



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:41 am BST

PDB ID : 6Q2T  
Title : Human sterol 14a-demethylase (CYP51) in complex with the functionally irreversible inhibitor (R)-N-(1-(3-chloro-4'-fluoro-[1,1'-biphenyl]-4-yl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-(3-fluoro-5-(5-fluoropyrimidin-4-yl)phenyl)-1,3,4-oxadiazol-2-yl)benzamide  
Authors : Friggeri, L.; Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.  
Deposited on : 2019-08-08  
Resolution : 2.80 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](mailto: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.

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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

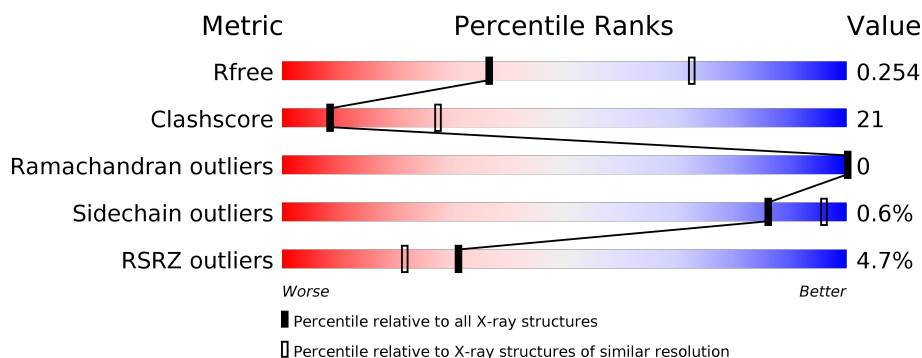
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	446	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> </div>
1	B	446	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> </div>

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
4	DXC	A	603	X	-	-	-
4	DXC	A	604	X	-	-	-
4	DXC	A	605	X	-	-	-
4	DXC	A	606	X	-	-	-
4	DXC	A	607	X	-	-	-
4	DXC	A	608	X	-	-	-
4	DXC	A	609	X	-	-	-
4	DXC	A	610	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7658 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.

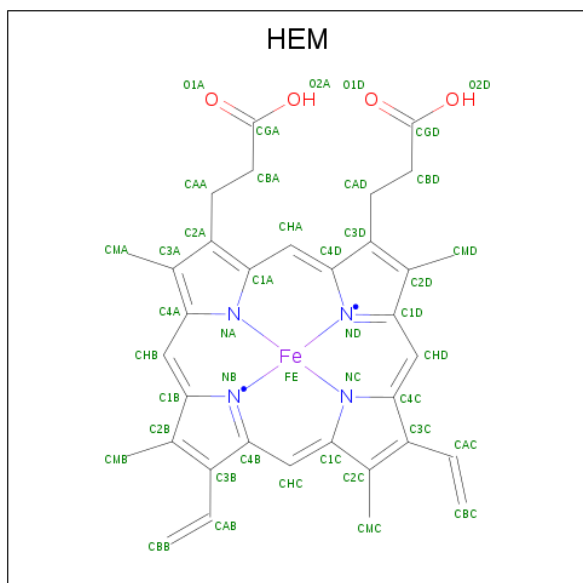
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	B	444	Total	C	N	O	S	0	0	0
			3584	2308	610	650	16			

There are 6 discrepancies between the modelled and reference sequences:

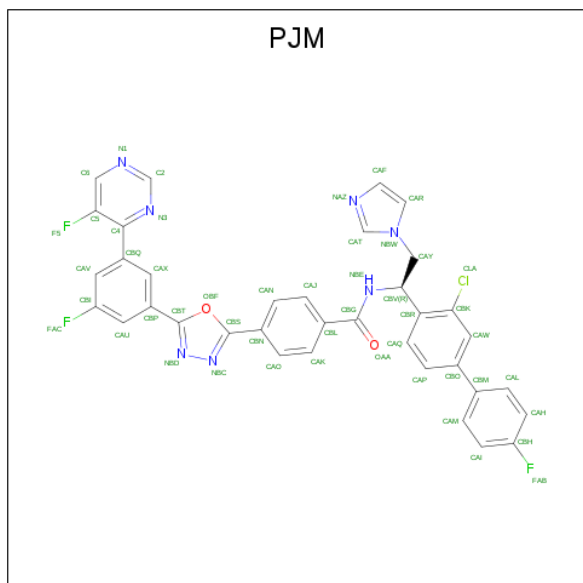
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	expression tag	UNP Q16850
A	59	LYS	-	expression tag	UNP Q16850
A	60	LEU	-	expression tag	UNP Q16850
B	58	GLY	-	expression tag	UNP Q16850
B	59	LYS	-	expression tag	UNP Q16850
B	60	LEU	-	expression tag	UNP Q16850

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



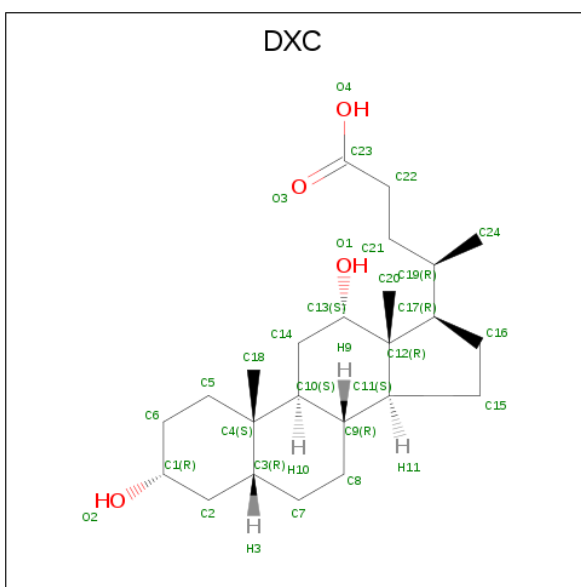
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N-[(1R)-1-(3-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)-2-(1H-imidazol-1-yl)ethyl]-4-{5-[3-fluoro-5-(5-fluoropyrimidin-4-yl)phenyl]-1,3,4-oxadiazol-2-yl}benzamide (three-letter code: PJM) (formula: C<sub>36</sub>H<sub>23</sub>ClF<sub>3</sub>N<sub>7</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 49	C 36	Cl 1	F 3	N 7	O 2	0	0
3	A	1	Total 49	C 36	Cl 1	F 3	N 7	O 2	0	0
3	B	1	Total 49	C 36	Cl 1	F 3	N 7	O 2	0	0

- Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0

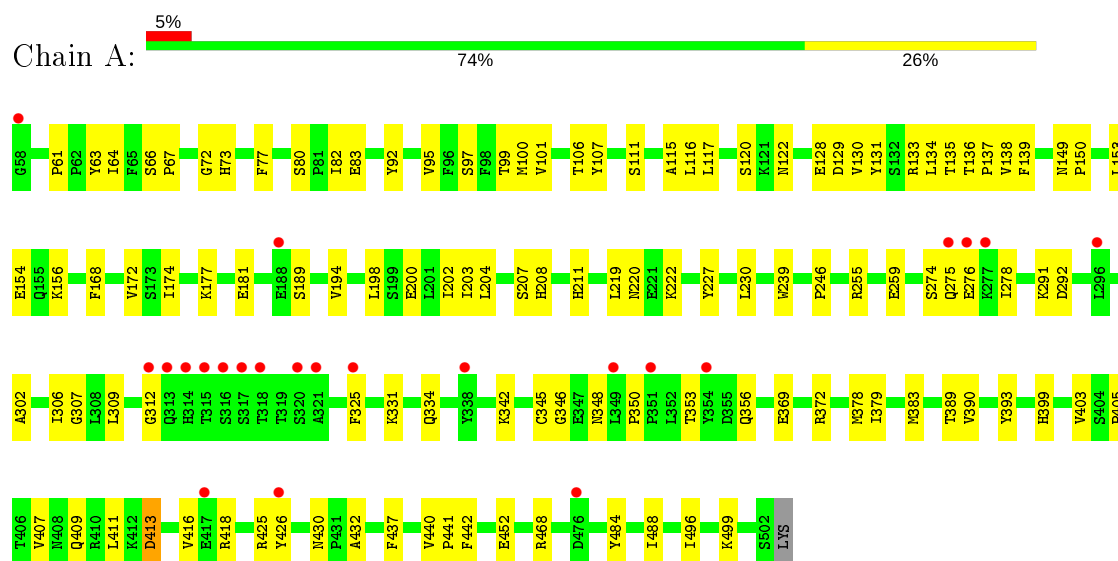
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total O 13 13	0	0
5	B	16	Total O 16 16	0	0

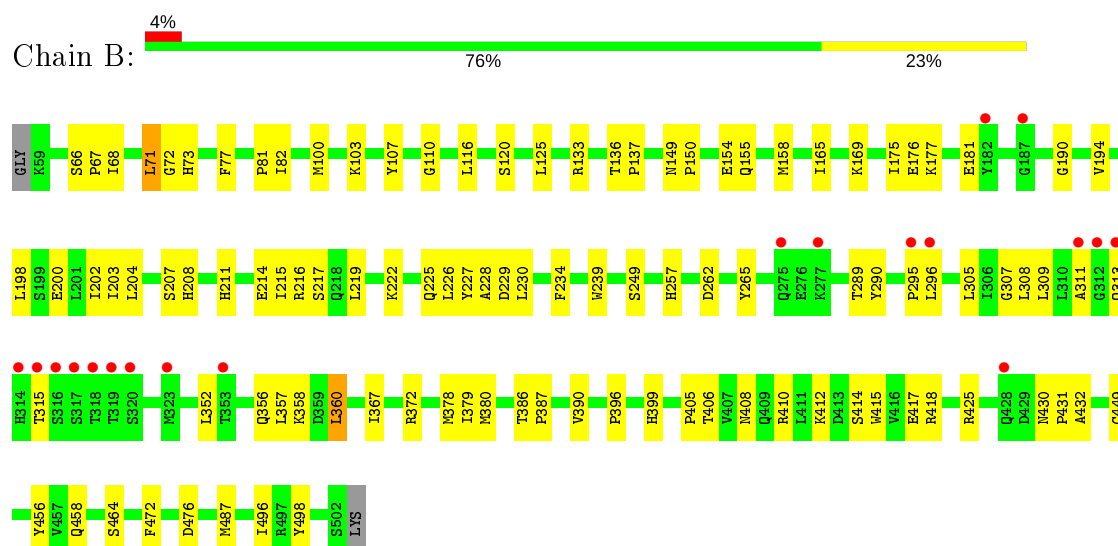
### 3 Residue-property plots [i](#)

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: Lanosterol 14-alpha demethylase



#### • Molecule 1: Lanosterol 14-alpha demethylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.66Å 117.66Å 157.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.10 – 2.80 28.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.10-2.80) 99.7 (28.08-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.227 , 0.256 0.227 , 0.254	Depositor DCC
$R_{free}$ test set	1258 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.63	0/3681	0.63	0/4986
1	B	0.63	0/3677	0.62	0/4981
All	All	0.63	0/7358	0.63	0/9967

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

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	3588	0	3581	124	0
1	B	3584	0	3578	108	0
2	A	43	0	30	6	0
2	B	43	0	30	7	0
3	A	98	0	0	13	0
3	B	49	0	0	8	0
4	A	224	0	312	74	0
5	A	13	0	0	3	0
5	B	16	0	0	5	0
All	All	7658	0	7531	316	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 21.

