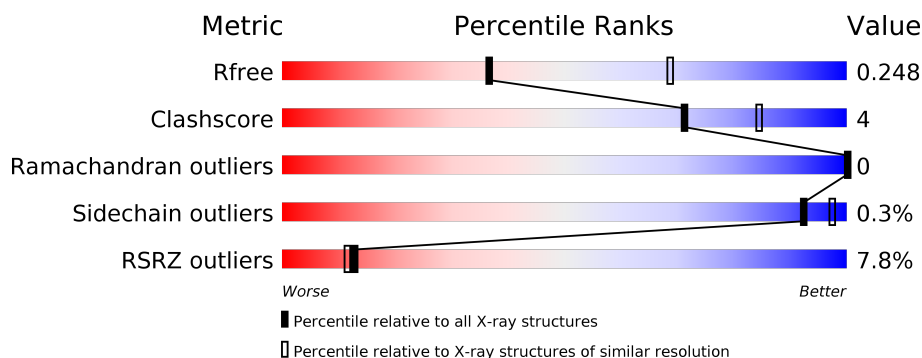
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	479	<div> <div>9%</div> <div>89% 8%</div> </div>
1	B	479	<div> <div>5%</div> <div>88% 8%</div> </div>
1	C	479	<div> <div>8%</div> <div>83% 10% 7%</div> </div>
1	D	479	<div> <div>8%</div> <div>88% 7% 5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	B	460	Total	C	N	O	S	0	0	0
			3642	2334	646	648	14			
1	C	447	Total	C	N	O	S	0	0	0
			3542	2269	628	631	14			
1	D	453	Total	C	N	O	S	0	0	0
			3586	2298	636	638	14			

There are 60 discrepancies between the modelled and reference sequences:

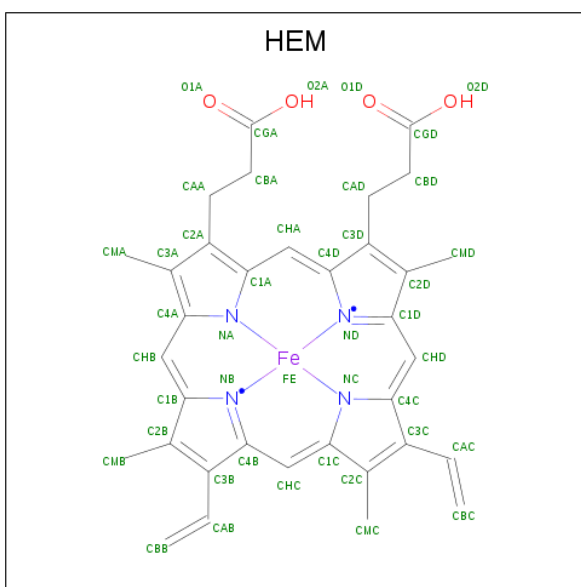
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	initiating methionine	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	initiating methionine	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	initiating methionine	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

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

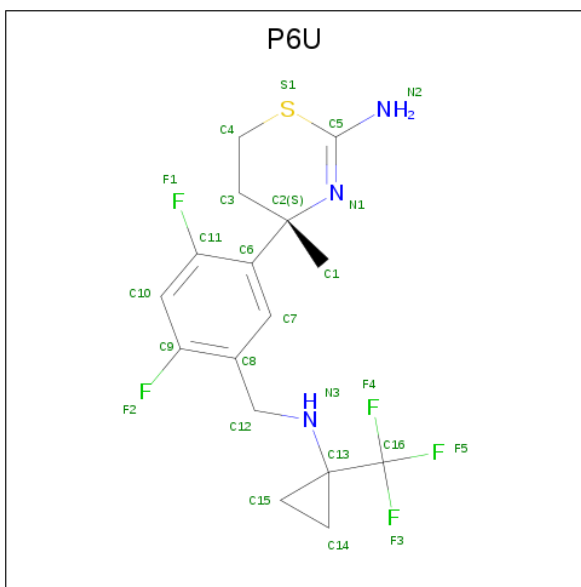


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	2	Total Zn 2 2	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is (4S)-4-[2,4-difluoro-5-([1-(trifluoromethyl)cyclopropyl]amino)methyl]phenyl]-4-methyl-5,6-dihydro-4H-1,3-thiazin-2-amine (three-letter code: P6U) (formula: $\text{C}_{16}\text{H}_{18}\text{F}_5\text{N}_3\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	S	0	0
			25	16	5	3	1		
4	B	1	Total	C	F	N	S	0	0
			25	16	5	3	1		
4	C	1	Total	C	F	N	S	0	0
			25	16	5	3	1		
4	D	1	Total	C	F	N	S	0	0
			25	16	5	3	1		

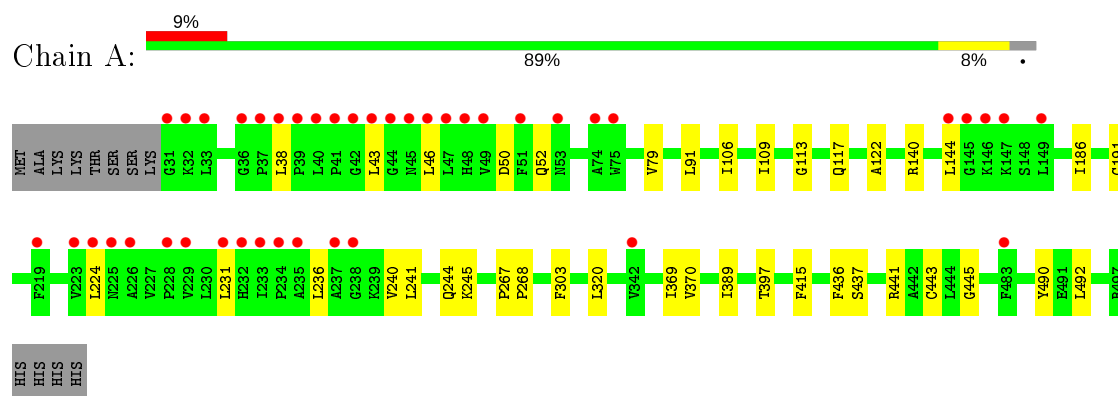
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	12	Total	O	0	0
			12	12		
5	C	10	Total	O	0	0
			10	10		
5	D	7	Total	O	0	0
			7	7		

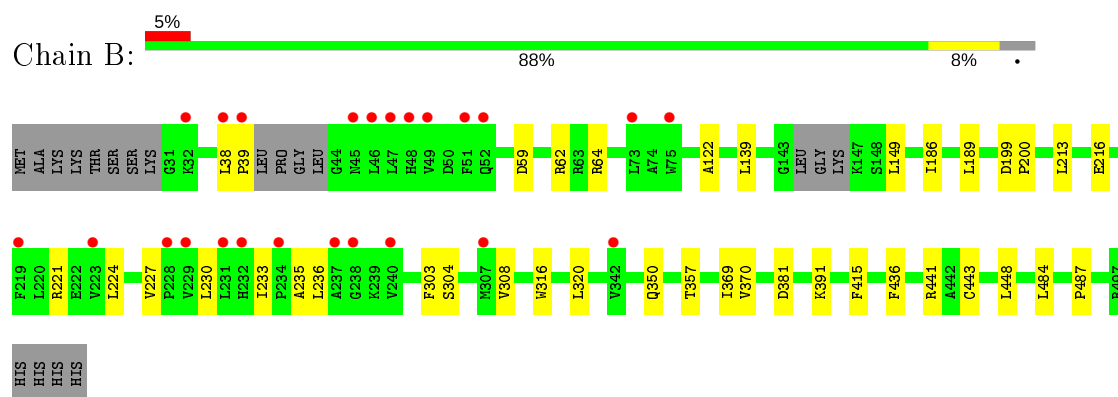
3 Residue-property plots [i](#)

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.

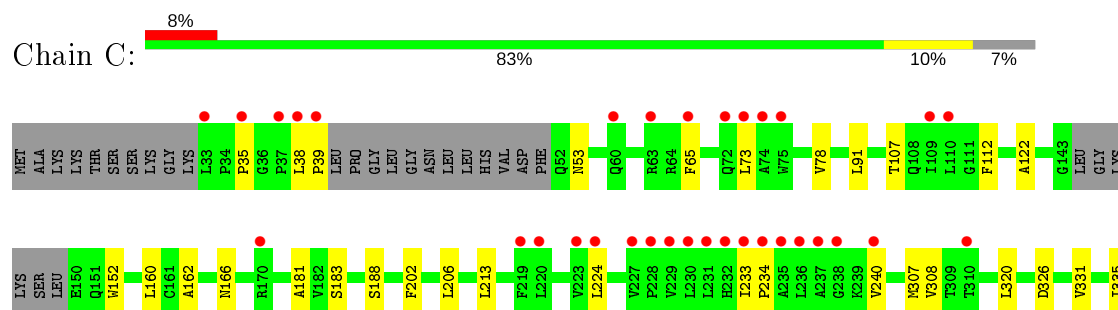
• Molecule 1: Cytochrome P450 2D6

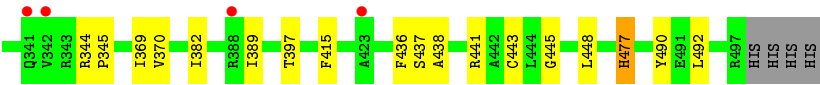


• Molecule 1: Cytochrome P450 2D6

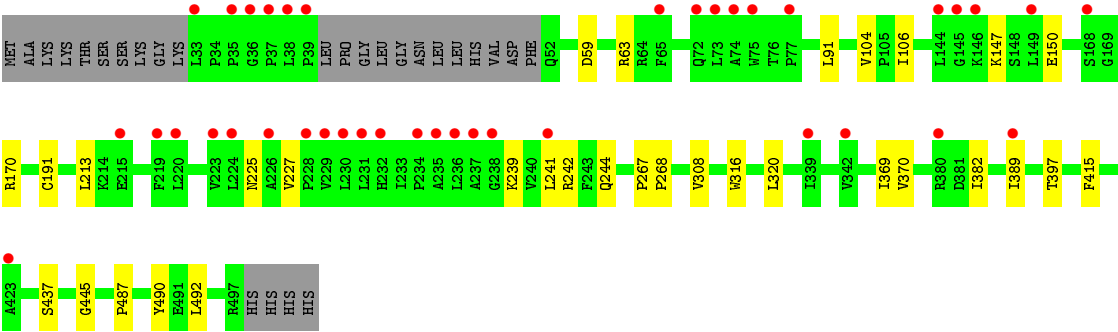
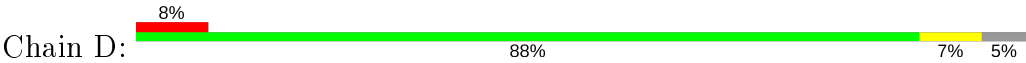


• Molecule 1: Cytochrome P450 2D6





● Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.47Å 192.56Å 247.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.24 – 2.71 39.24 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.24-2.71) 99.5 (39.24-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.245 0.213 , 0.248	Depositor DCC
R_{free} test set	3768 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14779	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9974e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HEM, ZN, P6U

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	0.22	0/3790	0.38	0/5155
1	B	0.22	0/3739	0.37	0/5083
1	C	0.22	0/3637	0.37	0/4947
1	D	0.22	0/3682	0.37	0/5007
All	All	0.22	0/14848	0.37	0/20192

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	3690	0	3679	25	0
1	B	3642	0	3618	24	0
1	C	3542	0	3513	29	0
1	D	3586	0	3570	18	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	6	0
2	D	43	0	30	5	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	1	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	13	0	0	1	0
5	B	12	0	0	0	0
5	C	10	0	0	0	0
5	D	7	0	0	1	0
All	All	14779	0	14500	103	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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG21	1:A:303:PHE:HA	1.60	0.80
1:B:186:ILE:HG21	1:B:303:PHE:HA	1.67	0.75
1:C:122:ALA:O	1:C:441:ARG:NH2	2.22	0.72
1:D:191:CYS:SG	5:D:707:HOH:O	2.51	0.68
1:B:122:ALA:O	1:B:441:ARG:NH2	2.28	0.67
1:A:122:ALA:O	1:A:441:ARG:NH2	2.23	0.66
1:B:441:ARG:NH1	2:B:601:HEM:O2D	2.32	0.63
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.81	0.61
1:B:213:LEU:HD22	1:B:308:VAL:HG21	1.81	0.60
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.84	0.59
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.85	0.59
1:C:477:HIS:CD2	1:C:477:HIS:H	2.21	0.59
1:B:64:ARG:HH22	1:C:53:ASN:HD22	1.50	0.58
1:D:490:TYR:HE1	1:D:492:LEU:HD23	1.69	0.58
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.86	0.57
1:A:240:VAL:HG12	1:A:241:LEU:HG	1.87	0.57
1:C:490:TYR:HE1	1:C:492:LEU:HD23	1.72	0.55
1:D:147:LYS:HG2	1:D:150:GLU:HB2	1.88	0.55
1:A:43:LEU:HD23	1:A:46:LEU:HD22	1.87	0.55
1:C:441:ARG:NH1	2:C:601:HEM:O2D	2.40	0.55
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.89	0.55
1:B:216:GLU:HA	1:B:221:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.89	0.55
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.90	0.54
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.90	0.52
1:C:213:LEU:HD22	1:C:308:VAL:HG21	1.92	0.52
1:A:109:ILE:HD11	1:A:231:LEU:HD22	1.92	0.51
1:A:224:LEU:HD21	1:A:236:LEU:HD21	1.93	0.51
1:C:35:PRO:HG2	1:C:65:PHE:HB3	1.91	0.51
1:B:381:ASP:OD1	1:B:391:LYS:N	2.43	0.50
1:C:38:LEU:HD12	1:C:39:PRO:HD2	1.92	0.50
1:C:152:TRP:CD1	1:C:188:SER:HB3	2.46	0.50
1:C:91:LEU:HD11	1:C:397:THR:HG21	1.93	0.49
1:A:140:ARG:HG2	1:A:144:LEU:HD23	1.94	0.49
1:D:213:LEU:HD22	1:D:308:VAL:HG21	1.94	0.49
1:C:224:LEU:HD11	1:C:240:VAL:HG11	1.95	0.48
1:D:91:LEU:HD11	1:D:397:THR:HG21	1.95	0.48
1:A:79:VAL:HG21	1:A:389:ILE:HD12	1.94	0.48
1:B:149:LEU:HD11	1:B:448:LEU:HD13	1.94	0.48
1:A:490:TYR:HE1	1:A:492:LEU:HD23	1.78	0.48
1:C:326:ASP:OD1	1:C:326:ASP:N	2.46	0.48
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.94	0.48
1:C:437:SER:OG	1:C:438:ALA:N	2.42	0.48
1:B:59:ASP:HA	1:B:62:ARG:HG2	1.97	0.47
1:A:241:LEU:HB3	1:A:244:GLN:HB2	1.95	0.47
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.95	0.47
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.96	0.46
1:D:59:ASP:O	1:D:63:ARG:HG2	2.15	0.46
1:C:445:GLY:HA3	2:C:601:HEM:C3C	2.49	0.46
1:B:227:VAL:HG22	1:B:230:LEU:H	1.81	0.46
1:C:183:SER:OG	1:C:307:MET:SD	2.66	0.46
1:B:149:LEU:HD13	1:B:189:LEU:HD21	1.97	0.46
1:D:445:GLY:HA3	2:D:601:HEM:C3C	2.50	0.46
1:A:106:ILE:HG22	1:A:231:LEU:HD11	1.97	0.46
1:C:73:LEU:HD12	1:C:78:VAL:HG21	1.98	0.46
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.97	0.45
1:D:239:LYS:HD2	1:D:242:ARG:HD3	1.97	0.45
1:A:50:ASP:OD1	1:A:50:ASP:N	2.44	0.45
1:A:236:LEU:O	1:A:240:VAL:HG23	2.17	0.44
1:B:320:LEU:HD13	1:B:415:PHE:CD1	2.51	0.44
1:D:104:VAL:HG12	1:D:106:ILE:HG22	1.99	0.44
1:B:38:LEU:HD12	1:B:39:PRO:HD2	1.98	0.44
1:B:448:LEU:HD23	2:B:601:HEM:HBC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HG22	1:B:484:LEU:HD22	1.99	0.44
1:D:267:PRO:HA	1:D:268:PRO:HD3	1.91	0.44
1:C:160:LEU:HD13	1:C:181:ALA:HB2	1.98	0.44
1:B:139:LEU:HD22	1:B:189:LEU:HD13	2.00	0.43
1:C:162:ALA:O	1:C:166:ASN:ND2	2.48	0.43
1:C:320:LEU:HD13	1:C:415:PHE:CD1	2.53	0.43
1:C:448:LEU:HD23	2:C:601:HEM:HBC2	2.00	0.43
1:A:436:PHE:HB3	1:A:443:CYS:HB3	1.99	0.43
1:D:382:ILE:HG13	1:D:389:ILE:HB	1.99	0.43
1:C:107:THR:HB	1:C:112:PHE:CD2	2.54	0.43
1:D:320:LEU:HD13	1:D:415:PHE:CD1	2.54	0.43
1:C:344:ARG:HA	1:C:345:PRO:HD3	1.91	0.43
1:D:316:TRP:CD2	1:D:487:PRO:HG3	2.53	0.42
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	2.01	0.42
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.93	0.42
1:C:233:ILE:HA	1:C:234:PRO:HD3	1.92	0.42
1:C:437:SER:HB3	2:C:601:HEM:HBA1	2.01	0.42
1:A:437:SER:HB3	2:A:601:HEM:HBA1	2.02	0.42
1:A:191:CYS:SG	5:A:713:HOH:O	2.53	0.42
1:A:320:LEU:HD13	1:A:415:PHE:CE1	2.55	0.42
1:B:304:SER:HB2	4:B:603:P6U:C10	2.50	0.42
1:A:113:GLY:O	1:A:117:GLN:HG2	2.19	0.42
1:D:241:LEU:HB3	1:D:244:GLN:HB2	2.01	0.42
1:B:436:PHE:HB3	1:B:443:CYS:HB3	2.02	0.41
1:D:104:VAL:HG13	1:D:225:ASN:HD21	1.85	0.41
1:A:443:CYS:HB2	2:A:601:HEM:NA	2.34	0.41
1:D:437:SER:HB3	2:D:601:HEM:HBA1	2.02	0.41
1:C:436:PHE:HB3	1:C:443:CYS:HB3	2.02	0.41
1:A:50:ASP:C	1:A:52:GLN:H	2.24	0.41
1:D:369:ILE:HD11	2:D:601:HEM:HMB2	2.02	0.41
1:B:224:LEU:HD11	1:B:236:LEU:HD23	2.03	0.41
1:B:233:ILE:HG22	1:B:235:ALA:H	1.85	0.41
1:B:199:ASP:HA	1:B:200:PRO:HD3	1.88	0.41
1:B:350:GLN:HE21	1:B:357:THR:HG23	1.86	0.41
1:C:382:ILE:HG13	1:C:389:ILE:HB	2.02	0.41
1:A:109:ILE:HG22	1:A:245:LYS:HE3	2.02	0.40
1:C:202:PHE:O	1:C:206:LEU:HG	2.21	0.40
1:A:445:GLY:HA3	2:A:601:HEM:C3C	2.57	0.40
1:B:316:TRP:CD2	1:B:487:PRO:HG3	2.55	0.40
1:C:331:VAL:O	1:C:335:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/479 (97%)	452 (97%)	13 (3%)	0	100	100
1	B	454/479 (95%)	442 (97%)	12 (3%)	0	100	100
1	C	441/479 (92%)	432 (98%)	9 (2%)	0	100	100
1	D	449/479 (94%)	435 (97%)	14 (3%)	0	100	100
All	All	1809/1916 (94%)	1761 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/409 (97%)	397 (100%)	1 (0%)	92	97
1	B	393/409 (96%)	393 (100%)	0	100	100
1	C	382/409 (93%)	381 (100%)	1 (0%)	92	97
1	D	387/409 (95%)	385 (100%)	2 (0%)	88	95
All	All	1560/1636 (95%)	1556 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	C	477	HIS