All (316) 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:204:LEU:HD23	1:A:219:LEU:CD2	1.66	1.24
1:A:204:LEU:CD2	1:A:219:LEU:HD23	1.68	1.23
4:A:608:DXC:C8	4:A:608:DXC:H61	1.72	1.19
4:A:608:DXC:H82	4:A:608:DXC:C6	1.75	1.16
4:A:606:DXC:H203	4:A:606:DXC:H242	1.14	1.12
4:A:610:DXC:H242	4:A:610:DXC:O1	1.49	1.11
1:A:156:LYS:HD3	5:A:710:HOH:O	1.49	1.10
1:A:153:LEU:HD23	5:A:710:HOH:O	1.53	1.07
1:A:204:LEU:CD2	1:A:219:LEU:CD2	2.31	1.07
1:B:412:LYS:HG3	5:B:709:HOH:O	1.53	1.06
1:B:77:PHE:CB	1:B:100:MET:HE1	1.85	1.05
4:A:610:DXC:H61	4:A:610:DXC:H82	1.37	1.04
1:B:155:GLN:HA	1:B:158:MET:HE2	1.40	1.04
1:B:194:VAL:CG1	1:B:496:ILE:HG21	1.87	1.03
1:B:77:PHE:CG	1:B:100:MET:HE1	1.94	1.02
1:B:194:VAL:HG13	1:B:496:ILE:CG2	1.89	1.01
1:B:120:SER:OG	1:B:125:LEU:HD12	1.65	0.96
1:B:357:LEU:HA	1:B:360:LEU:HD12	1.46	0.94
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.50	0.94
1:A:198:LEU:O	1:A:202:ILE:HG12	1.66	0.94
4:A:606:DXC:C20	4:A:606:DXC:H242	1.96	0.93
1:B:194:VAL:HG13	1:B:496:ILE:HG22	1.48	0.93
4:A:606:DXC:H61	4:A:606:DXC:H82	1.50	0.93
1:B:77:PHE:CB	1:B:100:MET:CE	2.47	0.92
1:A:307:GLY:HA3	3:A:602:PJM:CAH	2.00	0.91
1:B:307:GLY:HA3	3:B:602:PJM:CAH	2.01	0.91
1:A:77:PHE:CB	1:A:100:MET:HE1	2.02	0.90
1:A:77:PHE:CG	1:A:100:MET:CE	2.55	0.89
1:B:198:LEU:O	1:B:202:ILE:HG12	1.72	0.87
1:B:77:PHE:HB3	1:B:100:MET:HE1	1.56	0.87
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.55	0.87
4:A:610:DXC:H61	4:A:610:DXC:C8	2.03	0.87
1:A:77:PHE:CG	1:A:100:MET:HE1	2.09	0.86
1:A:204:LEU:HD23	1:A:219:LEU:HD21	1.55	0.86
4:A:606:DXC:H203	4:A:606:DXC:C24	2.04	0.86
1:A:66:SER:OG	1:A:99:THR:CG2	2.24	0.86
1:B:194:VAL:CG1	1:B:496:ILE:CG2	2.50	0.85
1:B:120:SER:CB	1:B:125:LEU:HD12	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLY:CA	3:A:602:PJM:CAL	2.55	0.84
1:A:77:PHE:HB3	1:A:100:MET:HE1	1.60	0.83
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.60	0.83
4:A:604:DXC:H10	4:A:604:DXC:H201	1.61	0.83
1:A:307:GLY:HA3	3:A:602:PJM:CAL	2.08	0.83
4:A:605:DXC:H1	4:A:607:DXC:H241	1.62	0.81
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.61	0.80
1:B:357:LEU:HA	1:B:360:LEU:CD1	2.11	0.80
1:A:115:ALA:HA	1:A:437:PHE:CE2	2.18	0.79
4:A:603:DXC:H222	4:A:606:DXC:H243	1.65	0.79
4:A:610:DXC:H82	4:A:610:DXC:C6	2.14	0.78
1:A:82:ILE:HD12	1:A:484:TYR:OH	1.84	0.78
1:B:67:PRO:HD2	1:B:72:GLY:O	1.84	0.77
1:A:307:GLY:C	3:A:602:PJM:CAL	2.52	0.77
1:B:77:PHE:CG	1:B:100:MET:CE	2.68	0.76
1:B:307:GLY:HA3	3:B:602:PJM:CAL	2.16	0.75
1:A:77:PHE:CB	1:A:100:MET:CE	2.64	0.75
1:B:208:HIS:CD2	1:B:216:ARG:HG2	2.22	0.75
1:A:77:PHE:CD2	1:A:100:MET:HE1	2.22	0.74
4:A:610:DXC:H61	4:A:610:DXC:C7	2.18	0.74
1:B:214:GLU:HG2	1:B:215:ILE:N	2.02	0.74
1:A:66:SER:OG	1:A:99:THR:HG21	1.88	0.72
1:B:77:PHE:HB2	1:B:100:MET:CE	2.18	0.72
1:A:204:LEU:HD22	1:A:219:LEU:HD23	1.71	0.72
1:A:413:ASP:OD1	1:A:413:ASP:N	2.20	0.72
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.19	0.72
1:A:77:PHE:CG	1:A:100:MET:HE3	2.23	0.72
1:B:204:LEU:HD23	1:B:219:LEU:HD23	1.72	0.72
1:B:307:GLY:CA	3:B:602:PJM:CAL	2.68	0.71
1:A:153:LEU:CD2	5:A:710:HOH:O	2.22	0.71
4:A:604:DXC:C14	4:A:604:DXC:H61	2.20	0.71
1:A:82:ILE:HG12	1:A:378:MET:CE	2.20	0.71
4:A:608:DXC:H241	4:A:608:DXC:O4	1.90	0.71
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.20	0.71
1:B:380:MET:HE2	1:B:405:PRO:HD3	1.73	0.70
1:A:426:TYR:HA	1:A:430:ASN:ND2	2.06	0.70
4:A:604:DXC:H61	4:A:604:DXC:H142	1.71	0.70
4:A:605:DXC:H201	4:A:605:DXC:H10	1.74	0.69
1:B:194:VAL:HG11	1:B:496:ILE:HG21	1.72	0.69
1:B:472:PHE:HB3	1:B:496:ILE:HD11	1.74	0.69
1:A:138:VAL:HG13	1:A:230:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:DXC:H82	4:A:608:DXC:H61	0.81	0.69
4:A:606:DXC:H201	4:A:606:DXC:H10	1.74	0.69
4:A:606:DXC:H61	4:A:606:DXC:C8	2.21	0.69
1:A:307:GLY:CA	3:A:602:PJM:CAH	2.71	0.69
1:A:135:THR:HB	1:A:139:PHE:CD2	2.28	0.69
2:B:601:HEM:CMC	2:B:601:HEM:HBC2	2.23	0.69
1:B:155:GLN:HA	1:B:158:MET:CE	2.21	0.68
1:B:66:SER:HB2	1:B:72:GLY:HA2	1.74	0.68
1:A:276:GLU:OE2	1:A:278:ILE:HD11	1.92	0.68
4:A:608:DXC:H52	4:A:608:DXC:O1	1.92	0.68
1:A:378:MET:HG2	1:A:379:ILE:HG13	1.74	0.68
1:A:194:VAL:HG13	1:A:496:ILE:CG2	2.24	0.68
1:A:66:SER:OG	1:A:99:THR:HG22	1.94	0.67
1:A:77:PHE:CD2	1:A:100:MET:CE	2.78	0.66
1:A:348:ASN:OD1	1:A:350:PRO:HD3	1.96	0.66
4:A:606:DXC:H13	4:A:606:DXC:H241	1.76	0.66
4:A:608:DXC:H52	4:A:608:DXC:H11	1.76	0.66
1:A:416:VAL:O	1:A:425:ARG:NH2	2.28	0.66
1:B:307:GLY:C	3:B:602:PJM:CAL	2.65	0.65
1:B:77:PHE:CD2	1:B:100:MET:HE3	2.32	0.65
4:A:610:DXC:C7	4:A:610:DXC:C6	2.74	0.65
1:B:66:SER:HB2	1:B:72:GLY:CA	2.26	0.65
4:A:610:DXC:O1	4:A:610:DXC:C24	2.36	0.65
1:B:77:PHE:CE1	1:B:81:PRO:HB3	2.32	0.65
1:B:77:PHE:CD1	1:B:81:PRO:HB3	2.32	0.65
1:B:107:TYR:OH	1:B:379:ILE:HD12	1.97	0.64
1:A:378:MET:O	1:A:405:PRO:HD2	1.98	0.63
1:B:357:LEU:CA	1:B:360:LEU:HD12	2.23	0.63
1:B:77:PHE:CD2	1:B:100:MET:CE	2.82	0.63
1:A:220:ASN:OD1	1:A:222:LYS:HB3	1.98	0.63
2:B:601:HEM:CMB	2:B:601:HEM:HBB2	2.27	0.63
1:B:77:PHE:HB3	1:B:100:MET:CE	2.25	0.63
1:B:410:ARG:O	1:B:418:ARG:HD2	1.99	0.63
4:A:606:DXC:H241	4:A:606:DXC:C13	2.29	0.62
1:A:115:ALA:CB	1:A:437:PHE:CE2	2.82	0.62
1:A:130:VAL:HG23	1:A:131:TYR:CD1	2.35	0.62
4:A:609:DXC:H203	4:A:609:DXC:H242	1.82	0.62
1:B:165:ILE:HG22	1:B:169:LYS:HE2	1.81	0.62
4:A:607:DXC:H10	4:A:607:DXC:H201	1.81	0.61
4:A:608:DXC:C6	4:A:608:DXC:C8	2.55	0.61
1:B:367:ILE:HG21	1:B:456:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLN:HG2	5:B:713:HOH:O	1.99	0.61
1:A:194:VAL:HG13	1:A:496:ILE:HG22	1.82	0.61
1:A:274:SER:OG	1:A:276:GLU:HB3	2.01	0.61
1:B:307:GLY:CA	3:B:602:PJM:CAH	2.75	0.61
1:A:246:PRO:HG3	4:A:610:DXC:H142	1.83	0.60
1:A:194:VAL:CG1	1:A:496:ILE:HG21	2.31	0.60
4:A:610:DXC:H11	4:A:610:DXC:H52	1.84	0.60
1:B:367:ILE:CG2	1:B:456:TYR:CE1	2.85	0.60
1:B:82:ILE:HD11	1:B:406:THR:HG21	1.82	0.60
1:A:274:SER:OG	1:A:276:GLU:CB	2.50	0.59
4:A:604:DXC:H152	4:A:608:DXC:H142	1.85	0.59
1:A:407:VAL:HG12	1:A:411:LEU:HD21	1.84	0.59
4:A:604:DXC:H203	4:A:604:DXC:H242	1.85	0.59
4:A:604:DXC:C6	4:A:604:DXC:H142	2.29	0.59
1:A:72:GLY:HA3	1:A:99:THR:HG23	1.83	0.59
1:B:204:LEU:HD23	1:B:219:LEU:CD2	2.31	0.59
1:B:378:MET:O	1:B:405:PRO:HD2	2.03	0.59
1:B:82:ILE:CD1	1:B:406:THR:HG21	2.33	0.59
1:A:82:ILE:CG1	1:A:378:MET:CE	2.81	0.58
1:A:115:ALA:CB	1:A:437:PHE:HE2	2.16	0.58
1:A:149:ASN:N	1:A:150:PRO:CD	2.67	0.58
1:A:220:ASN:OD1	1:A:222:LYS:N	2.36	0.58
1:A:133:ARG:HH22	1:A:239:TRP:HA	1.69	0.58
1:A:407:VAL:O	1:A:411:LEU:HG	2.04	0.57
1:A:115:ALA:CA	1:A:437:PHE:CE2	2.87	0.57
1:A:66:SER:HB3	1:A:72:GLY:HA2	1.85	0.57
4:A:604:DXC:H221	4:A:604:DXC:H161	1.85	0.57
1:B:120:SER:HG	1:B:125:LEU:HD12	1.64	0.57
1:A:82:ILE:HG12	1:A:378:MET:HE1	1.85	0.57
1:A:442:PHE:CE2	1:A:452:GLU:HA	2.40	0.56
4:A:610:DXC:C8	4:A:610:DXC:C6	2.79	0.56
1:A:82:ILE:CG1	1:A:378:MET:HE1	2.36	0.56
4:A:608:DXC:C5	4:A:608:DXC:H11	2.35	0.56
1:A:307:GLY:C	3:A:602:PJM:CAH	2.74	0.56
1:A:116:LEU:HD22	1:A:390:VAL:HB	1.86	0.56
1:A:302:ALA:O	1:A:306:ILE:HG13	2.05	0.56
1:A:129:ASP:HB2	1:A:383:MET:HB3	1.88	0.56
4:A:606:DXC:C24	4:A:606:DXC:C13	2.84	0.55
1:B:116:LEU:HD22	1:B:390:VAL:HB	1.88	0.55
1:A:111:SER:HA	1:A:437:PHE:HB2	1.88	0.55
1:B:107:TYR:OH	1:B:379:ILE:CD1	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:603:DXC:H10	4:A:603:DXC:H201	1.89	0.55
1:B:158:MET:SD	1:B:296:LEU:HD11	2.46	0.55
1:B:262:ASP:O	1:B:265:TYR:HB2	2.07	0.55
1:A:426:TYR:HA	1:A:430:ASN:HD22	1.71	0.54
3:A:611:PJM:CAY	3:A:611:PJM:CLA	2.91	0.54
1:B:67:PRO:CD	1:B:72:GLY:O	2.55	0.54
1:A:207:SER:O	1:A:211:HIS:HB2	2.07	0.54
1:A:276:GLU:CD	1:A:278:ILE:HD11	2.27	0.54
1:A:331:LYS:HE3	1:A:334:GLN:NE2	2.22	0.54
1:A:220:ASN:OD1	1:A:222:LYS:CB	2.55	0.54
1:A:101:VAL:O	1:A:101:VAL:HG12	2.07	0.54
1:B:200:GLU:O	1:B:203:ILE:HG22	2.07	0.54
1:A:204:LEU:HD21	1:A:219:LEU:HD23	1.76	0.54
1:A:115:ALA:HB2	1:A:437:PHE:CE2	2.43	0.53
3:A:602:PJM:N1	4:A:609:DXC:O4	2.41	0.53
1:B:430:ASN:OD1	1:B:432:ALA:HB3	2.08	0.53
4:A:606:DXC:H13	4:A:606:DXC:C24	2.39	0.53
1:B:311:ALA:O	1:B:315:THR:OG1	2.26	0.53
1:A:135:THR:HB	1:A:139:PHE:CE2	2.44	0.53
1:A:122:ASN:HD21	1:A:128:GLU:CD	2.12	0.52
1:A:107:TYR:OH	1:A:379:ILE:HD13	2.09	0.52
1:B:207:SER:O	1:B:211:HIS:HB2	2.09	0.52
4:A:604:DXC:C10	4:A:604:DXC:H201	2.32	0.52
1:A:200:GLU:O	1:A:203:ILE:HG22	2.10	0.51
1:A:67:PRO:HD3	1:A:73:HIS:NE2	2.26	0.51
4:A:604:DXC:C14	4:A:604:DXC:C6	2.87	0.51
4:A:610:DXC:H241	4:A:610:DXC:O3	2.10	0.51
1:B:120:SER:HB3	1:B:125:LEU:HD12	1.90	0.50
1:A:488:ILE:O	1:A:488:ILE:HG23	2.12	0.50
2:A:601:HEM:HMC2	2:A:601:HEM:CBC	2.37	0.50
1:B:449:CYS:HA	2:B:601:HEM:C4D	2.47	0.50
1:A:312:GLY:HA2	2:A:601:HEM:HMC1	1.94	0.49
1:A:139:PHE:HE1	3:A:602:PJM:CAW	2.25	0.49
1:A:331:LYS:HE3	1:A:334:GLN:HE22	1.77	0.49
1:B:410:ARG:NH1	5:B:701:HOH:O	2.37	0.49
1:A:139:PHE:CE1	3:A:602:PJM:CAW	2.95	0.49
4:A:606:DXC:H61	4:A:606:DXC:C7	2.41	0.49
1:B:133:ARG:HH12	1:B:239:TRP:HA	1.77	0.49
4:A:606:DXC:H201	4:A:606:DXC:C10	2.42	0.49
1:B:305:LEU:O	1:B:308:LEU:HB2	2.12	0.49
1:B:222:LYS:O	1:B:226:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HA	1:B:356:GLN:OE1	2.13	0.49
1:A:353:THR:N	1:A:356:GLN:OE1	2.40	0.49
1:A:372:ARG:NH2	1:A:418:ARG:O	2.46	0.48
1:A:67:PRO:HD3	1:A:73:HIS:CE1	2.48	0.48
1:A:136:THR:N	1:A:137:PRO:CD	2.77	0.48
1:B:177:LYS:HE2	1:B:181:GLU:OE2	2.13	0.48
1:A:117:LEU:O	1:A:120:SER:OG	2.30	0.48
3:A:611:PJM:CAV	3:A:611:PJM:F5	2.51	0.48
1:A:246:PRO:CG	4:A:610:DXC:H142	2.43	0.48
4:A:610:DXC:C5	4:A:610:DXC:C8	2.91	0.48
4:A:603:DXC:C22	4:A:606:DXC:H243	2.41	0.47
1:A:227:TYR:CE1	1:A:309:LEU:HD23	2.49	0.47
4:A:607:DXC:H201	4:A:607:DXC:C10	2.43	0.47
1:A:80:SER:OG	1:A:83:GLU:HB2	2.15	0.47
1:B:386:THR:HB	1:B:387:PRO:HD2	1.95	0.47
1:A:154:GLU:OE1	1:A:291:LYS:HG3	2.14	0.47
1:A:372:ARG:HA	1:A:409:GLN:NE2	2.30	0.47
1:B:116:LEU:O	1:B:120:SER:HB3	2.13	0.47
1:B:208:HIS:HD2	1:B:216:ARG:HG2	1.77	0.47
1:B:372:ARG:HD2	1:B:415:TRP:CZ3	2.50	0.47
1:A:430:ASN:OD1	1:A:432:ALA:HB3	2.15	0.47
1:B:414:SER:O	1:B:431:PRO:CG	2.63	0.47
4:A:606:DXC:H81	4:A:607:DXC:H162	1.97	0.47
1:B:214:GLU:CG	1:B:215:ILE:N	2.76	0.47
4:A:610:DXC:H61	4:A:610:DXC:H72	1.95	0.47
1:B:103:LYS:HG3	5:B:716:HOH:O	2.14	0.47
1:B:307:GLY:C	3:B:602:PJM:CAH	2.83	0.46
4:A:609:DXC:H13	4:A:609:DXC:H242	1.97	0.46
1:A:440:VAL:N	1:A:441:PRO:CD	2.78	0.46
1:A:389:THR:HA	1:A:393:TYR:O	2.15	0.46
4:A:610:DXC:H82	4:A:610:DXC:C5	2.46	0.46
1:B:175:ILE:HD13	1:B:458:GLN:HA	1.97	0.46
1:B:68:ILE:O	1:B:72:GLY:HA2	2.14	0.46
1:A:345:CYS:SG	1:A:468:ARG:NH2	2.88	0.46
4:A:608:DXC:H183	4:A:608:DXC:H141	1.61	0.46
1:A:82:ILE:CG1	1:A:378:MET:HE3	2.46	0.46
1:B:396:PRO:HG2	1:B:399:HIS:CD2	2.51	0.46
4:A:607:DXC:C13	4:A:607:DXC:H242	2.46	0.46
1:B:67:PRO:HG2	1:B:72:GLY:O	2.15	0.46
4:A:608:DXC:H221	4:A:608:DXC:H243	1.72	0.46
1:A:134:LEU:HD11	1:A:239:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:610:DXC:H243	4:A:610:DXC:H221	1.70	0.46
1:B:214:GLU:O	1:B:217:SER:OG	2.26	0.45
1:B:315:THR:HB	2:B:601:HEM:CAB	2.46	0.45
1:A:342:LYS:HA	1:A:346:GLY:O	2.16	0.45
1:A:61:PRO:HA	1:A:393:TYR:CD1	2.50	0.45
2:B:601:HEM:CBC	2:B:601:HEM:HMC2	2.40	0.45
1:B:417:GLU:O	1:B:425:ARG:NH2	2.49	0.45
4:A:607:DXC:H13	4:A:607:DXC:H242	1.99	0.45
1:B:136:THR:HB	1:B:137:PRO:HD3	1.98	0.45
1:B:227:TYR:CZ	1:B:309:LEU:HD22	2.52	0.45
1:B:289:THR:HG22	1:B:295:PRO:HB3	1.98	0.45
4:A:606:DXC:C8	4:A:607:DXC:H162	2.47	0.44
1:B:120:SER:CB	1:B:125:LEU:CD1	2.88	0.44
1:B:149:ASN:N	1:B:150:PRO:CD	2.80	0.44
1:B:410:ARG:O	1:B:410:ARG:HG3	2.16	0.44
1:B:249:SER:HB2	5:B:708:HOH:O	2.17	0.44
1:B:67:PRO:CG	1:B:72:GLY:O	2.65	0.44
4:A:608:DXC:H19	4:A:608:DXC:H203	1.76	0.44
4:A:605:DXC:H201	4:A:605:DXC:C10	2.42	0.44
1:A:246:PRO:HD3	4:A:610:DXC:O1	2.18	0.44
1:B:214:GLU:HG2	1:B:215:ILE:H	1.80	0.44
3:B:602:PJM:CAV	3:B:602:PJM:F5	2.55	0.44
1:A:255:ARG:NH2	1:A:259:GLU:OE2	2.51	0.44
1:A:115:ALA:HB2	1:A:437:PHE:HE2	1.82	0.44
1:B:67:PRO:HD3	1:B:73:HIS:CE1	2.52	0.44
1:A:139:PHE:CE1	1:A:307:GLY:HA2	2.52	0.43
1:B:77:PHE:CE1	1:B:81:PRO:CB	3.01	0.43
1:B:230:LEU:HD21	1:B:257:HIS:HB2	1.99	0.43
1:A:135:THR:HG22	1:A:139:PHE:HE2	1.83	0.43
4:A:604:DXC:H13	4:A:604:DXC:H242	2.00	0.43
1:B:414:SER:O	1:B:431:PRO:HG3	2.19	0.43
1:B:234:PHE:O	1:B:487:MET:HG3	2.18	0.43
1:A:168:PHE:O	1:A:172:VAL:HG23	2.19	0.43
4:A:610:DXC:H242	4:A:610:DXC:H1O1	1.75	0.43
1:A:136:THR:HB	1:A:137:PRO:HD3	2.00	0.43
1:A:117:LEU:HD13	1:A:403:VAL:HG23	2.01	0.43
1:A:134:LEU:HD22	3:A:602:PJM:NBC	2.33	0.43
4:A:608:DXC:C6	4:A:608:DXC:H11	2.49	0.43
1:A:61:PRO:HB3	1:A:95:VAL:HG12	2.01	0.43
4:A:604:DXC:H82	4:A:604:DXC:H22	1.71	0.43
4:A:608:DXC:H241	4:A:608:DXC:C23	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:HE3	1:A:239:TRP:O	2.02	0.42
1:A:135:THR:HB	1:A:139:PHE:HD2	1.79	0.42
1:A:239:TRP:C	1:A:239:TRP:CE3	2.92	0.42
1:A:369:GLU:HA	1:A:369:GLU:OE1	2.20	0.42
1:A:64:ILE:HG23	1:A:92:TYR:CZ	2.54	0.42
1:B:225:GLN:O	1:B:228:ALA:HB3	2.19	0.42
1:B:289:THR:HG22	1:B:295:PRO:CA	2.49	0.42
3:A:602:PJM:CAV	3:A:602:PJM:F5	2.57	0.42
1:A:63:TYR:OH	1:A:99:THR:HB	2.20	0.42
1:B:487:MET:HE1	3:B:602:PJM:CAO	2.50	0.42
1:A:246:PRO:HG3	4:A:610:DXC:C14	2.50	0.42
1:A:275:GLN:HG2	1:A:276:GLU:N	2.35	0.42
1:A:325:PHE:CE1	1:A:496:ILE:HD13	2.54	0.42
4:A:603:DXC:H161	4:A:603:DXC:H211	1.87	0.41
4:A:609:DXC:H82	4:A:609:DXC:H22	1.71	0.41
1:B:136:THR:N	1:B:137:PRO:CD	2.83	0.41
1:B:110:GLY:N	1:B:408:ASN:OD1	2.52	0.41
1:A:106:THR:OG1	1:A:399:HIS:ND1	2.40	0.41
1:A:174:ILE:HG23	1:A:208:HIS:CE1	2.56	0.41
1:A:177:LYS:HE2	1:A:181:GLU:OE2	2.21	0.41
1:B:358:LYS:HD2	1:B:358:LYS:N	2.36	0.41
1:B:190:GLY:O	1:B:498:TYR:CD1	2.73	0.41
4:A:606:DXC:C7	4:A:606:DXC:C6	2.96	0.41
4:A:607:DXC:H142	4:A:607:DXC:H51	1.81	0.40
1:B:352:LEU:HD21	1:B:464:SER:HB3	2.02	0.40
1:B:66:SER:HB2	1:B:72:GLY:HA3	2.00	0.40
1:A:189:SER:HB3	1:A:499:LYS:HA	2.03	0.40
1:A:63:TYR:HA	1:A:97:SER:O	2.21	0.40
1:B:176:GLU:HG3	1:B:177:LYS:N	2.36	0.40
1:B:226:LEU:O	1:B:229:ASP:HB2	2.22	0.40
1:B:154:GLU:OE1	1:B:290:TYR:HD1	2.04	0.40
1:B:71:LEU:HG	1:B:71:LEU:H	1.58	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	443/446 (99%)	424 (96%)	19 (4%)	0	100	100
1	B	442/446 (99%)	424 (96%)	18 (4%)	0	100	100
All	All	885/892 (99%)	848 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/390 (100%)	387 (100%)	2 (0%)	88	96
1	B	389/390 (100%)	386 (99%)	3 (1%)	81	94
All	All	778/780 (100%)	773 (99%)	5 (1%)	86	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ASP
1	A	413	ASP
1	B	71	LEU
1	B	360	LEU
1	B	476	ASP