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Mol	Chain	Res	Type
1	D	170	ARG
1	D	227	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	341	GLN
1	C	477	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](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	601	1	27,50,50	1.71	4 (14%)	17,82,82	1.48	4 (23%)
4	P6U	A	604	-	24,27,27	0.24	0	27,43,43	1.40	2 (7%)
4	P6U	D	603	-	24,27,27	0.23	0	27,43,43	1.35	2 (7%)
4	P6U	B	603	-	24,27,27	0.24	0	27,43,43	1.38	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	601	1	27,50,50	1.72	4 (14%)	17,82,82	1.38	3 (17%)
2	HEM	C	601	1	27,50,50	1.73	4 (14%)	17,82,82	1.40	3 (17%)
2	HEM	B	601	1	27,50,50	1.73	5 (18%)	17,82,82	1.44	4 (23%)
4	P6U	C	603	-	24,27,27	0.23	0	27,43,43	1.34	2 (7%)

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	1	-	0/6/54/54	-
4	P6U	A	604	-	-	4/15/37/37	0/3/3/3
4	P6U	D	603	-	-	1/15/37/37	0/3/3/3
4	P6U	B	603	-	-	3/15/37/37	0/3/3/3
2	HEM	A	601	1	-	0/6/54/54	-
2	HEM	C	601	1	-	0/6/54/54	-
2	HEM	B	601	1	-	0/6/54/54	-
4	P6U	C	603	-	-	3/15/37/37	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-CAC	3.92	1.55	1.47
2	B	601	HEM	C3C-CAC	3.89	1.55	1.47
2	D	601	HEM	C3C-CAC	3.88	1.55	1.47
2	C	601	HEM	C3C-CAC	3.83	1.55	1.47
2	D	601	HEM	C3B-CAB	3.80	1.55	1.47
2	B	601	HEM	C3B-CAB	3.74	1.55	1.47
2	C	601	HEM	C3B-CAB	3.74	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.73	1.35	1.40
2	C	601	HEM	C3C-C2C	-3.72	1.35	1.40
2	A	601	HEM	C3B-CAB	3.70	1.55	1.47
2	A	601	HEM	C3C-C2C	-3.69	1.35	1.40
2	C	601	HEM	C3B-C2B	-3.69	1.35	1.40
2	B	601	HEM	C3C-C2C	-3.63	1.35	1.40
2	A	601	HEM	C3B-C2B	-3.61	1.35	1.40
2	D	601	HEM	C3C-C2C	-3.60	1.35	1.40
2	D	601	HEM	C3B-C2B	-3.53	1.35	1.40
2	B	601	HEM	CAA-C2A	2.09	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	P6U	C15-C13-N3	5.53	123.16	115.64
4	D	603	P6U	C15-C13-N3	5.49	123.11	115.64
4	C	603	P6U	C15-C13-N3	5.42	123.01	115.64
4	A	604	P6U	C15-C13-N3	5.36	122.93	115.64
4	A	604	P6U	C14-C13-N3	4.09	121.20	115.64
4	B	603	P6U	C14-C13-N3	3.82	120.83	115.64
4	C	603	P6U	C14-C13-N3	3.56	120.48	115.64
4	D	603	P6U	C14-C13-N3	3.53	120.44	115.64
2	D	601	HEM	CAA-CBA-CGA	-2.48	108.51	112.67
2	D	601	HEM	CMB-C2B-C3B	2.44	129.24	124.68
2	C	601	HEM	CAA-CBA-CGA	-2.41	108.62	112.67
2	B	601	HEM	CMB-C2B-C3B	2.31	128.99	124.68
2	B	601	HEM	CMC-C2C-C3C	2.21	128.81	124.68
2	D	601	HEM	CMC-C2C-C3C	2.16	128.72	124.68
2	C	601	HEM	CMC-C2C-C3C	2.14	128.69	124.68
2	A	601	HEM	CMB-C2B-C3B	2.14	128.69	124.68
2	A	601	HEM	CAA-CBA-CGA	-2.14	109.08	112.67
2	D	601	HEM	CBD-CAD-C3D	-2.12	108.57	112.48
2	C	601	HEM	CMB-C2B-C3B	2.10	128.60	124.68
2	B	601	HEM	CAD-CBD-CGD	-2.09	109.17	112.67
2	B	601	HEM	CAA-CBA-CGA	-2.00	109.31	112.67
2	A	601	HEM	CMC-C2C-C3C	2.00	128.42	124.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

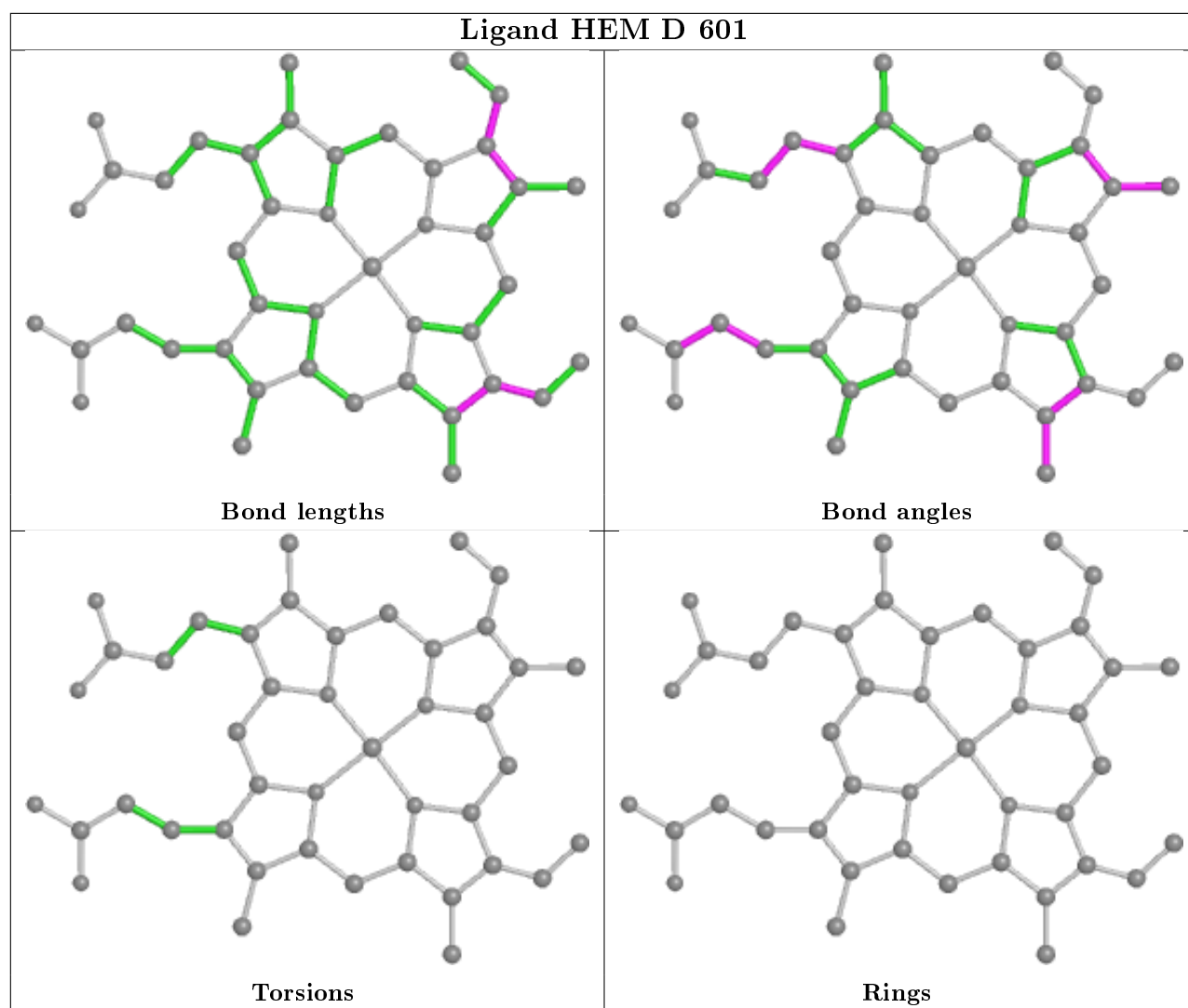
Mol	Chain	Res	Type	Atoms
4	B	603	P6U	C15-C13-C16-F3
4	B	603	P6U	C15-C13-C16-F4
4	B	603	P6U	C15-C13-C16-F5
4	A	604	P6U	C15-C13-C16-F3
4	A	604	P6U	C15-C13-C16-F5
4	C	603	P6U	C15-C13-C16-F3
4	C	603	P6U	C15-C13-C16-F4
4	C	603	P6U	C15-C13-C16-F5
4	A	604	P6U	C15-C13-C16-F4
4	D	603	P6U	C8-C12-N3-C13
4	A	604	P6U	N3-C12-C8-C9

There are no ring outliers.