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

Mol	Chain	Res	Type
1	A	489	HIS
1	B	73	HIS
1	B	269	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 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$
4	DXC	A	606	-	28,31,31	0.95	1 (3%)	46,49,49	2.62	16 (34%)
4	DXC	A	610	-	28,31,31	0.96	2 (7%)	46,49,49	2.15	18 (39%)
2	HEM	B	601	1,3	27,50,50	0.86	2 (7%)	17,82,82	1.15	0
3	PJM	B	602	2	46,55,55	2.70	9 (19%)	67,78,78	1.75	9 (13%)
4	DXC	A	607	-	28,31,31	0.89	2 (7%)	46,49,49	2.76	18 (39%)
3	PJM	A	602	2	46,55,55	2.73	9 (19%)	67,78,78	1.75	11 (16%)
4	DXC	A	608	-	28,31,31	1.06	3 (10%)	46,49,49	2.25	13 (28%)
4	DXC	A	603	-	28,31,31	0.84	1 (3%)	46,49,49	2.48	20 (43%)
2	HEM	A	601	1,3	27,50,50	0.87	2 (7%)	17,82,82	1.14	1 (5%)
4	DXC	A	604	-	28,31,31	0.80	1 (3%)	46,49,49	2.24	16 (34%)
4	DXC	A	609	-	28,31,31	0.96	1 (3%)	46,49,49	2.83	21 (45%)
3	PJM	A	611	-	46,55,55	3.19	9 (19%)	67,78,78	1.97	15 (22%)
4	DXC	A	605	-	28,31,31	0.86	1 (3%)	46,49,49	2.30	19 (41%)

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
4	DXC	A	606	-	1/1/11/11	7/7/71/71	1/4/4/4
4	DXC	A	610	-	1/1/11/11	7/7/71/71	1/4/4/4
2	HEM	B	601	1,3	-	0/6/54/54	-
3	PJM	B	602	2	-	5/28/32/32	0/7/7/7
4	DXC	A	607	-	1/1/11/11	1/7/71/71	1/4/4/4
3	PJM	A	602	2	-	5/28/32/32	0/7/7/7
4	DXC	A	608	-	1/1/11/11	7/7/71/71	1/4/4/4
4	DXC	A	603	-	1/1/11/11	6/7/71/71	0/4/4/4
2	HEM	A	601	1,3	-	0/6/54/54	-
4	DXC	A	604	-	1/1/11/11	3/7/71/71	0/4/4/4
4	DXC	A	609	-	1/1/11/11	2/7/71/71	1/4/4/4
3	PJM	A	611	-	-	13/28/32/32	0/7/7/7
4	DXC	A	605	-	1/1/11/11	0/7/71/71	1/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	PJM	NBC-NBD	-15.34	1.07	1.37
3	A	602	PJM	NBC-NBD	-10.44	1.17	1.37
3	B	602	PJM	NBC-NBD	-9.66	1.18	1.37
3	A	611	PJM	CBQ-C4	-9.26	1.38	1.49
3	B	602	PJM	CBR-CBV	-8.81	1.38	1.52
3	A	602	PJM	CBR-CBV	-8.58	1.38	1.52
3	B	602	PJM	CBQ-C4	-8.49	1.39	1.49
3	A	602	PJM	CBQ-C4	-8.32	1.39	1.49
3	A	611	PJM	CBR-CBV	-7.48	1.40	1.52
3	A	611	PJM	CBL-CBG	-5.52	1.38	1.50
3	B	602	PJM	CBL-CBG	-5.31	1.39	1.50
3	A	602	PJM	CBL-CBG	-5.19	1.39	1.50
3	A	602	PJM	CBM-CBO	-4.18	1.38	1.49
3	B	602	PJM	CBM-CBO	-4.12	1.38	1.49
3	A	611	PJM	CBM-CBO	-3.69	1.39	1.49
3	B	602	PJM	C2-N3	3.45	1.40	1.33
3	A	602	PJM	C2-N3	3.44	1.40	1.33
3	B	602	PJM	C2-N1	3.42	1.40	1.33
3	A	611	PJM	C2-N1	3.42	1.40	1.33
3	A	602	PJM	C2-N1	3.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	PJM	C2-N3	3.31	1.40	1.33
4	A	608	DXC	C12-C11	-3.02	1.50	1.55
4	A	609	DXC	C12-C11	-2.80	1.50	1.55
3	B	602	PJM	C6-N1	2.80	1.40	1.34
3	A	611	PJM	C6-N1	2.77	1.40	1.34
3	A	602	PJM	C6-N1	2.76	1.40	1.34
2	A	601	HEM	C3B-C2B	-2.66	1.36	1.40
4	A	606	DXC	C12-C11	-2.66	1.51	1.55
4	A	607	DXC	C12-C11	-2.62	1.51	1.55
4	A	610	DXC	C12-C11	-2.54	1.51	1.55
2	B	601	HEM	C3B-C2B	-2.53	1.36	1.40
4	A	605	DXC	C12-C11	-2.41	1.51	1.55
3	A	602	PJM	CAR-NBW	-2.35	1.33	1.37
4	A	610	DXC	C4-C3	-2.34	1.51	1.55
4	A	604	DXC	C12-C11	-2.33	1.51	1.55
3	B	602	PJM	CAR-NBW	-2.30	1.33	1.37
4	A	608	DXC	C12-C17	-2.29	1.51	1.55
4	A	607	DXC	C8-C9	-2.24	1.49	1.53
3	A	611	PJM	CAR-NBW	-2.22	1.33	1.37
4	A	608	DXC	C12-C13	-2.21	1.51	1.54
4	A	603	DXC	C12-C11	-2.19	1.51	1.55
2	A	601	HEM	C4D-C3D	2.06	1.47	1.42
2	B	601	HEM	C4D-C3D	2.05	1.47	1.42

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	609	DXC	C14-C10-C4	-8.85	104.60	113.73
4	A	608	DXC	C12-C17-C19	-8.45	109.41	119.50
4	A	607	DXC	C12-C17-C19	-8.43	109.43	119.50
3	A	611	PJM	N1-C2-N3	-7.66	119.28	127.70
4	A	606	DXC	C14-C10-C4	-7.57	105.92	113.73
3	B	602	PJM	N1-C2-N3	-7.43	119.53	127.70
3	A	602	PJM	N1-C2-N3	-7.01	119.99	127.70
4	A	607	DXC	C10-C4-C3	6.22	117.32	108.58
4	A	608	DXC	C12-C11-C9	-6.17	107.90	114.71
4	A	610	DXC	C17-C12-C11	-6.02	94.03	100.09
4	A	607	DXC	C22-C21-C19	-5.99	106.66	114.72
4	A	606	DXC	C17-C12-C13	-5.87	112.31	117.67
4	A	603	DXC	C10-C4-C3	5.75	116.65	108.58
4	A	609	DXC	C10-C4-C3	5.74	116.64	108.58
4	A	604	DXC	C12-C17-C19	-5.70	112.69	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	DXC	C12-C17-C19	-5.58	112.83	119.50
3	A	611	PJM	CAO-CBN-CBS	-5.57	111.94	120.44
4	A	607	DXC	C14-C10-C4	-5.33	108.23	113.73
4	A	606	DXC	C10-C4-C3	5.31	116.03	108.58
4	A	605	DXC	C12-C17-C19	-5.09	113.42	119.50
4	A	609	DXC	C15-C11-C9	-5.02	110.81	119.08
4	A	605	DXC	C10-C4-C3	4.94	115.52	108.58
4	A	606	DXC	C22-C21-C19	-4.79	108.27	114.72
4	A	607	DXC	C4-C10-C9	4.75	117.42	112.42
4	A	603	DXC	C12-C17-C19	-4.66	113.93	119.50
4	A	604	DXC	C10-C4-C3	4.64	115.10	108.58
3	B	602	PJM	CAQ-CBR-CBK	4.63	121.42	116.81
4	A	603	DXC	C4-C10-C9	4.57	117.22	112.42
4	A	609	DXC	C4-C10-C9	4.55	117.20	112.42
4	A	603	DXC	C14-C10-C4	-4.51	109.08	113.73
4	A	605	DXC	C17-C12-C13	-4.50	113.55	117.67
4	A	609	DXC	C10-C14-C13	4.37	120.07	114.30
4	A	607	DXC	C17-C12-C13	-4.30	113.74	117.67
4	A	603	DXC	C17-C12-C13	-4.28	113.75	117.67
4	A	607	DXC	C12-C11-C9	-4.26	110.01	114.71
4	A	607	DXC	C7-C8-C9	-4.25	105.14	112.14
4	A	605	DXC	C15-C11-C9	-4.19	112.18	119.08
4	A	604	DXC	C15-C11-C9	-4.18	112.19	119.08
3	A	602	PJM	CAQ-CBR-CBK	4.18	120.97	116.81
4	A	608	DXC	C17-C12-C13	-4.16	113.87	117.67
4	A	609	DXC	C17-C12-C13	-4.15	113.88	117.67
4	A	609	DXC	C8-C9-C11	-4.14	105.01	112.08
4	A	603	DXC	C15-C11-C9	-4.12	112.30	119.08
4	A	606	DXC	C8-C9-C11	-4.11	105.06	112.08
4	A	610	DXC	C2-C3-C4	-4.08	108.32	112.66
4	A	603	DXC	C7-C8-C9	-4.00	105.55	112.14
4	A	610	DXC	C15-C11-C12	-3.97	99.66	103.55
3	B	602	PJM	CBV-NBE-CBG	-3.95	117.25	122.34
4	A	610	DXC	C14-C10-C4	-3.94	109.66	113.73
4	A	610	DXC	C12-C17-C19	-3.93	114.80	119.50
4	A	609	DXC	C7-C8-C9	-3.91	105.70	112.14
4	A	603	DXC	C5-C4-C10	-3.89	105.23	111.35
4	A	604	DXC	C7-C8-C9	-3.87	105.76	112.14
4	A	603	DXC	C2-C3-C4	-3.86	108.55	112.66
4	A	603	DXC	C3-C2-C1	-3.83	107.14	112.76
3	A	602	PJM	CBV-NBE-CBG	-3.81	117.43	122.34
4	A	604	DXC	C2-C1-C6	-3.79	106.03	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	DXC	C2-C3-C4	-3.75	108.67	112.66
4	A	605	DXC	C7-C8-C9	-3.71	106.02	112.14
4	A	607	DXC	C15-C11-C9	-3.70	112.99	119.08
4	A	606	DXC	C15-C11-C9	-3.69	113.00	119.08
4	A	609	DXC	C11-C9-C10	3.65	113.98	109.09
4	A	609	DXC	C2-C3-C4	-3.64	108.79	112.66
4	A	604	DXC	C10-C14-C13	-3.63	109.50	114.30
4	A	606	DXC	C20-C12-C13	3.54	112.67	109.07
4	A	609	DXC	C8-C7-C3	-3.54	104.74	111.84
4	A	605	DXC	C8-C9-C11	-3.52	106.07	112.08
3	A	611	PJM	CAU-CBI-CAV	-3.49	119.11	123.52
4	A	608	DXC	C15-C11-C9	-3.49	113.33	119.08
4	A	604	DXC	C17-C12-C13	-3.45	114.52	117.67
4	A	610	DXC	C12-C11-C9	-3.44	110.92	114.71
4	A	608	DXC	C14-C10-C4	-3.43	110.19	113.73
4	A	604	DXC	C18-C4-C10	-3.42	106.47	111.18
4	A	605	DXC	C14-C10-C4	-3.40	110.22	113.73
4	A	609	DXC	C14-C10-C9	3.40	116.33	110.82
4	A	605	DXC	C3-C2-C1	-3.36	107.83	112.76
4	A	610	DXC	C8-C9-C10	3.33	114.62	110.49
4	A	606	DXC	C5-C6-C1	-3.31	106.22	110.47
3	A	611	PJM	CBL-CBG-NBE	-3.30	110.74	117.06
4	A	609	DXC	C12-C17-C19	-3.30	115.56	119.50
4	A	610	DXC	C16-C17-C12	-3.25	100.36	103.55
4	A	604	DXC	C12-C11-C9	-3.24	111.14	114.71
4	A	605	DXC	C4-C10-C9	3.23	115.81	112.42
4	A	606	DXC	C18-C4-C10	-3.16	106.82	111.18
4	A	607	DXC	C2-C3-C4	-3.14	109.32	112.66
3	A	602	PJM	CAY-NBW-CAT	-3.11	119.63	125.76
4	A	609	DXC	C21-C22-C23	-3.10	106.94	113.59
4	A	605	DXC	C22-C21-C19	-3.09	110.56	114.72
3	A	611	PJM	CAU-CBP-CAX	3.08	122.87	118.31
4	A	608	DXC	C21-C22-C23	-3.06	107.02	113.59
4	A	605	DXC	C21-C22-C23	-3.05	107.03	113.59
4	A	606	DXC	C2-C3-C4	-3.04	109.43	112.66
4	A	604	DXC	C8-C9-C11	-3.03	106.91	112.08
4	A	603	DXC	C8-C9-C11	-3.01	106.94	112.08
3	A	611	PJM	C6-N1-C2	3.00	119.64	115.80
4	A	606	DXC	C21-C22-C23	-3.00	107.15	113.59
3	A	602	PJM	CAY-NBW-CAR	2.99	132.08	125.92
4	A	608	DXC	C14-C10-C9	2.95	115.60	110.82
4	A	607	DXC	C8-C9-C11	-2.94	107.07	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	611	PJM	CAN-CBN-CAO	2.93	123.43	117.59
3	A	611	PJM	CAX-CBP-CBT	-2.93	115.77	120.06
4	A	609	DXC	C3-C2-C1	-2.87	108.54	112.76
4	A	605	DXC	C12-C11-C9	-2.87	111.54	114.71
4	A	610	DXC	C24-C19-C17	-2.87	108.53	112.92
4	A	604	DXC	C5-C6-C1	-2.87	106.79	110.47
4	A	604	DXC	C8-C7-C3	-2.86	106.11	111.84
4	A	609	DXC	C5-C4-C10	-2.85	106.88	111.35
4	A	610	DXC	C21-C22-C23	-2.84	107.49	113.59
4	A	608	DXC	C22-C21-C19	-2.81	110.94	114.72
4	A	603	DXC	C6-C5-C4	2.79	117.57	112.78
3	A	602	PJM	CAU-CBI-CAV	-2.74	120.06	123.52
4	A	603	DXC	C12-C11-C9	-2.69	111.74	114.71
3	B	602	PJM	CAU-CBI-CAV	-2.68	120.13	123.52
3	A	611	PJM	CAJ-CBL-CAK	2.68	122.40	118.59
4	A	605	DXC	C20-C12-C13	2.68	111.79	109.07
3	A	611	PJM	CBN-CBS-NBC	-2.67	119.60	124.12
4	A	609	DXC	C20-C12-C13	2.62	111.73	109.07
4	A	608	DXC	C24-C19-C17	-2.58	108.98	112.92
4	A	609	DXC	C18-C4-C10	-2.55	107.67	111.18
4	A	605	DXC	C8-C7-C3	-2.54	106.75	111.84
3	A	602	PJM	CBK-CBR-CBV	-2.54	118.46	121.71
4	A	607	DXC	C17-C12-C11	2.53	102.64	100.09
4	A	610	DXC	C22-C21-C19	-2.52	111.33	114.72
4	A	604	DXC	C3-C2-C1	-2.51	109.07	112.76
3	A	611	PJM	CAK-CBL-CBG	-2.50	112.51	120.62
4	A	607	DXC	C8-C7-C3	-2.50	106.82	111.84
3	A	611	PJM	CAN-CBN-CBS	2.50	124.25	120.44
4	A	606	DXC	C7-C3-C4	2.49	116.77	112.31
4	A	603	DXC	C21-C22-C23	-2.46	108.31	113.59
4	A	603	DXC	C18-C4-C10	-2.46	107.80	111.18
4	A	603	DXC	C8-C9-C10	2.45	113.53	110.49
3	A	602	PJM	CAP-CBO-CAW	2.45	121.62	118.16
3	B	602	PJM	CAW-CBK-CBR	-2.44	119.50	122.41
3	A	611	PJM	CBP-CAX-CBQ	-2.43	117.47	121.31
3	B	602	PJM	C6-N1-C2	2.41	118.88	115.80
4	A	610	DXC	C14-C13-C12	-2.41	108.77	111.24
4	A	610	DXC	C20-C12-C13	2.40	111.51	109.07
4	A	605	DXC	C18-C4-C10	-2.39	107.88	111.18
4	A	606	DXC	C12-C11-C9	-2.39	112.07	114.71
4	A	608	DXC	C20-C12-C13	2.38	111.49	109.07
3	A	611	PJM	CAI-CBH-CAH	-2.38	119.67	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	PJM	CAP-CBO-CAW	2.38	121.52	118.16
4	A	610	DXC	C10-C14-C13	-2.37	111.17	114.30
4	A	606	DXC	C11-C12-C13	2.37	109.61	107.40
4	A	606	DXC	C2-C3-C7	-2.36	107.41	111.74
4	A	609	DXC	C8-C9-C10	2.34	113.39	110.49
4	A	607	DXC	C3-C2-C1	-2.33	109.33	112.76
4	A	607	DXC	C20-C12-C13	2.33	111.44	109.07
2	A	601	HEM	CAD-CBD-CGD	-2.33	108.76	112.67
4	A	609	DXC	C16-C17-C19	-2.31	108.58	112.15
3	A	611	PJM	CAJ-CAN-CBN	-2.30	117.82	121.13
4	A	603	DXC	C16-C17-C19	-2.28	108.61	112.15
3	A	602	PJM	C6-N1-C2	2.25	118.68	115.80
3	B	602	PJM	CAO-CBN-CBS	-2.25	117.00	120.44
3	B	602	PJM	C2-N3-C4	2.25	121.28	117.78
4	A	605	DXC	C8-C9-C10	2.24	113.28	110.49
4	A	610	DXC	C18-C4-C10	-2.23	108.11	111.18
4	A	609	DXC	C22-C21-C19	-2.22	111.73	114.72
4	A	608	DXC	C18-C4-C10	-2.22	108.13	111.18
4	A	605	DXC	C10-C14-C13	-2.20	111.40	114.30
4	A	607	DXC	C24-C19-C17	-2.19	109.57	112.92
4	A	604	DXC	C21-C22-C23	-2.18	108.90	113.59
4	A	610	DXC	C8-C9-C11	-2.17	108.38	112.08
4	A	608	DXC	C5-C4-C3	2.15	110.95	107.77
4	A	603	DXC	C8-C7-C3	-2.15	107.53	111.84
3	A	602	PJM	CAY-CBV-NBE	-2.14	106.72	110.45
4	A	607	DXC	C18-C4-C10	-2.13	108.25	111.18
4	A	603	DXC	C24-C19-C17	-2.13	109.66	112.92
4	A	605	DXC	C16-C17-C19	-2.11	108.88	112.15
4	A	610	DXC	C11-C9-C10	-2.10	106.28	109.09
4	A	610	DXC	C16-C15-C11	-2.10	100.97	105.13
3	A	602	PJM	C2-N3-C4	2.09	121.04	117.78
4	A	604	DXC	C16-C17-C19	-2.08	108.93	112.15
4	A	603	DXC	C10-C14-C13	-2.05	111.59	114.30
4	A	607	DXC	C5-C4-C10	-2.05	108.14	111.35
4	A	604	DXC	C5-C4-C3	2.04	110.79	107.77
4	A	608	DXC	C16-C17-C12	-2.03	101.56	103.55

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	606	DXC	C10
4	A	610	DXC	C10

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Mol	Chain	Res	Type	Atom
4	A	607	DXC	C10
4	A	608	DXC	C10
4	A	603	DXC	C10
4	A	604	DXC	C10
4	A	609	DXC	C10
4	A	605	DXC	C10

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	PJM	CBR-CBV-NBE-CBG
4	A	608	DXC	C12-C17-C19-C24
3	A	611	PJM	CAY-CBV-NBE-CBG
4	A	606	DXC	C16-C17-C19-C24
4	A	606	DXC	C12-C17-C19-C24
4	A	606	DXC	C16-C17-C19-C21
4	A	608	DXC	C12-C17-C19-C21
4	A	610	DXC	C24-C19-C21-C22
4	A	608	DXC	C24-C19-C21-C22
4	A	608	DXC	C16-C17-C19-C24
4	A	606	DXC	C12-C17-C19-C21
4	A	608	DXC	C16-C17-C19-C21
4	A	604	DXC	C24-C19-C21-C22
4	A	610	DXC	C12-C17-C19-C24
4	A	608	DXC	C17-C19-C21-C22
4	A	603	DXC	C24-C19-C21-C22
4	A	606	DXC	C17-C19-C21-C22
4	A	610	DXC	C17-C19-C21-C22
4	A	604	DXC	C17-C19-C21-C22
4	A	607	DXC	C19-C21-C22-C23
4	A	606	DXC	C24-C19-C21-C22
4	A	603	DXC	C12-C17-C19-C24
4	A	610	DXC	C12-C17-C19-C21
3	A	611	PJM	CAN-CBN-CBS-NBC
4	A	606	DXC	C19-C21-C22-C23
4	A	610	DXC	C19-C21-C22-C23
4	A	604	DXC	C19-C21-C22-C23
4	A	609	DXC	C16-C17-C19-C21
3	A	602	PJM	CBR-CBV-NBE-CBG
3	A	611	PJM	CAO-CBN-CBS-NBC
4	A	603	DXC	C12-C17-C19-C21
3	A	611	PJM	C5-C4-CBQ-CAX

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Mol	Chain	Res	Type	Atoms
3	B	602	PJM	N3-C4-CBQ-CAV
4	A	608	DXC	C19-C21-C22-C23
3	B	602	PJM	C5-C4-CBQ-CAV
3	A	611	PJM	C5-C4-CBQ-CAV
3	B	602	PJM	N3-C4-CBQ-CAX
3	A	602	PJM	N3-C4-CBQ-CAV
3	A	611	PJM	N3-C4-CBQ-CAX
3	A	602	PJM	N3-C4-CBQ-CAX
4	A	610	DXC	C16-C17-C19-C24
4	A	603	DXC	C16-C17-C19-C24
3	B	602	PJM	C5-C4-CBQ-CAX
3	A	611	PJM	CAQ-CBR-CBV-CAY
3	A	602	PJM	C5-C4-CBQ-CAV
4	A	603	DXC	C16-C17-C19-C21
4	A	610	DXC	C16-C17-C19-C21
3	A	611	PJM	OAA-CBG-CBL-CAJ
4	A	603	DXC	C19-C21-C22-C23
3	A	611	PJM	CBV-CAY-NBW-CAT
3	A	602	PJM	C5-C4-CBQ-CAX
3	A	611	PJM	N3-C4-CBQ-CAV
3	A	611	PJM	CBK-CBR-CBV-CAY
3	A	611	PJM	CAU-CBP-CBT-NBD
4	A	609	DXC	C16-C17-C19-C24
3	A	611	PJM	CBV-CAY-NBW-CAR

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	DXC	C1-C2-C3-C4-C5-C6
4	A	610	DXC	C1-C2-C3-C4-C5-C6
4	A	606	DXC	C1-C2-C3-C4-C5-C6
4	A	608	DXC	C1-C2-C3-C4-C5-C6
4	A	605	DXC	C1-C2-C3-C4-C5-C6
4	A	607	DXC	C1-C2-C3-C4-C5-C6

13 monomers are involved in 107 short contacts:

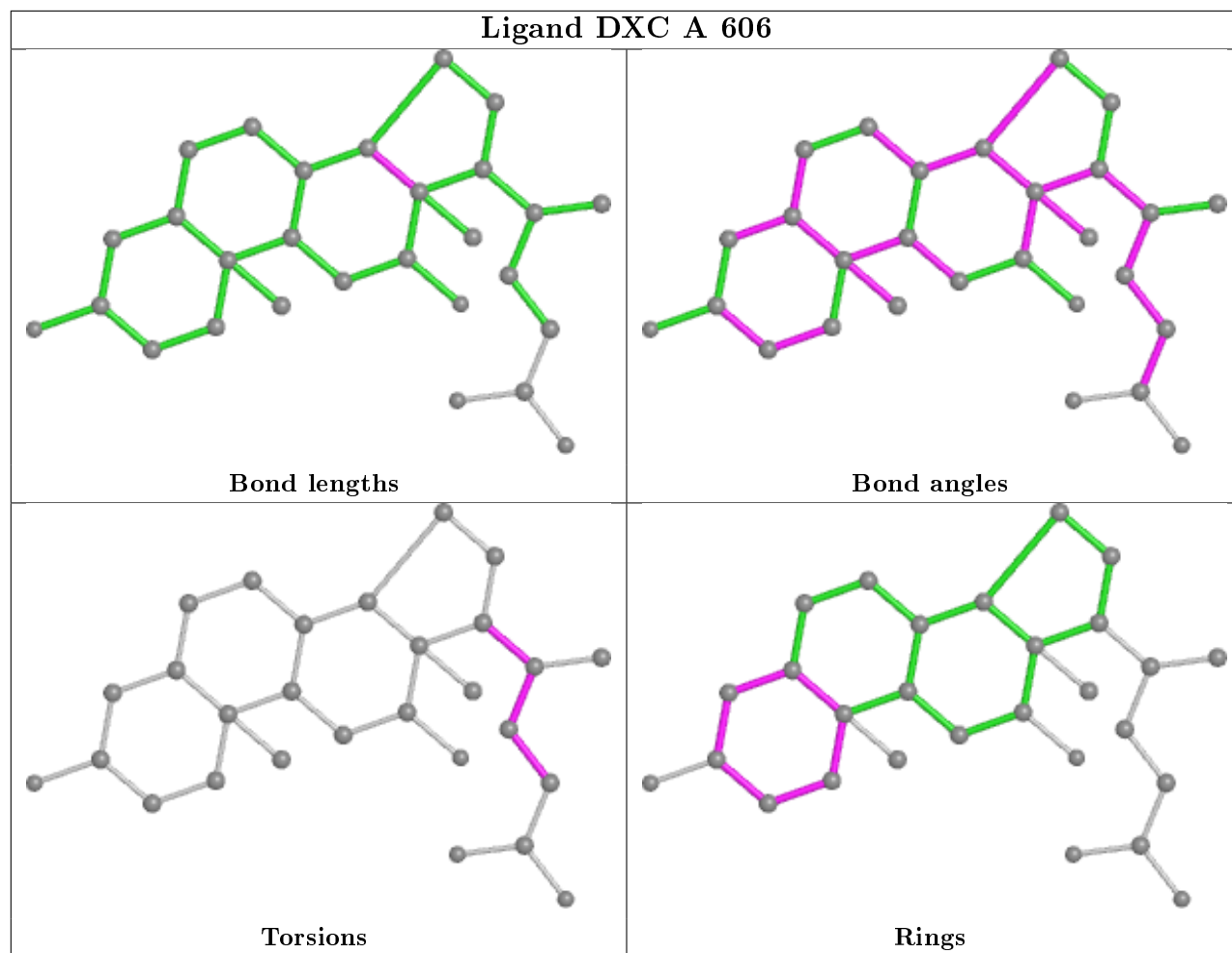
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	DXC	17	0
4	A	610	DXC	19	0
2	B	601	HEM	7	0
3	B	602	PJM	8	0