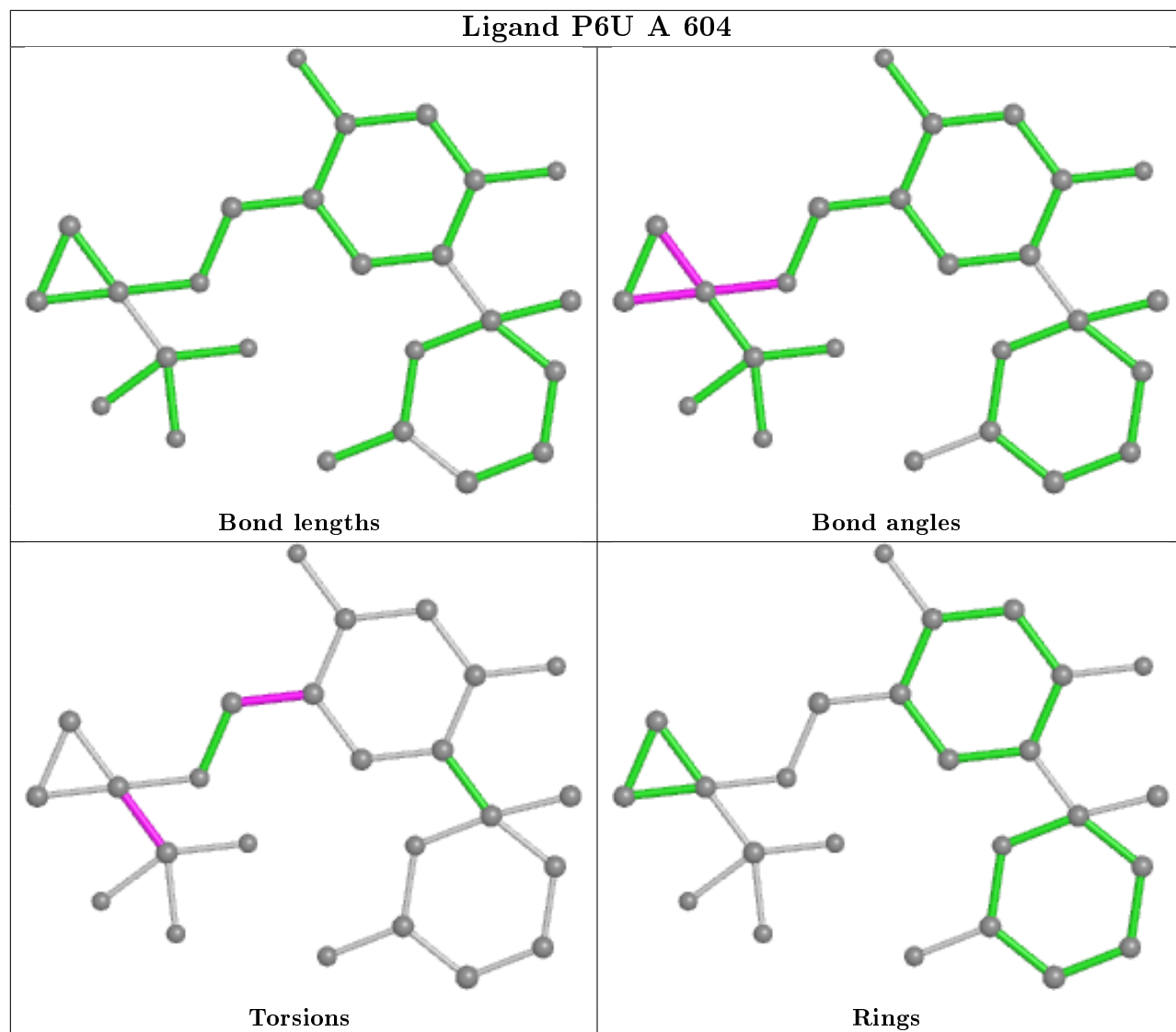
5 monomers are involved in 21 short contacts:

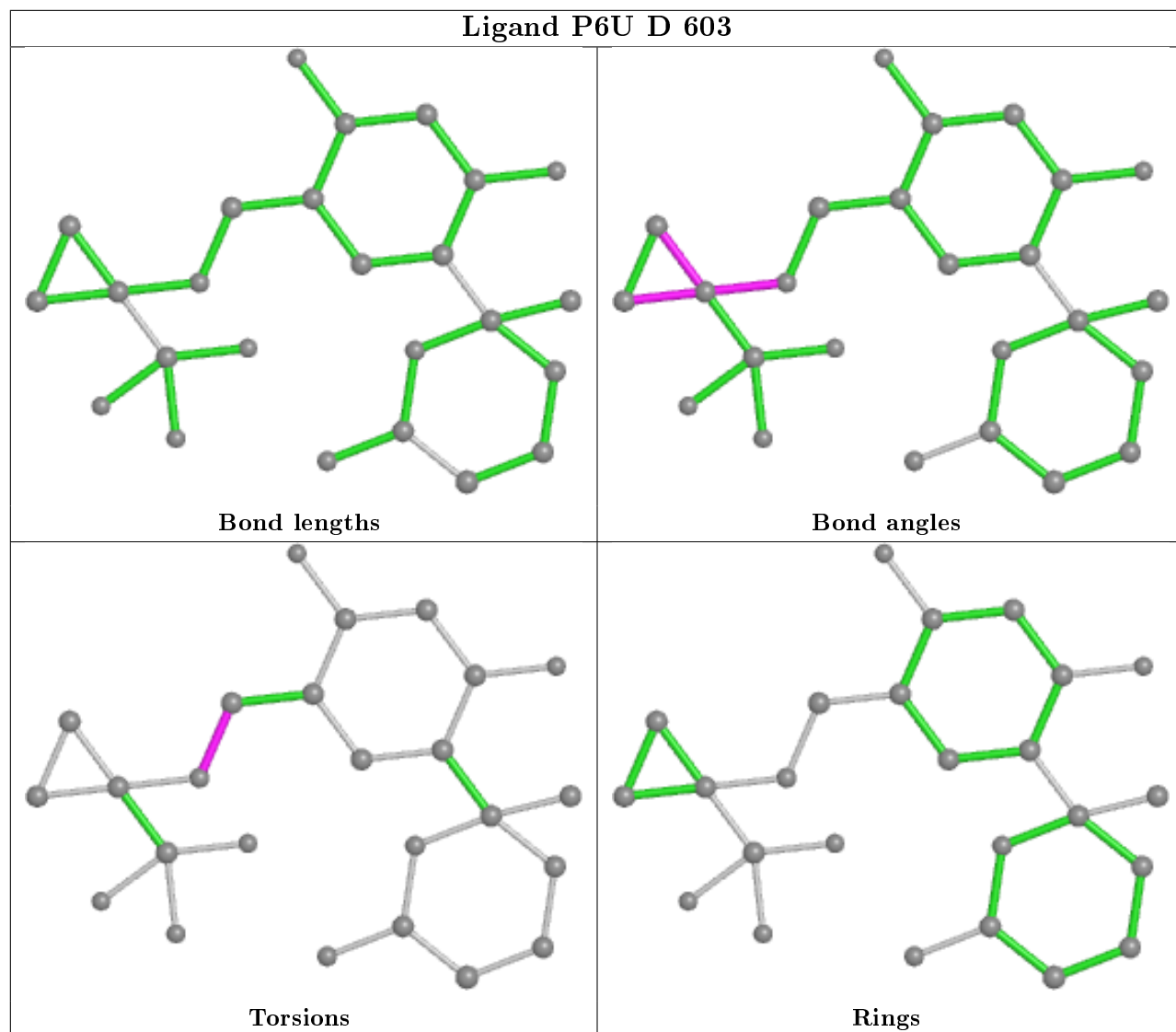
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	5	0
4	B	603	P6U	1	0
2	A	601	HEM	5	0
2	C	601	HEM	6	0
2	B	601	HEM	4	0

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.

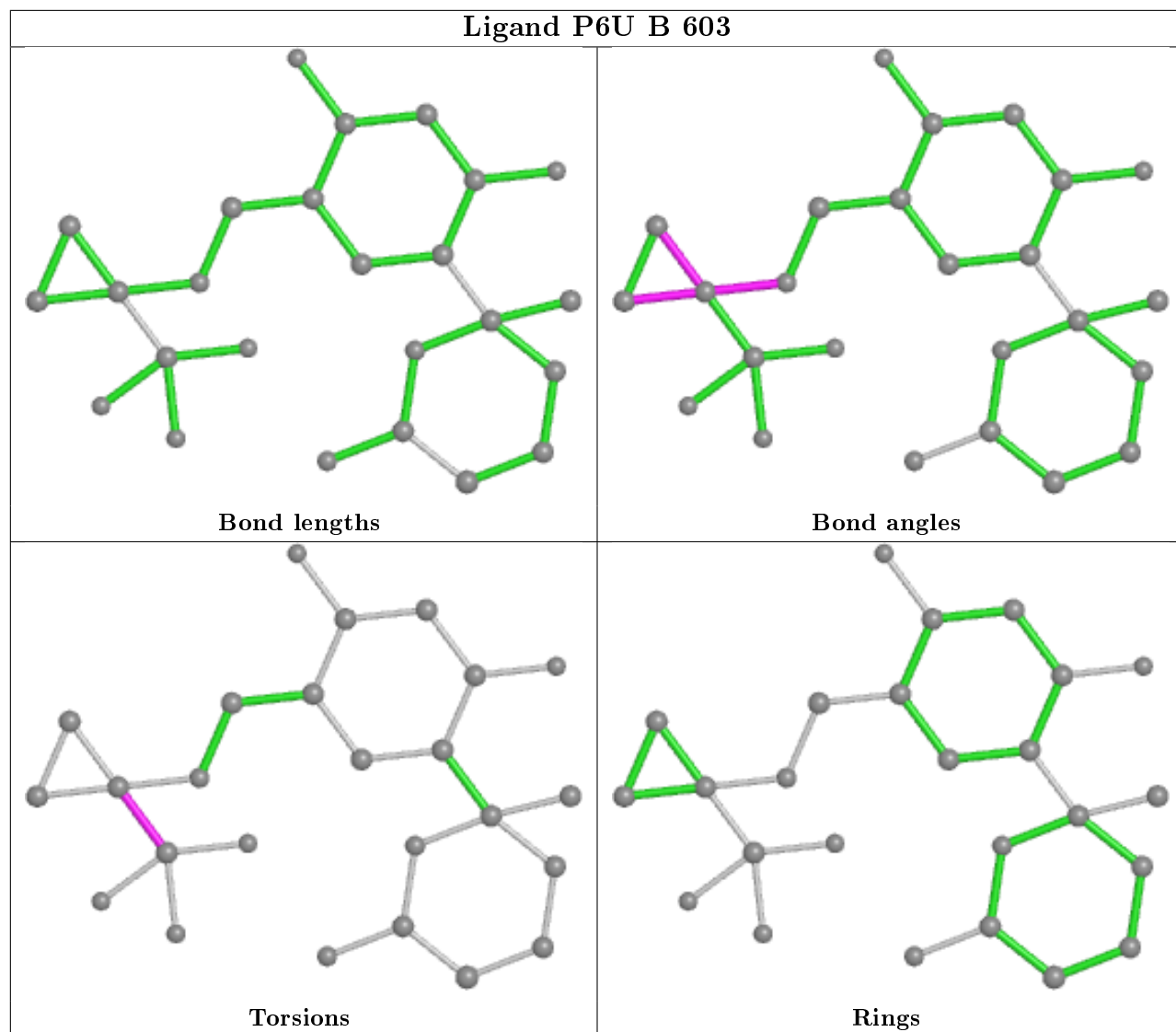


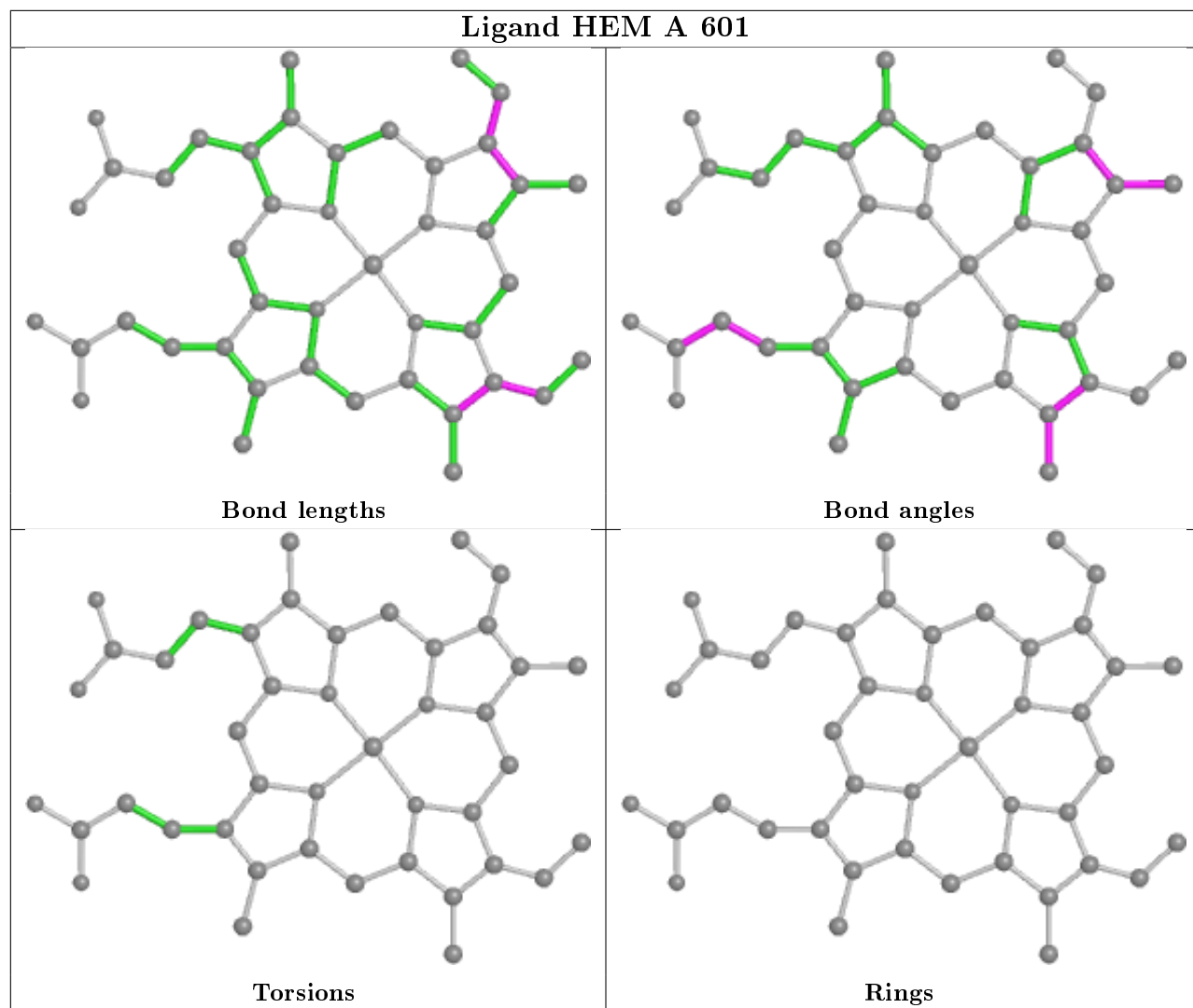
Ligand P6U A 604

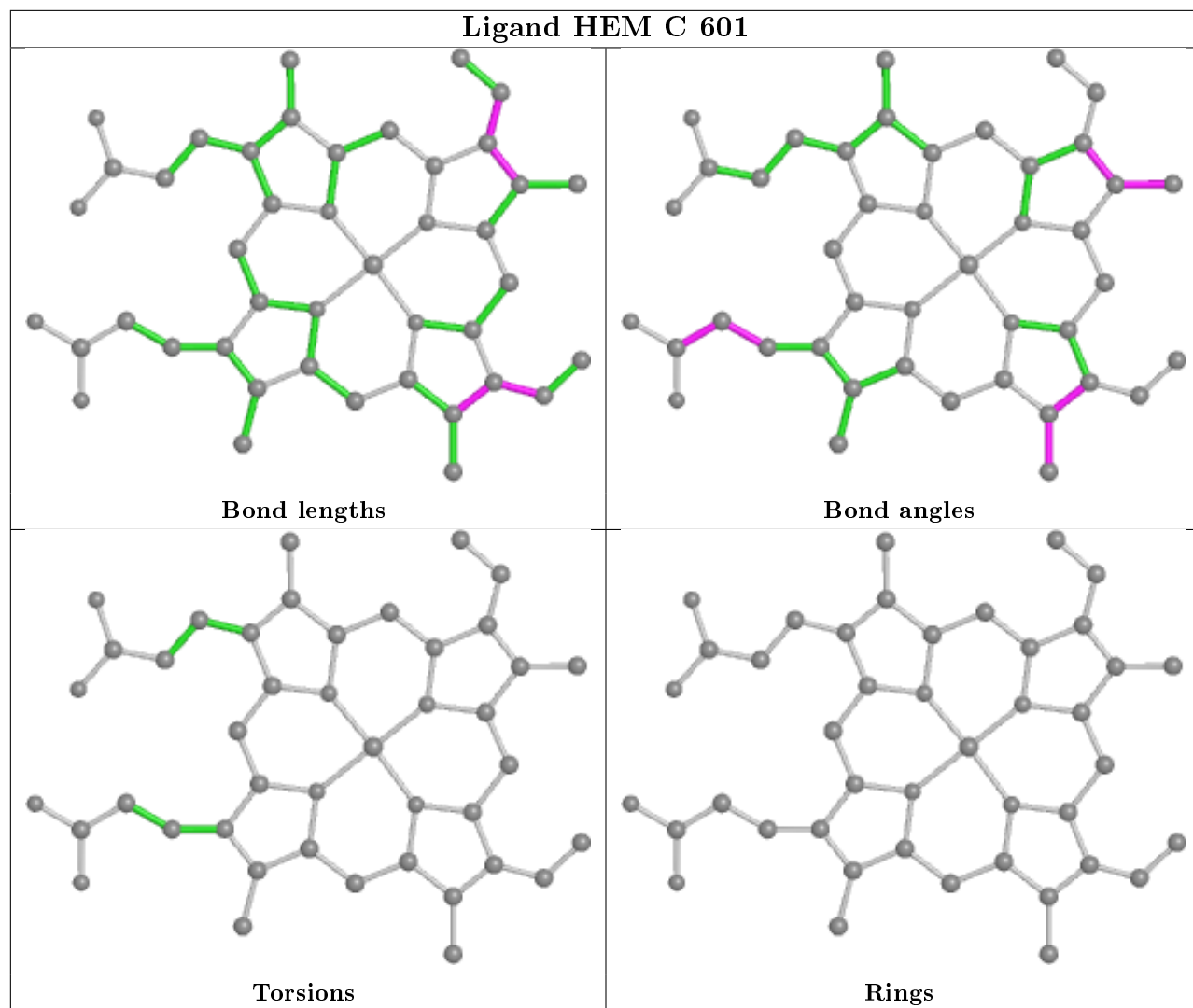


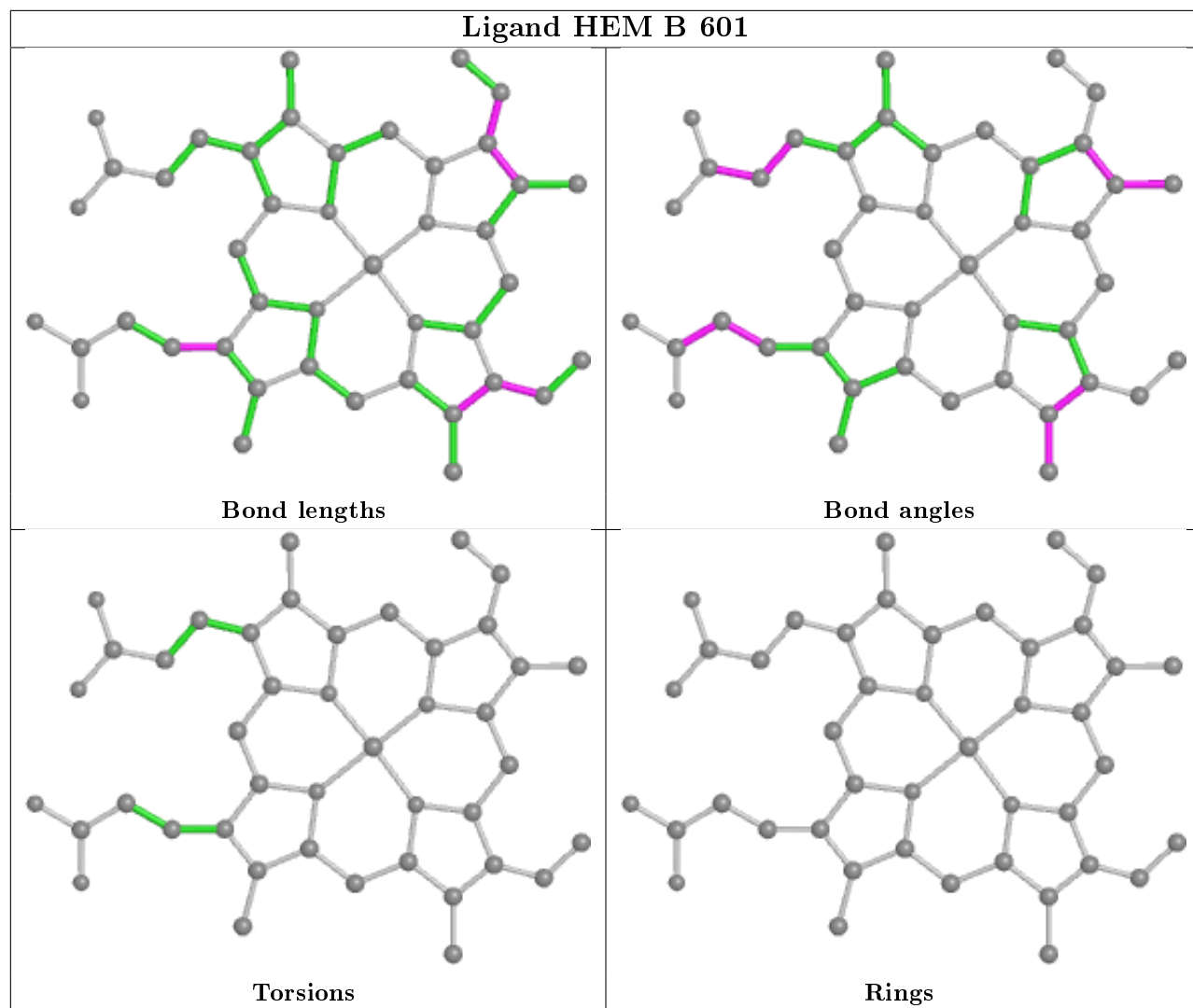


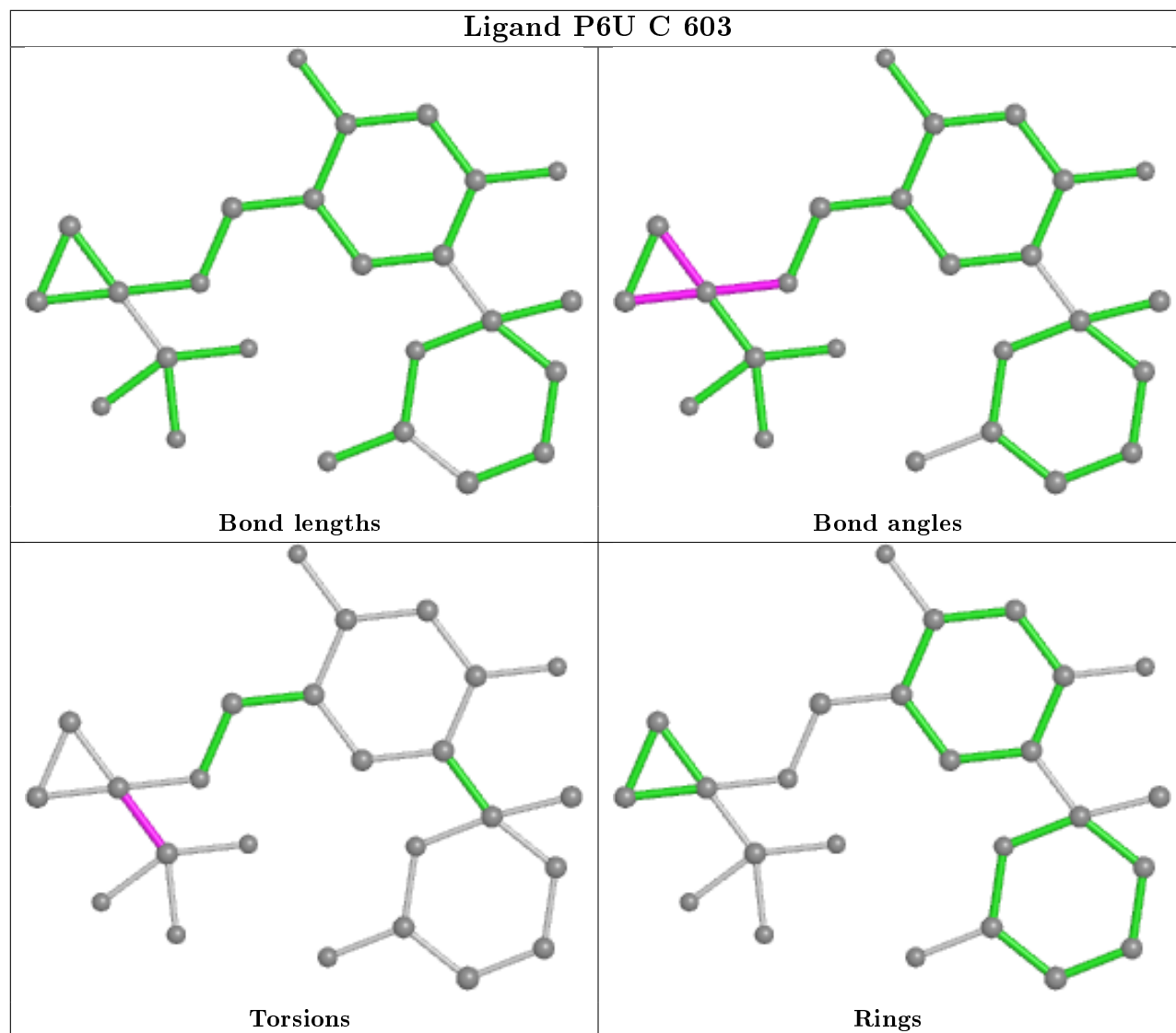
Ligand P6U B 603











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	467/479 (97%)	0.42	42 (8%) 9 8	21, 42, 101, 115	0
1	B	460/479 (96%)	0.24	24 (5%) 27 26	21, 42, 92, 118	0
1	C	447/479 (93%)	0.42	37 (8%) 11 10	25, 45, 95, 119	0
1	D	453/479 (94%)	0.44	39 (8%) 10 9	25, 49, 95, 119	0
All	All	1827/1916 (95%)	0.38	142 (7%) 13 11	21, 45, 97, 119	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	LEU	9.2
1	D	75	TRP	9.1
1	C	228	PRO	8.5
1	C	219	PHE	8.1
1	A	228	PRO	7.4
1	A	43	LEU	7.3
1	A	38	LEU	7.1
1	B	237	ALA	6.8
1	A	42	GLY	6.5
1	A	223	VAL	6.3
1	C	237	ALA	6.2
1	A	231	LEU	6.1
1	D	235	ALA	5.9
1	A	144	LEU	5.8
1	A	47	LEU	5.7
1	A	219	PHE	5.7
1	A	40	LEU	5.6
1	B	229	VAL	5.6
1	B	47	LEU	5.5
1	C	229	VAL	5.5
1	D	219	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	38	LEU	5.3
1	C	75	TRP	5.3
1	D	236	LEU	5.3
1	C	234	PRO	5.1
1	A	75	TRP	5.0
1	C	236	LEU	5.0
1	A	48	HIS	4.9
1	C	238	GLY	4.9
1	C	33	LEU	4.7
1	D	238	GLY	4.7
1	B	46	LEU	4.6
1	D	231	LEU	4.6
1	D	229	VAL	4.5
1	A	41	PRO	4.5
1	D	38	LEU	4.4
1	D	234	PRO	4.4
1	C	224	LEU	4.3
1	B	48	HIS	4.3
1	C	223	VAL	4.3
1	B	45	ASN	4.2
1	A	32	LYS	4.1
1	B	219	PHE	4.1
1	B	52	GLN	4.1
1	A	53	ASN	4.1
1	A	234	PRO	4.0
1	A	237	ALA	4.0
1	C	37	PRO	3.9
1	A	229	VAL	3.9
1	D	220	LEU	3.9
1	B	342	VAL	3.9
1	A	235	ALA	3.9
1	C	35	PRO	3.8
1	B	75	TRP	3.8