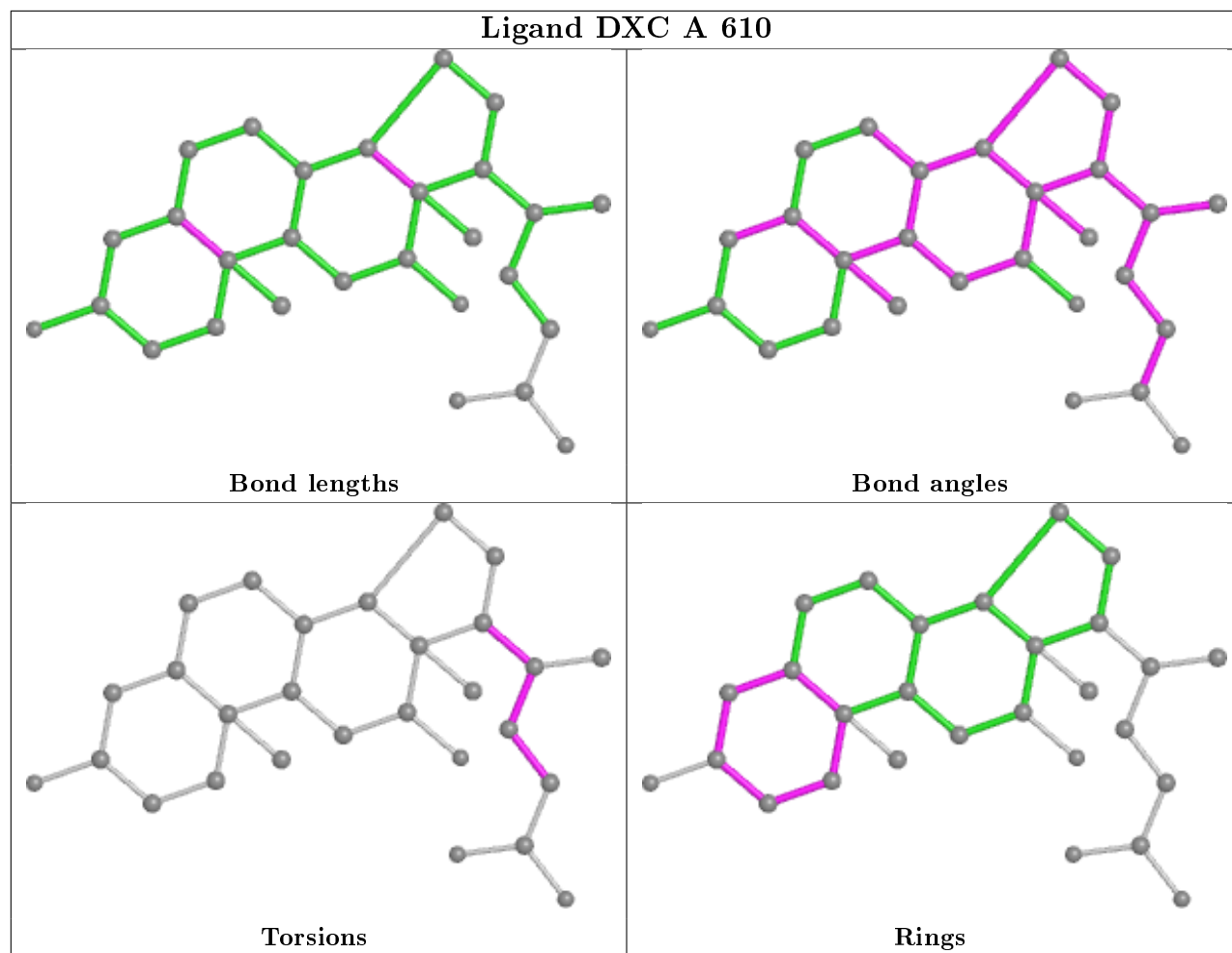
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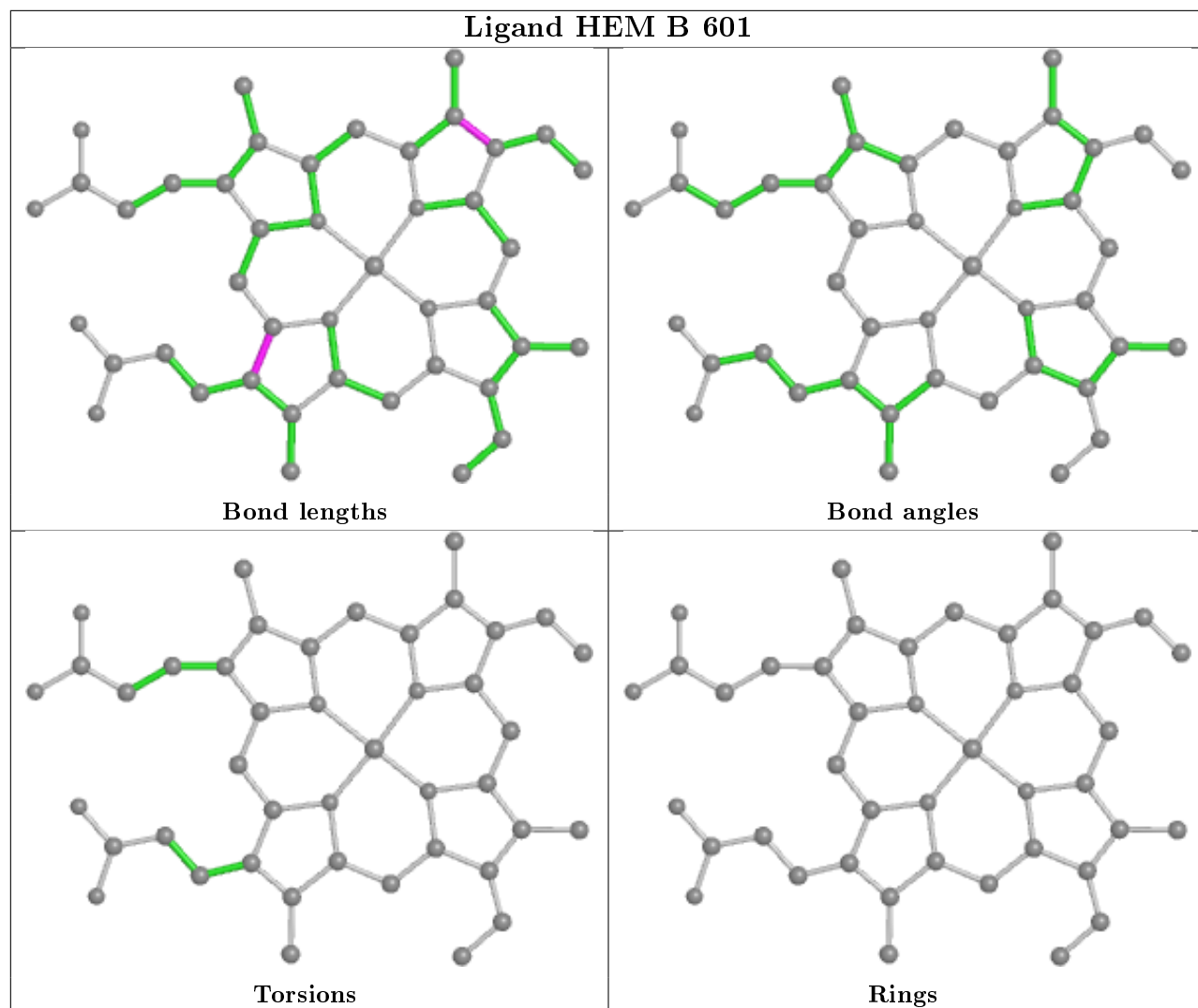
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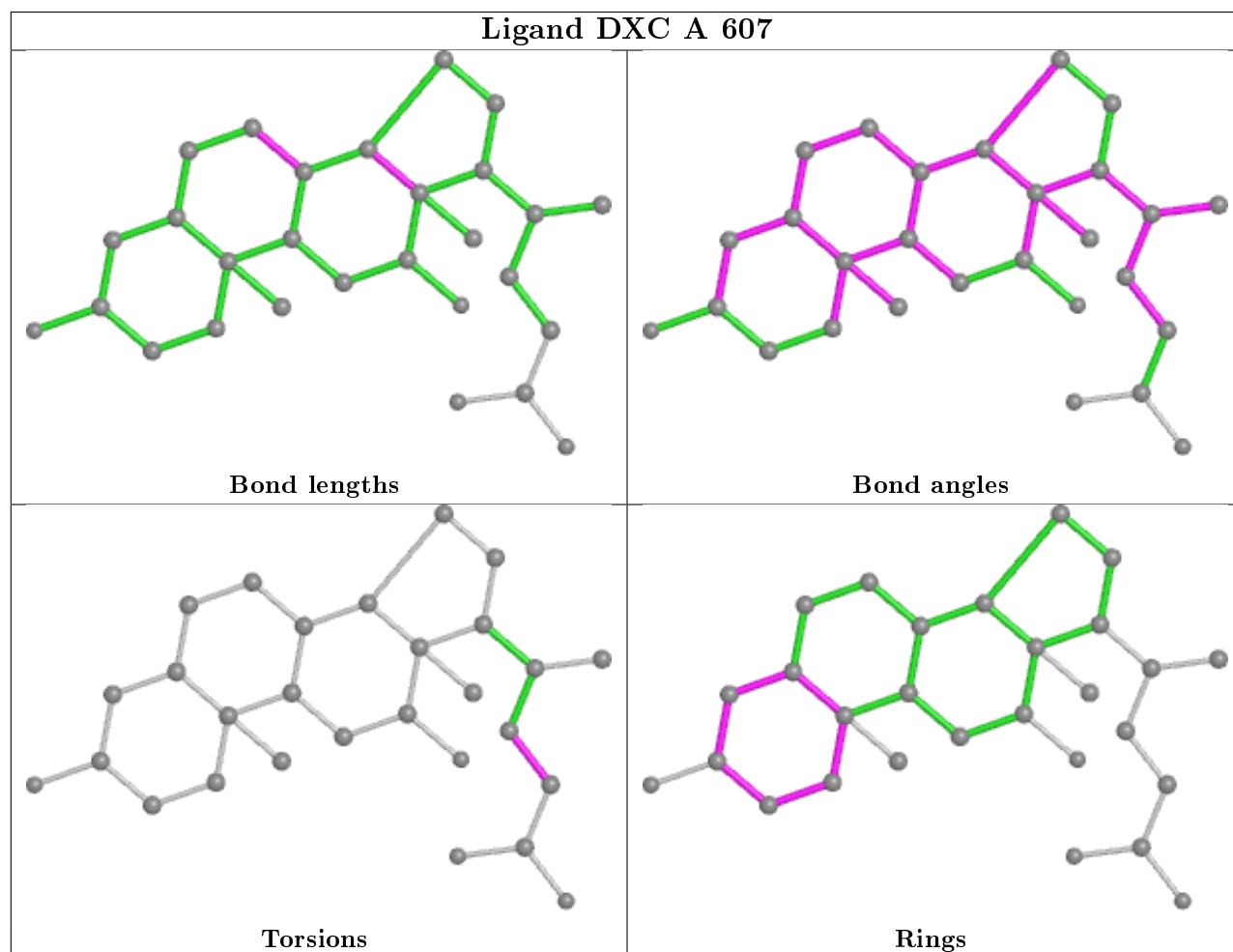
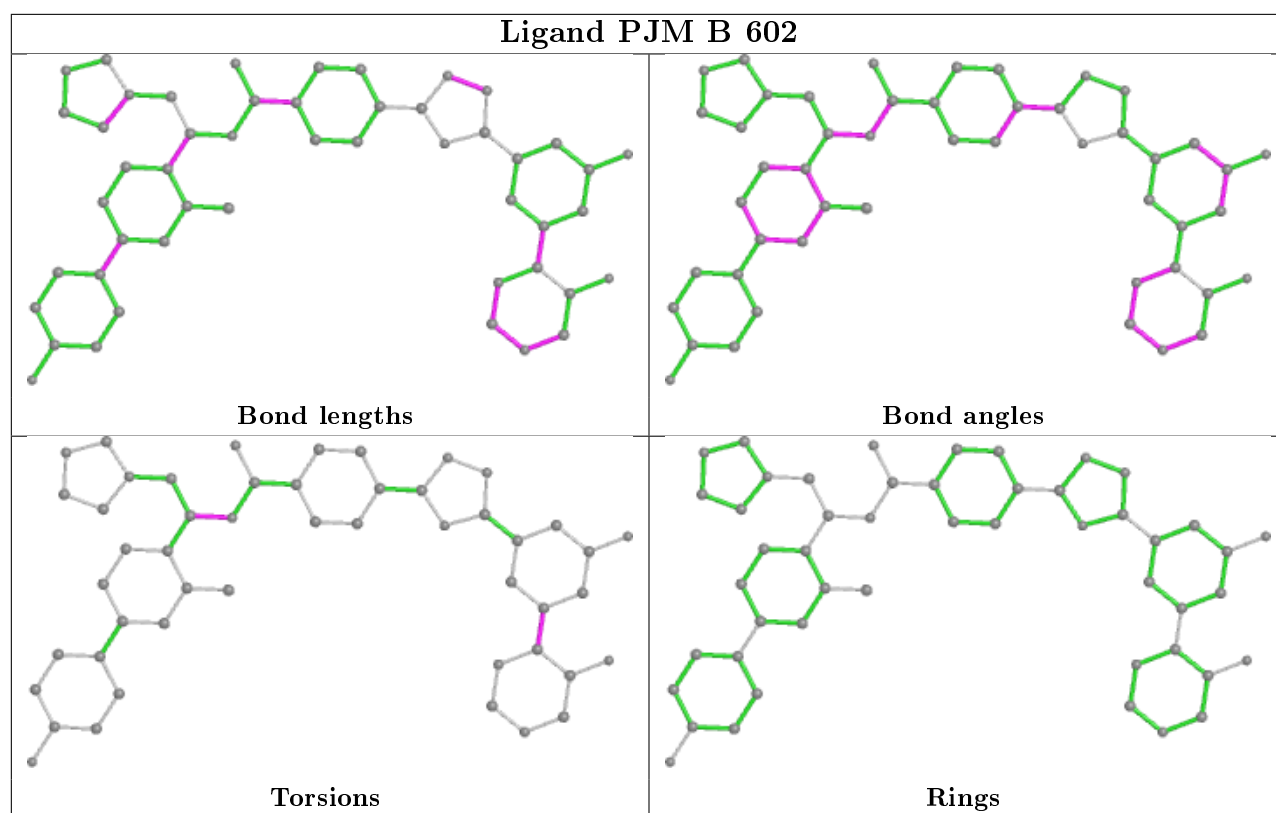
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	DXC	8	0
3	A	602	PJM	11	0
4	A	608	DXC	14	0
4	A	603	DXC	4	0
2	A	601	HEM	6	0
4	A	604	DXC	11	0
4	A	609	DXC	4	0
3	A	611	PJM	2	0
4	A	605	DXC	3	0

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.

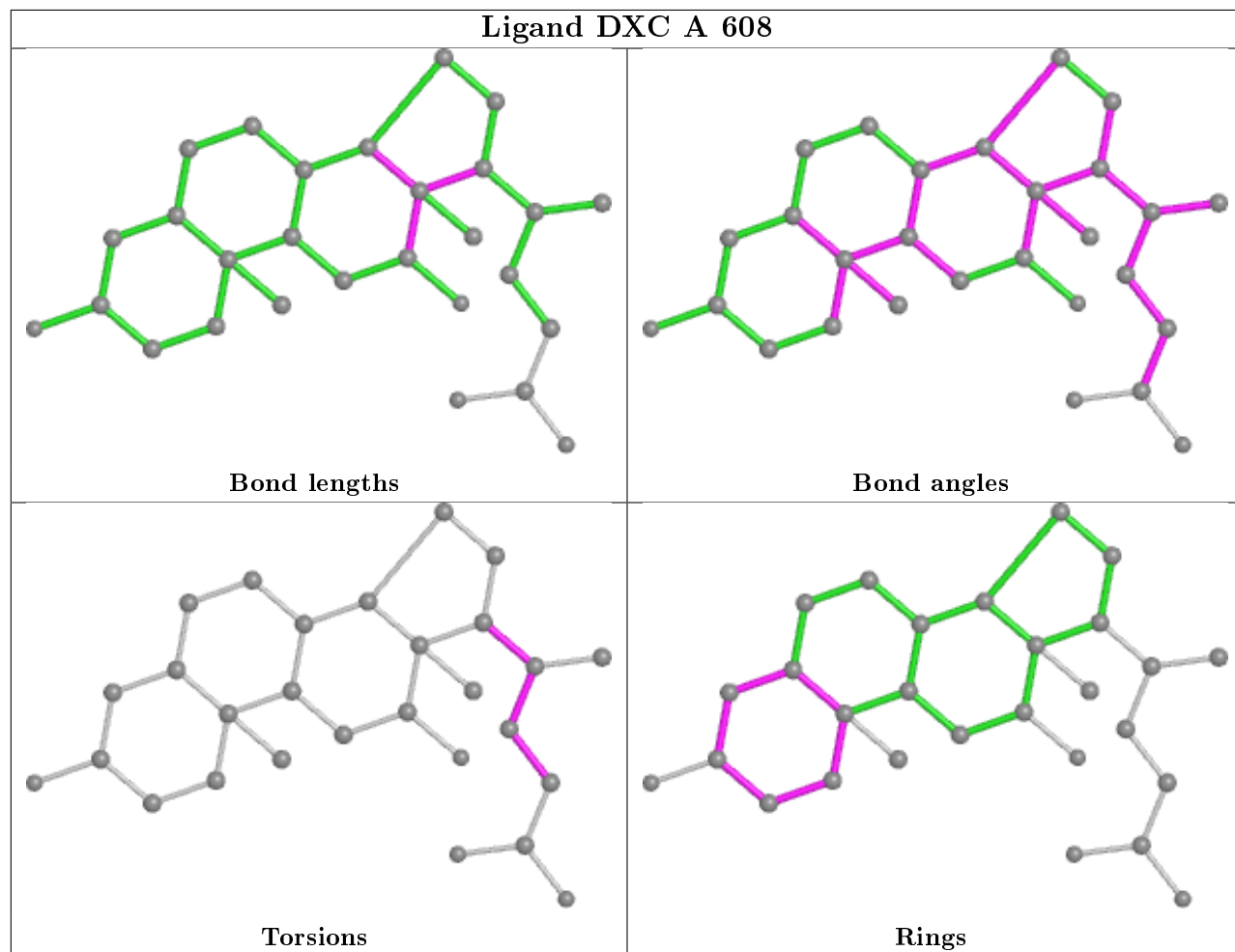
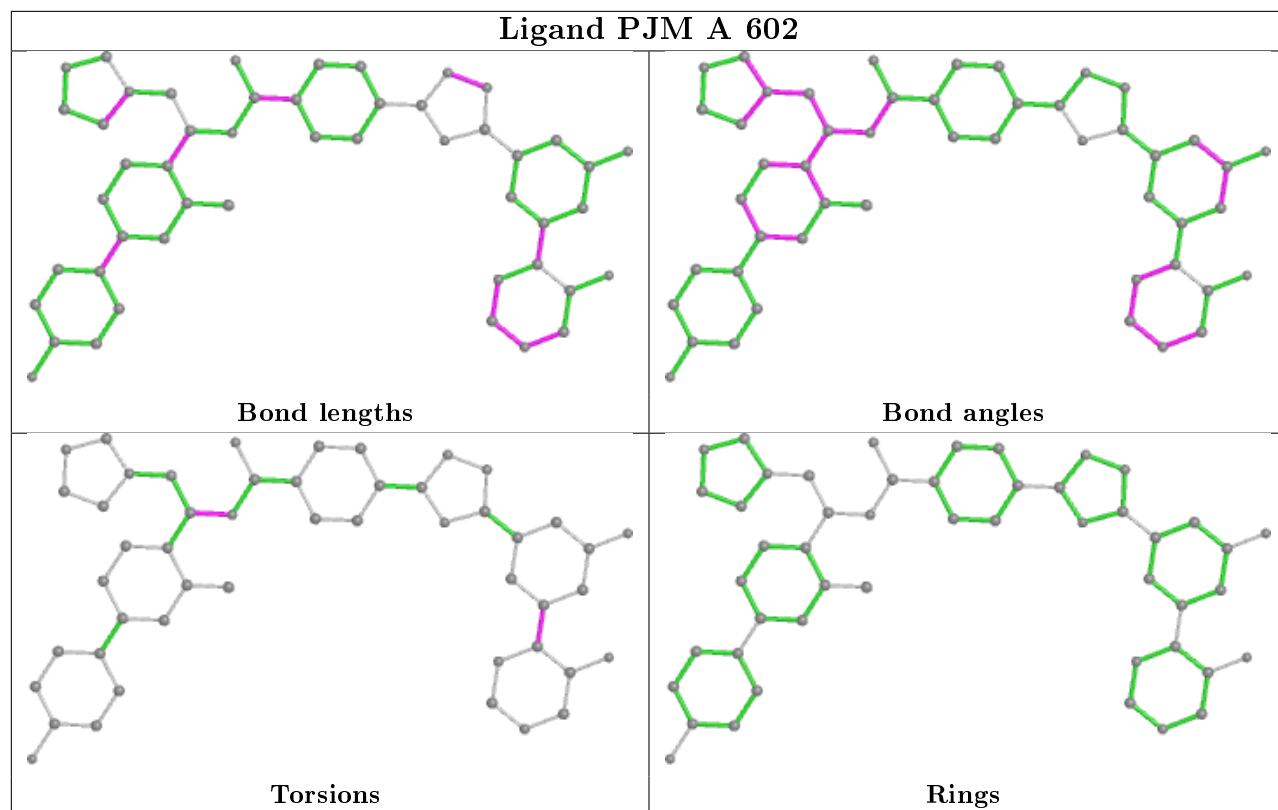