1	B	49	VAL	3.7
1	A	226	ALA	3.5
1	D	72	GLN	3.5
1	D	228	PRO	3.5
1	B	38	LEU	3.4
1	A	145	GLY	3.4
1	A	232	HIS	3.4
1	B	32	LYS	3.4
1	A	342	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	237	ALA	3.3
1	D	33	LEU	3.3
1	B	228	PRO	3.3
1	D	380	ARG	3.2
1	D	145	GLY	3.2
1	D	37	PRO	3.2
1	D	149	LEU	3.1
1	D	223	VAL	3.1
1	C	232	HIS	3.1
1	C	220	LEU	3.1
1	A	39	PRO	3.1
1	A	33	LEU	3.1
1	A	225	ASN	3.0
1	C	233	ILE	3.0
1	D	389	ILE	3.0
1	A	36	GLY	3.0
1	A	44	GLY	3.0
1	C	342	VAL	3.0
1	D	144	LEU	3.0
1	B	234	PRO	3.0
1	A	74	ALA	2.9
1	C	230	LEU	2.9
1	B	39	PRO	2.9
1	C	240	VAL	2.9
1	A	37	PRO	2.9
1	A	224	LEU	2.9
1	A	233	ILE	2.8
1	D	168	SER	2.8
1	D	65	PHE	2.8
1	D	232	HIS	2.8
1	D	77	PRO	2.8
1	A	146	LYS	2.8
1	A	238	GLY	2.7
1	C	235	ALA	2.7
1	B	51	PHE	2.7
1	D	226	ALA	2.7
1	C	39	PRO	2.6
1	A	147	LYS	2.6
1	D	342	VAL	2.5
1	A	51	PHE	2.5
1	A	483	PHE	2.5
1	D	146	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	73	LEU	2.5
1	B	232	HIS	2.5
1	A	149	LEU	2.4
1	B	73	LEU	2.4
1	A	46	LEU	2.4
1	A	45	ASN	2.3
1	C	109	ILE	2.3
1	C	72	GLN	2.3
1	D	73	LEU	2.3
1	C	423	ALA	2.3
1	B	238	GLY	2.3
1	B	240	VAL	2.3
1	C	170	ARG	2.2
1	D	74	ALA	2.2
1	C	310	THR	2.2
1	C	388	ARG	2.2
1	A	31	GLY	2.2
1	C	227	VAL	2.2
1	B	231	LEU	2.2
1	D	36	GLY	2.2
1	D	423	ALA	2.2
1	C	65	PHE	2.1
1	C	60	GLN	2.1
1	C	63	ARG	2.1
1	C	74	ALA	2.1
1	D	35	PRO	2.1
1	B	307	MET	2.1
1	D	215	GLU	2.1
1	C	341	GLN	2.1
1	D	339	ILE	2.1
1	D	39	PRO	2.1
1	C	110	LEU	2.0
1	B	223	VAL	2.0
1	D	224	LEU	2.0
1	D	230	LEU	2.0
1	D	241	LEU	2.0
1	A	49	VAL	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 ⓘ