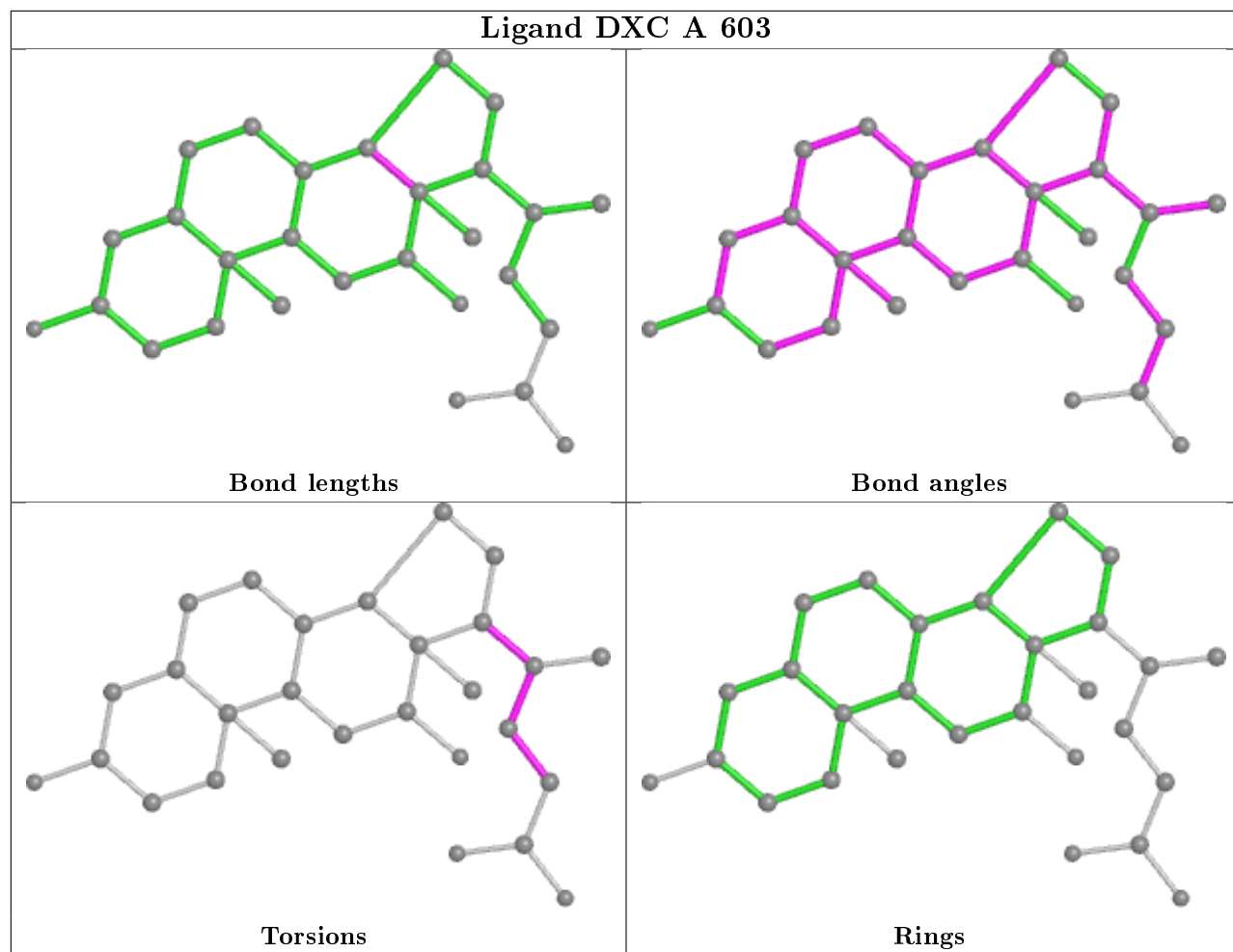


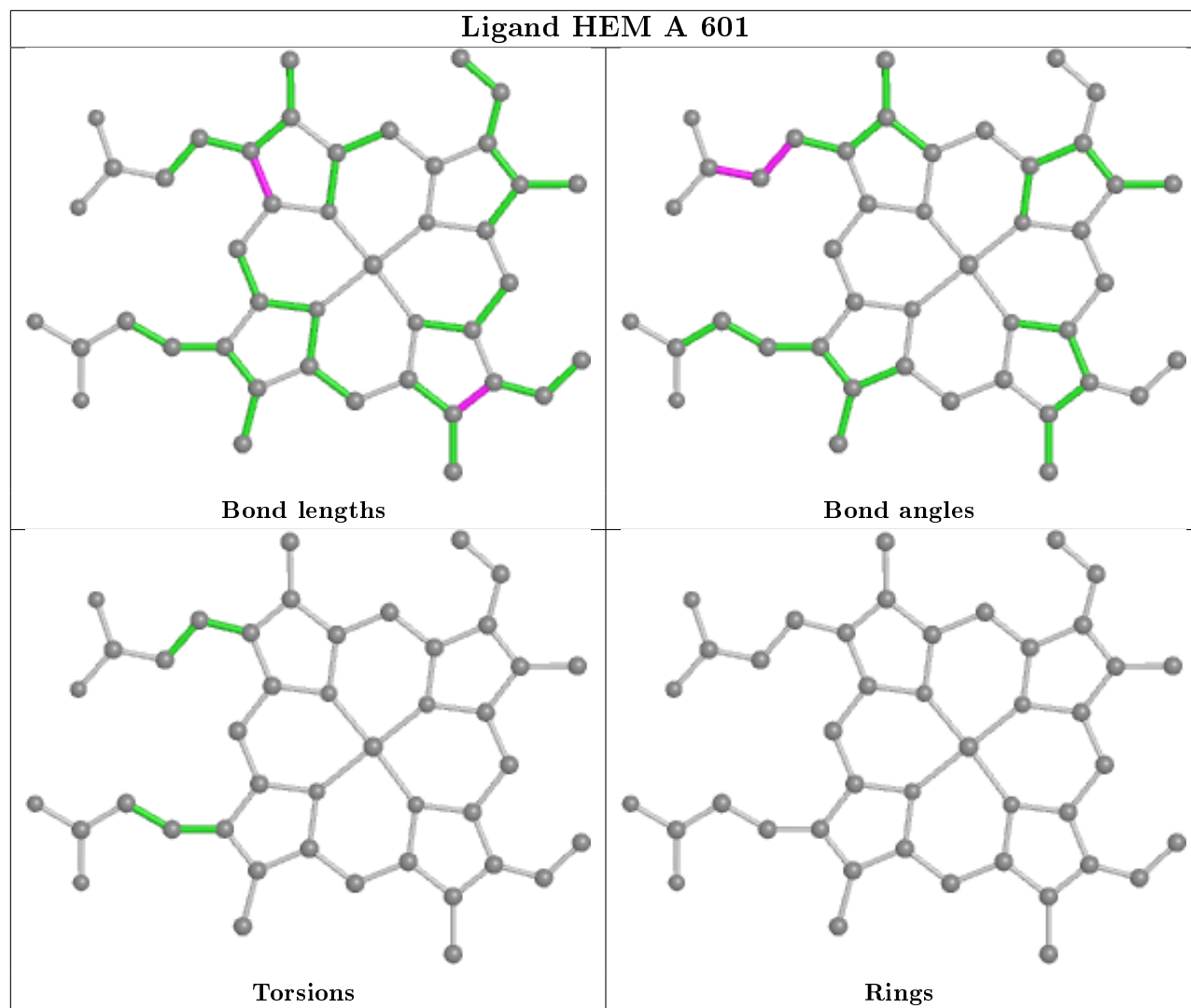


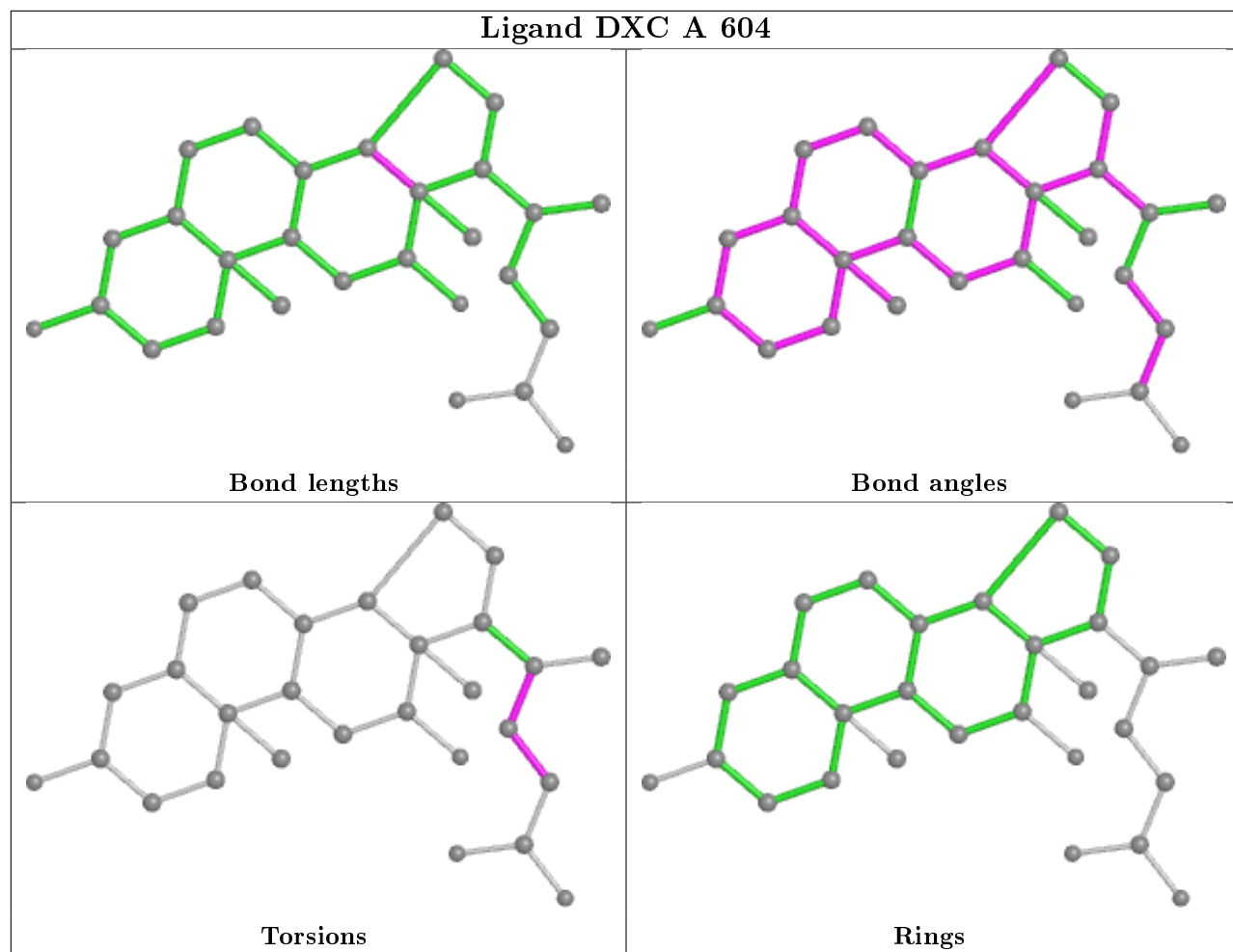


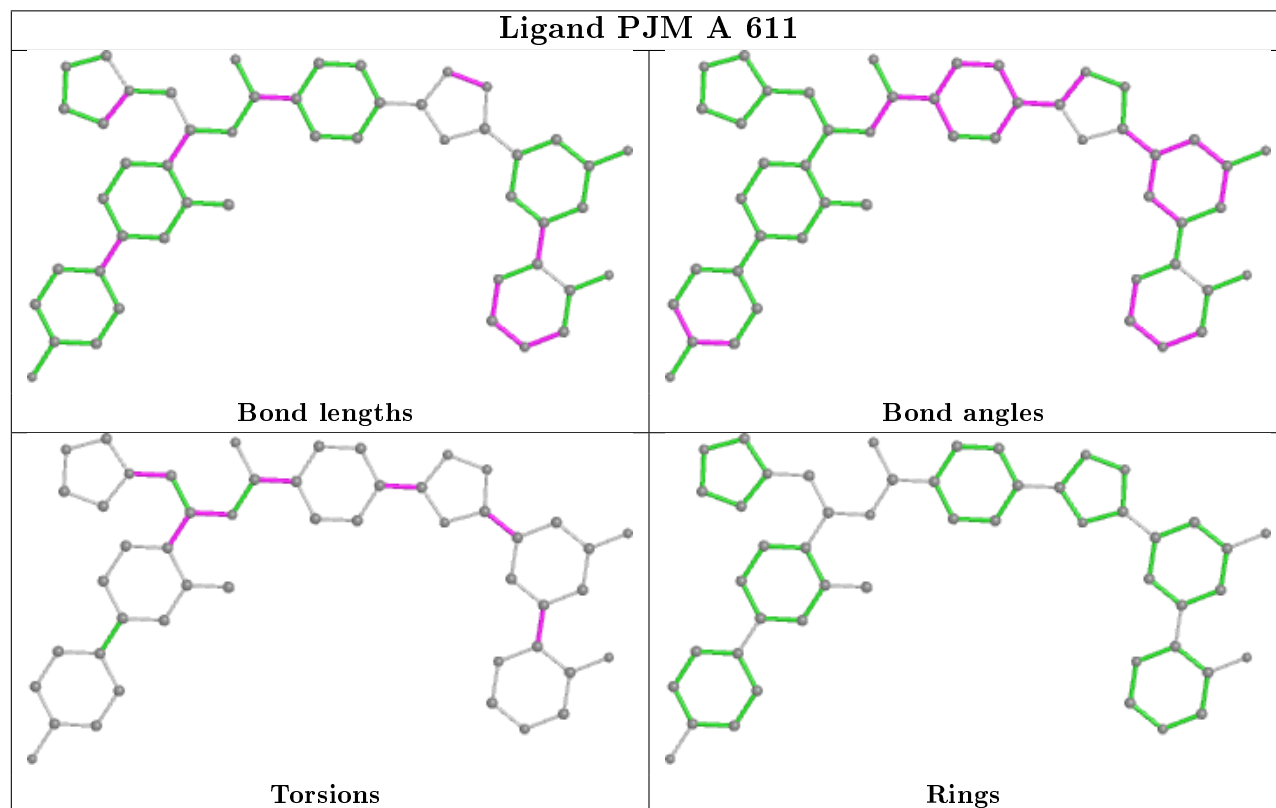
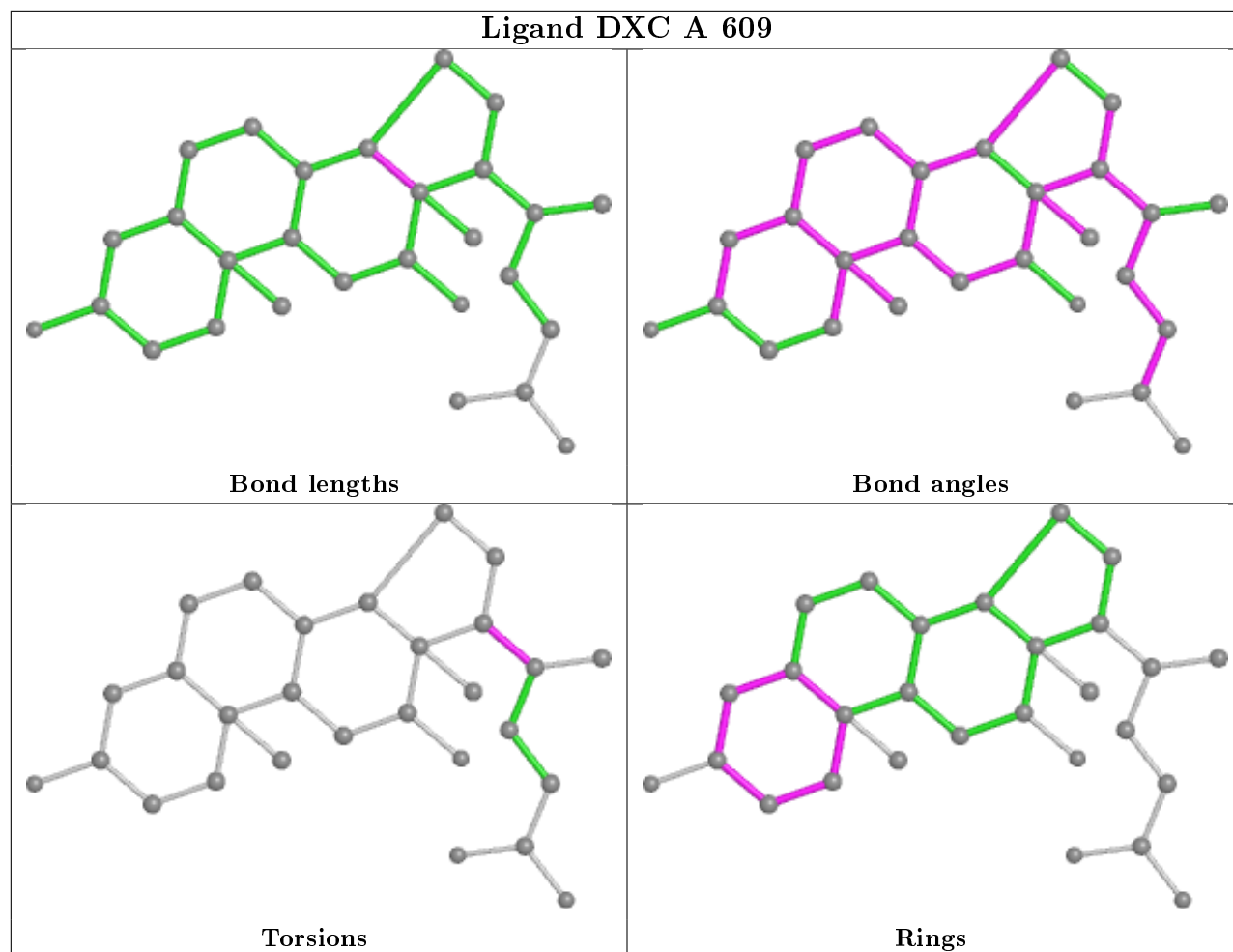


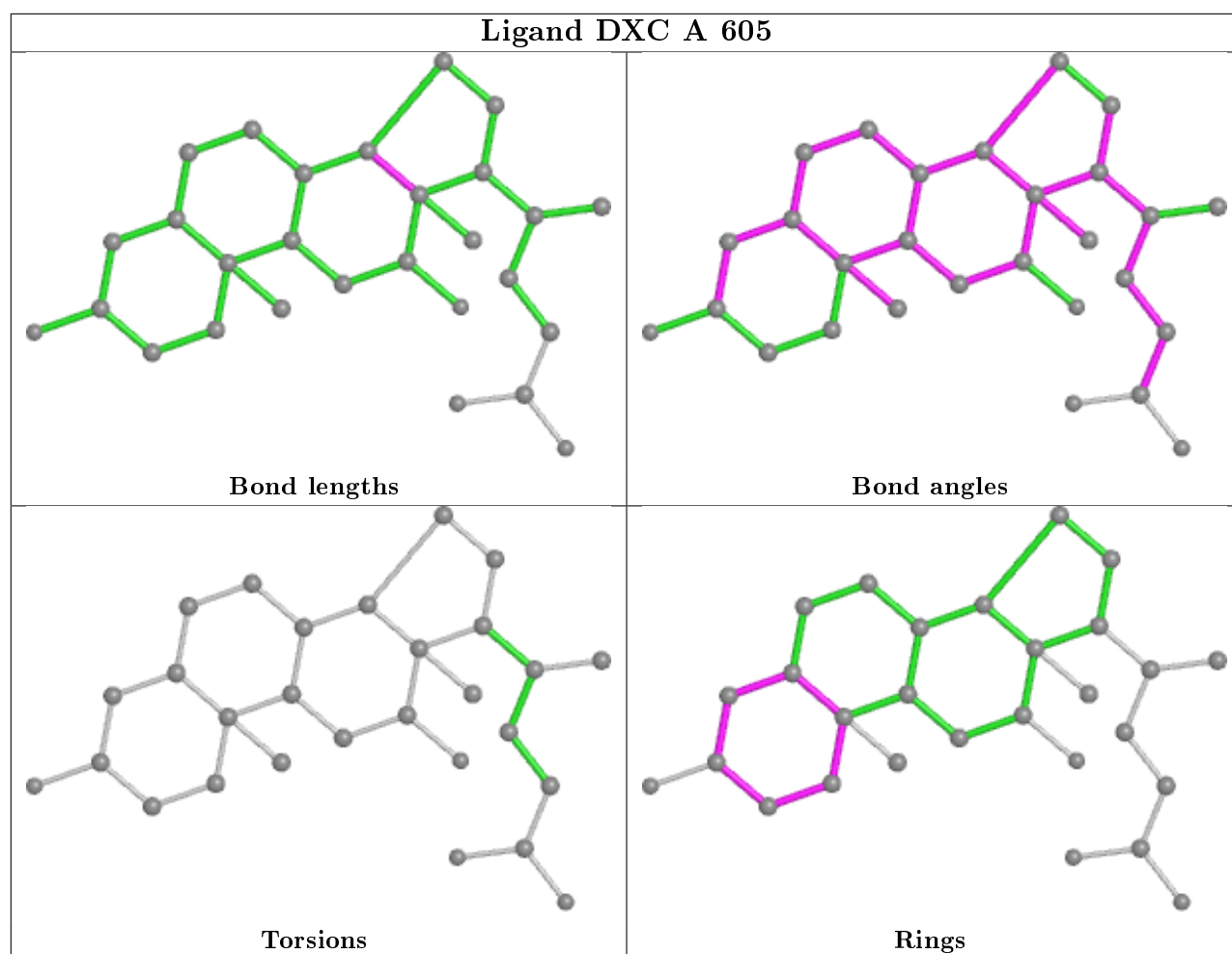












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	445/446 (99%)	0.06	23 (5%) 27 18	60, 103, 148, 194	0
1	B	444/446 (99%)	0.06	19 (4%) 35 25	59, 98, 141, 164	0
All	All	889/892 (99%)	0.06	42 (4%) 31 22	59, 101, 146, 194	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	GLN	4.8
1	A	354	TYR	4.6
1	B	312	GLY	4.5
1	A	277	LYS	4.1
1	B	277	LYS	4.1
1	B	315	THR	4.0
1	B	316	SER	4.0
1	A	320	SER	3.8
1	B	314	HIS	3.4
1	A	338	TYR	3.4
1	A	317	SER	3.3
1	B	313	GLN	3.3
1	A	314	HIS	3.3
1	B	317	SER	3.2
1	A	315	THR	3.2
1	A	351	PRO	2.9
1	B	187	GLY	2.8
1	A	276	GLU	2.7
1	A	58	GLY	2.7
1	A	188	GLU	2.7
1	A	313	GLN	2.6
1	B	275	GLN	2.6
1	B	311	ALA	2.5
1	B	320	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	319	THR	2.5
1	A	296	LEU	2.5
1	A	316	SER	2.4
1	B	295	PRO	2.3
1	B	182	TYR	2.3
1	A	312	GLY	2.3
1	B	428	GLN	2.3
1	A	426	TYR	2.3
1	B	318	THR	2.3
1	A	417	GLU	2.3
1	A	476	ASP	2.2
1	B	296	LEU	2.1
1	A	318	THR	2.1
1	A	349	LEU	2.1
1	A	325	PHE	2.1
1	A	321	ALA	2.0
1	B	323	MET	2.0
1	B	353	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PJM	A	611	49/49	0.75	0.26	71,107,150,207	0
3	PJM	A	602	49/49	0.88	0.22	77,110,126,128	0
4	DXC	A	606	28/28	0.90	0.26	61,73,82,101	0
4	DXC	A	608	28/28	0.91	0.24	87,110,132,144	0
3	PJM	B	602	49/49	0.91	0.21	70,109,122,131	0

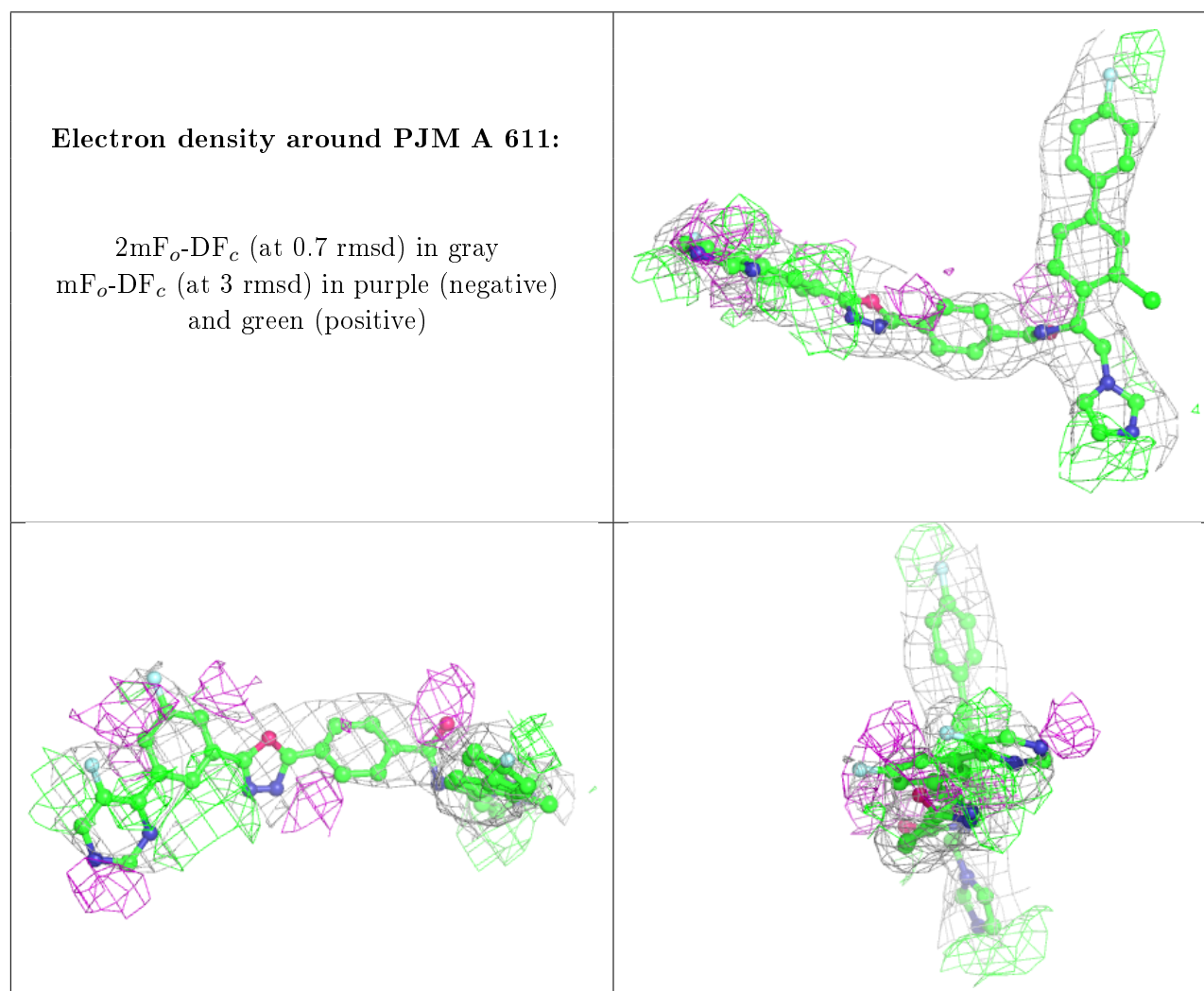
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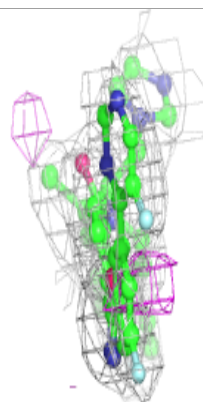
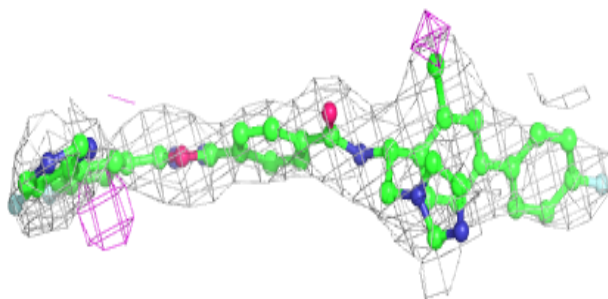
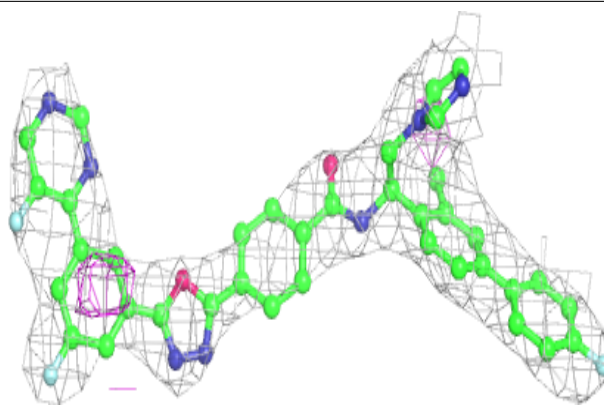
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DXC	A	610	28/28	0.92	0.23	76,104,124,133	0
4	DXC	A	609	28/28	0.94	0.16	75,82,102,114	0
4	DXC	A	603	28/28	0.96	0.16	43,53,78,84	0
2	HEM	B	601	43/43	0.96	0.23	65,76,85,90	0
4	DXC	A	607	28/28	0.96	0.15	48,55,68,77	0
4	DXC	A	604	28/28	0.97	0.14	46,52,56,66	0
4	DXC	A	605	28/28	0.97	0.13	42,52,69,76	0
2	HEM	A	601	43/43	0.98	0.18	62,77,87,100	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.