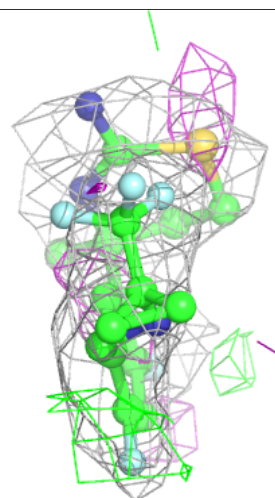
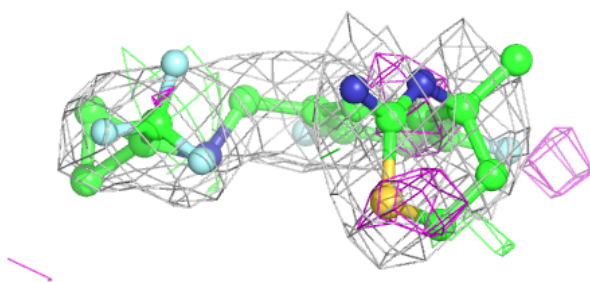
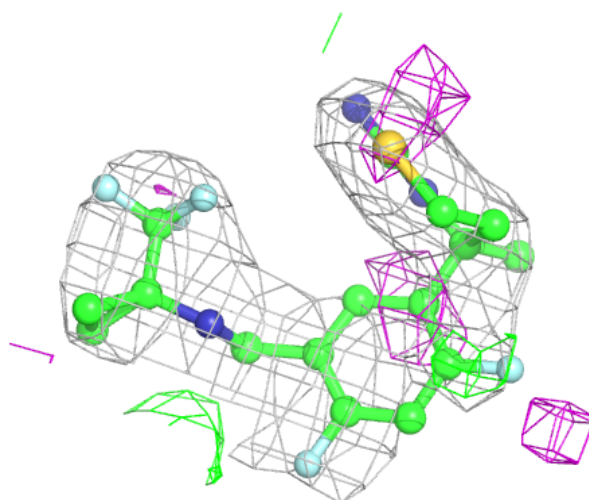
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	P6U	A	604	25/25	0.87	0.24	56,74,86,96	0
4	P6U	B	603	25/25	0.88	0.23	51,71,84,93	0
4	P6U	C	603	25/25	0.90	0.19	58,76,84,93	0
4	P6U	D	603	25/25	0.91	0.21	50,75,86,92	0
2	HEM	A	601	43/43	0.97	0.20	18,25,29,31	0
2	HEM	D	601	43/43	0.97	0.22	22,33,43,44	0
2	HEM	C	601	43/43	0.98	0.21	24,31,40,42	0
2	HEM	B	601	43/43	0.98	0.21	17,25,31,36	0
3	ZN	A	603	1/1	0.98	0.15	57,57,57,57	0
3	ZN	A	602	1/1	0.99	0.14	36,36,36,36	0
3	ZN	B	602	1/1	0.99	0.10	26,26,26,26	0
3	ZN	D	602	1/1	0.99	0.09	34,34,34,34	0
3	ZN	C	602	1/1	1.00	0.13	35,35,35,35	0

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

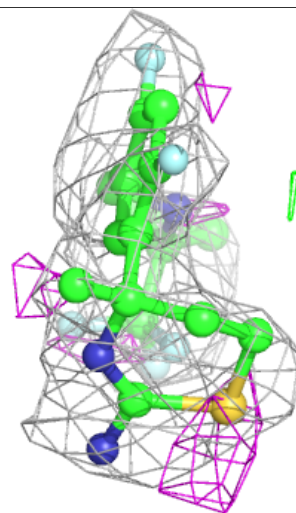
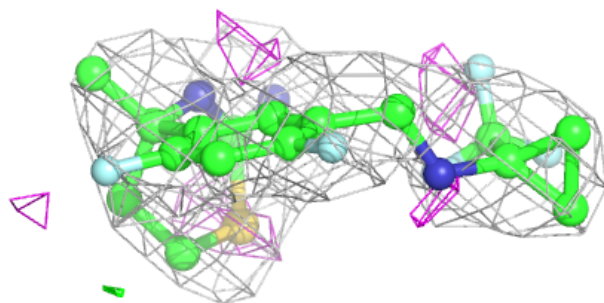
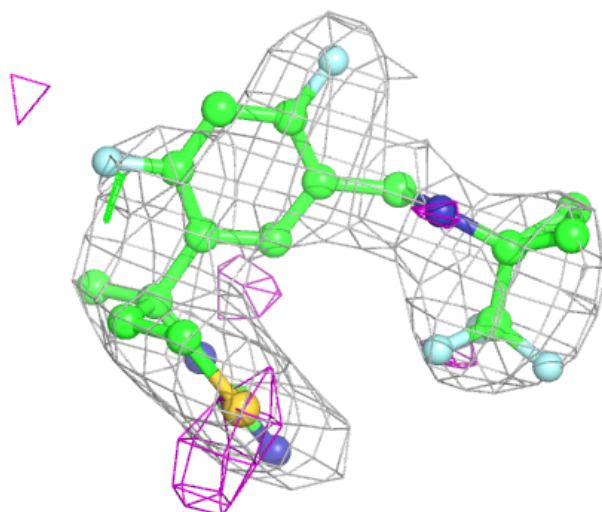
Electron density around P6U A 604:

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



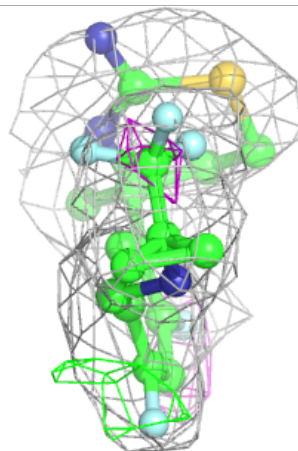
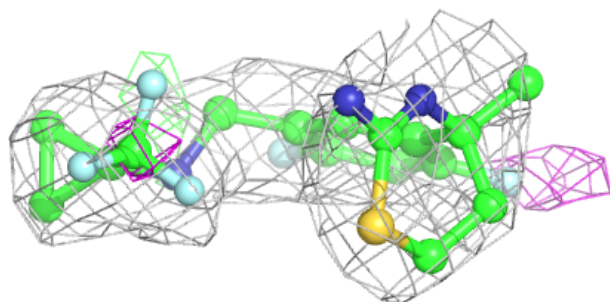
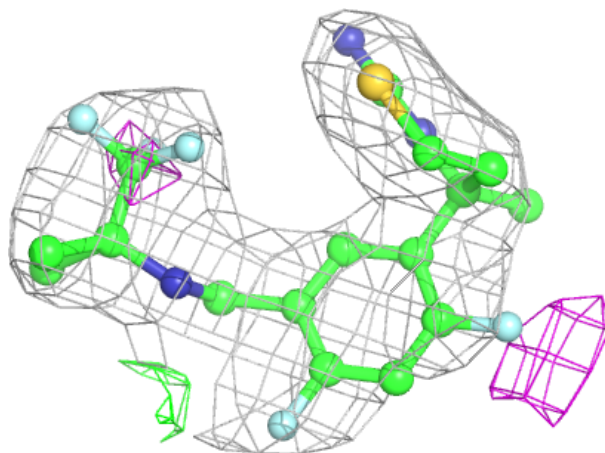
Electron density around P6U B 603:

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



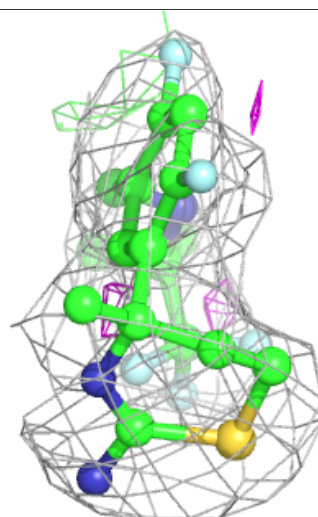
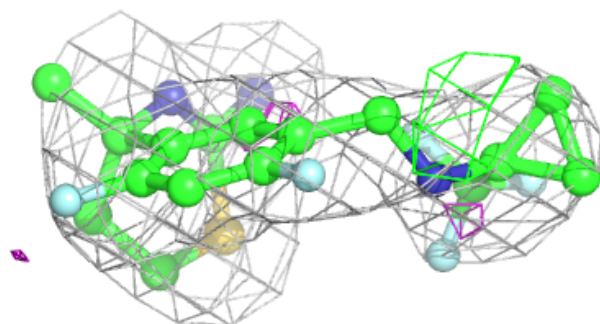
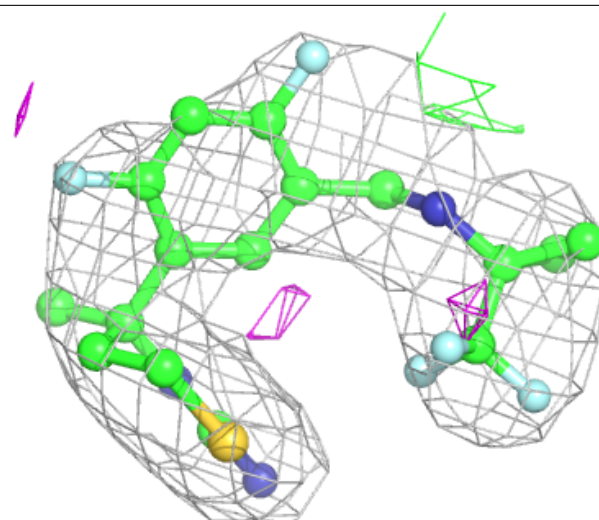
Electron density around P6U C 603:

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



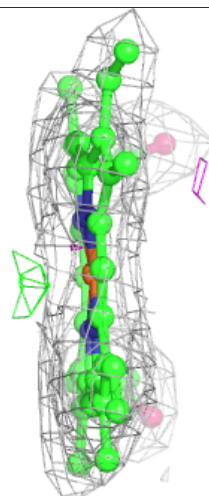
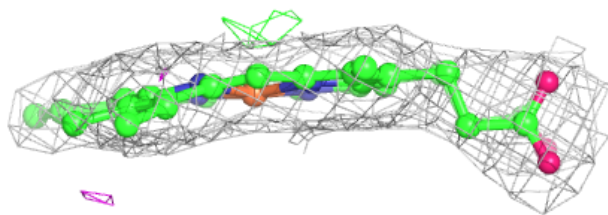
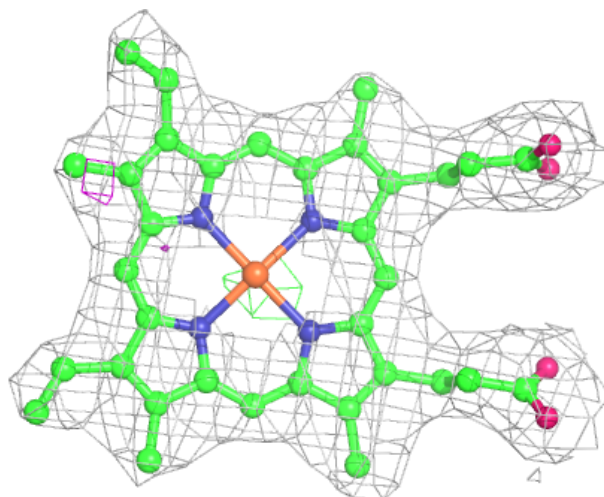
Electron density around P6U D 603:

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



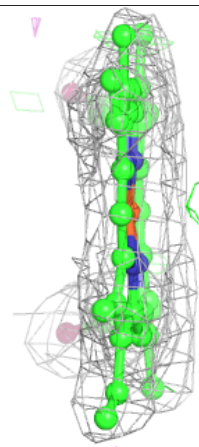
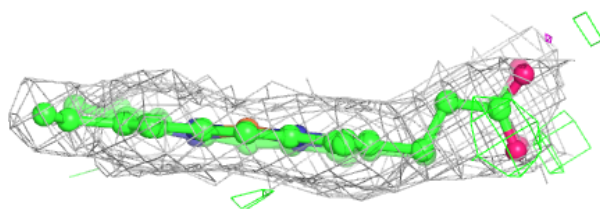
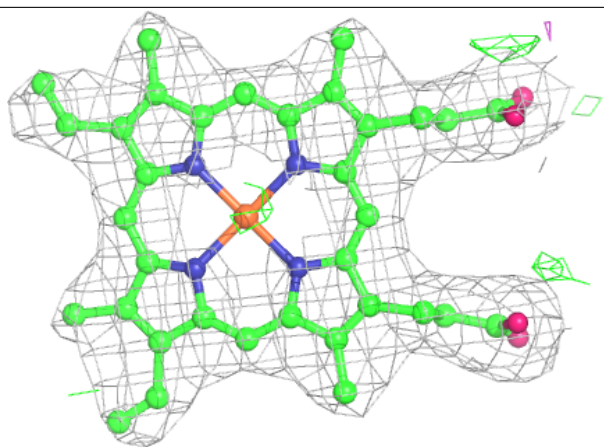
Electron density around HEM A 601:

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



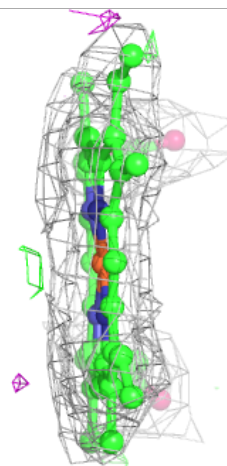
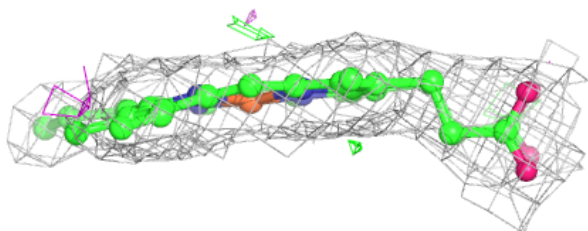
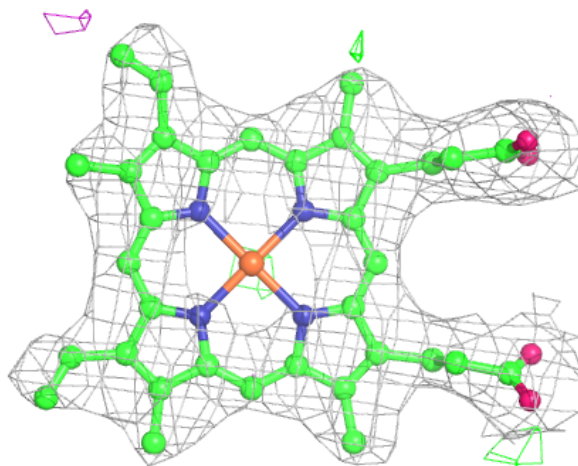
Electron density around HEM D 601:

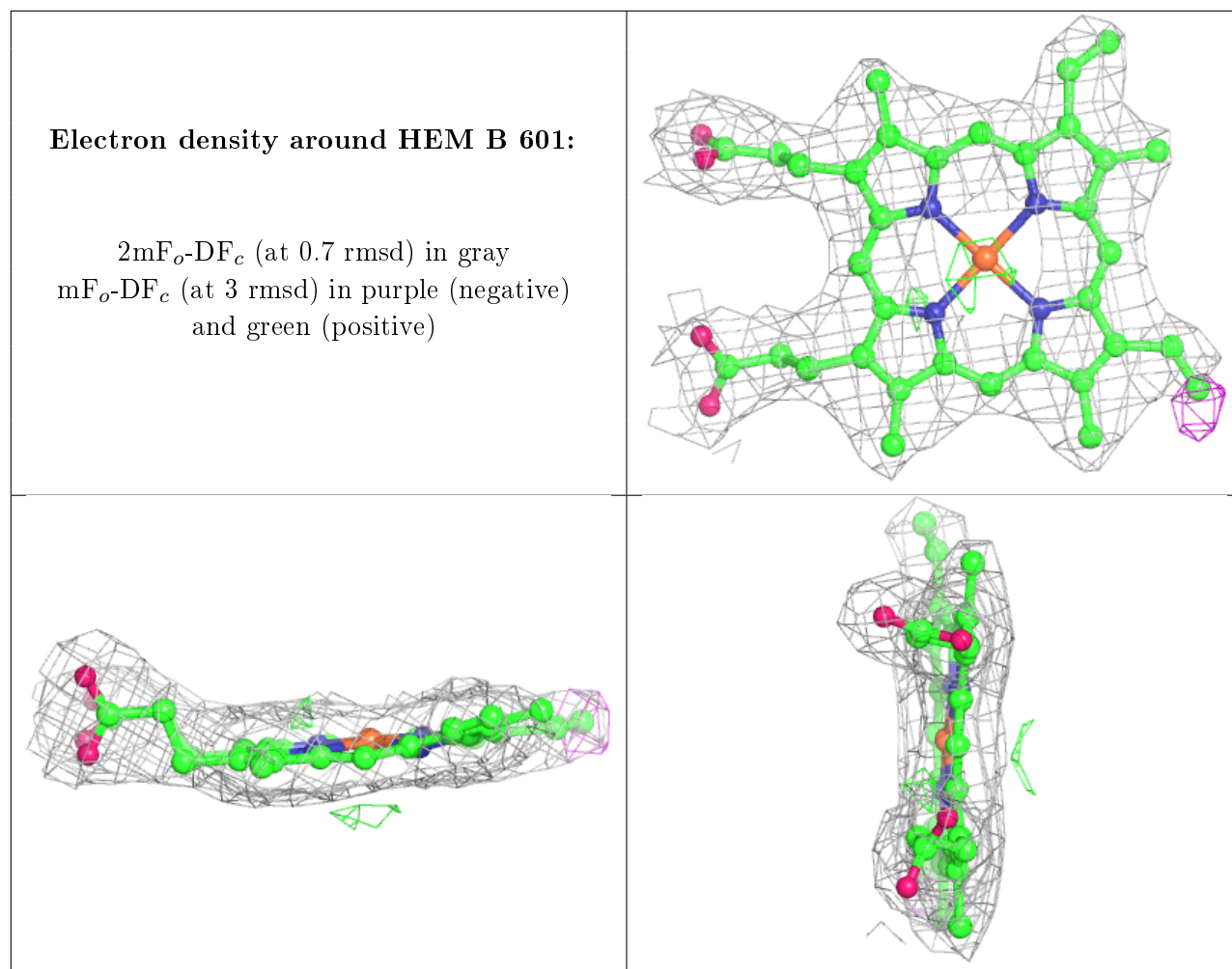
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 ⓘ

There are no such residues in this entry.