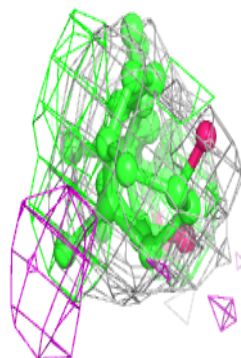
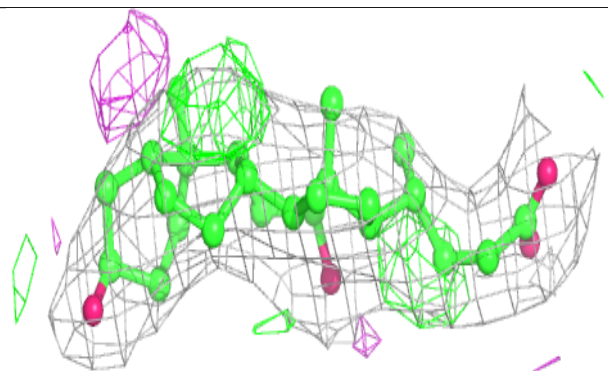
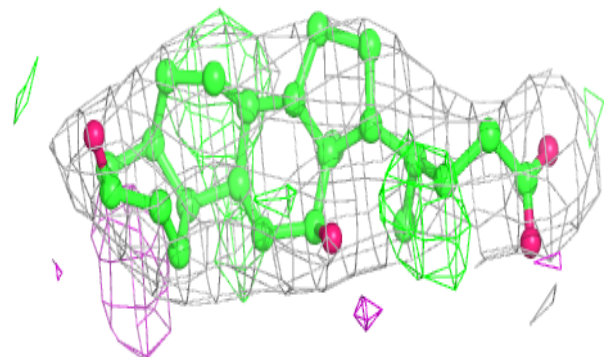


**Electron density around PJM A 602:**

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

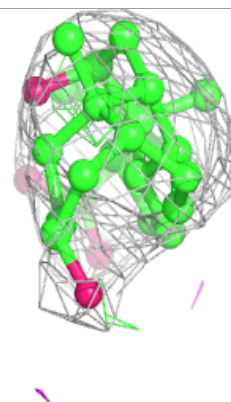
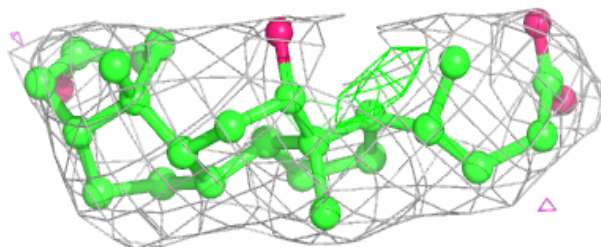
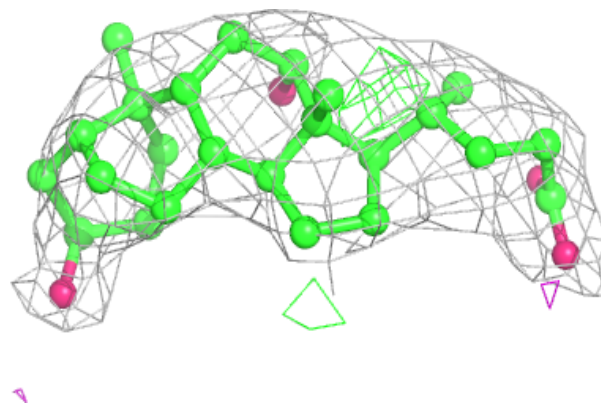
**Electron density around DXC A 606:**

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

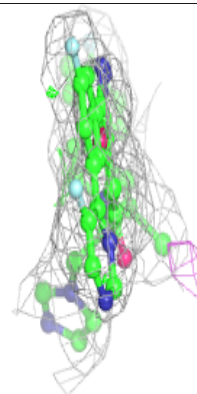
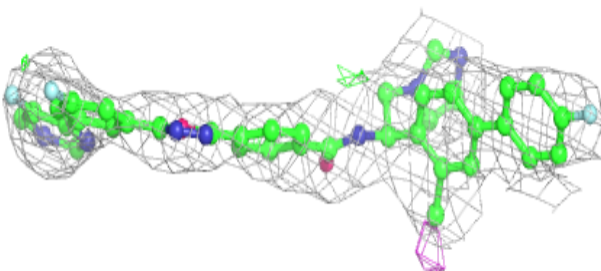
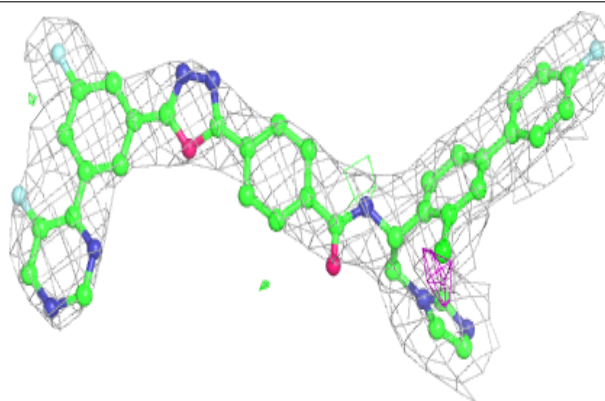


**Electron density around DXC A 608:**

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

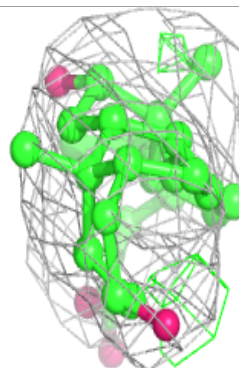
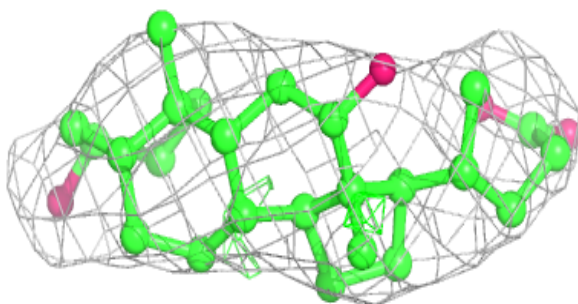
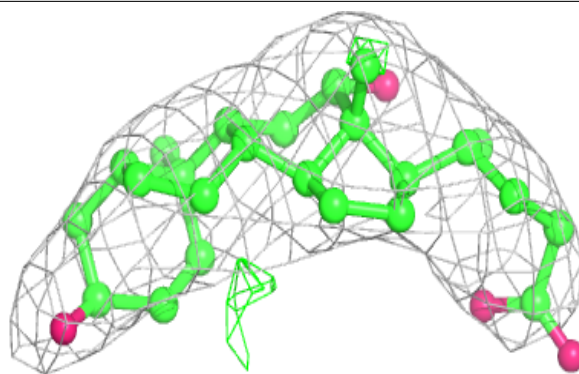
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

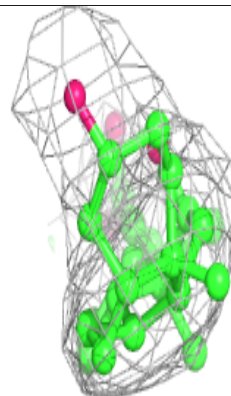
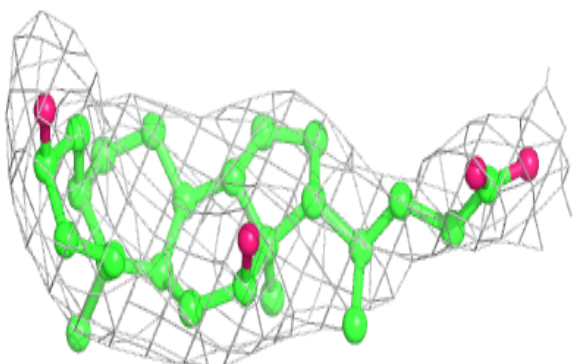
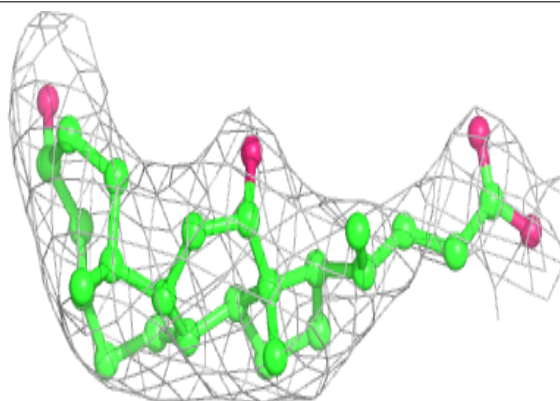


**Electron density around DXC A 610:**

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

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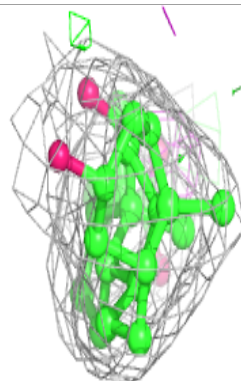
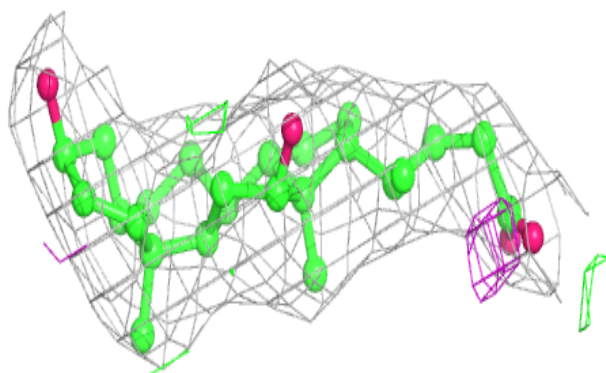
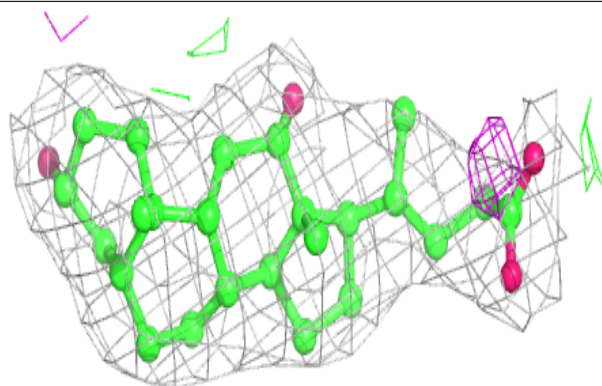
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



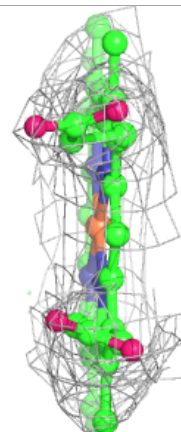
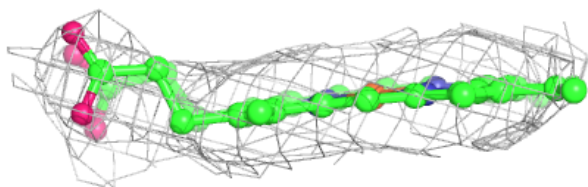
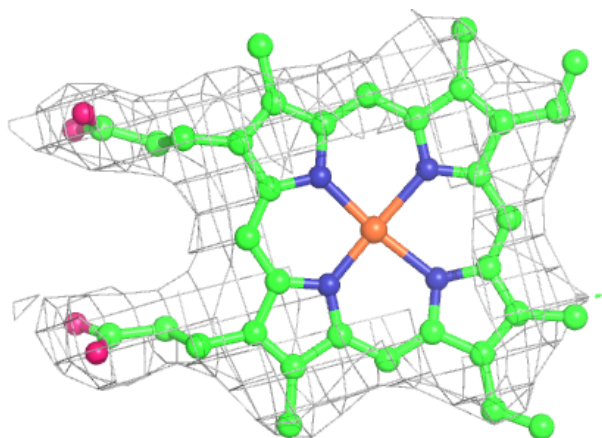


**Electron density around DXC A 603:**

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

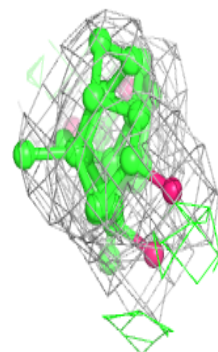
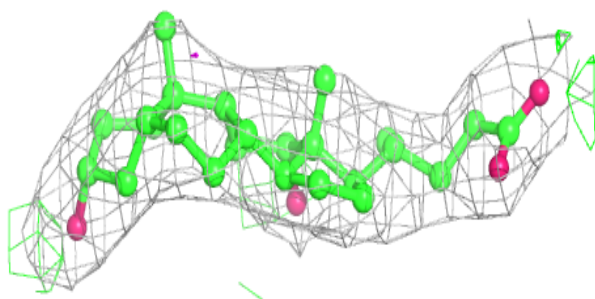
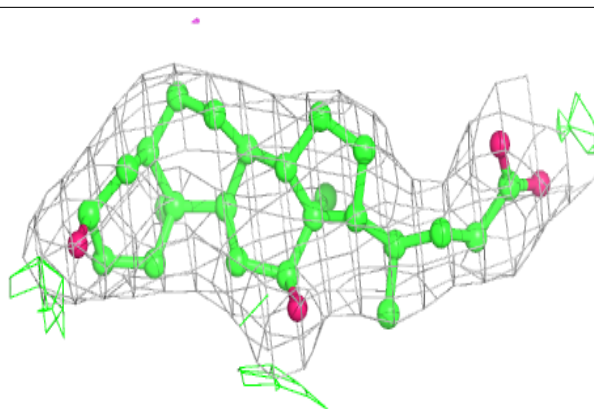
**Electron density around HEM B 601:**

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

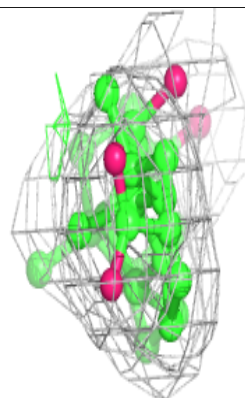
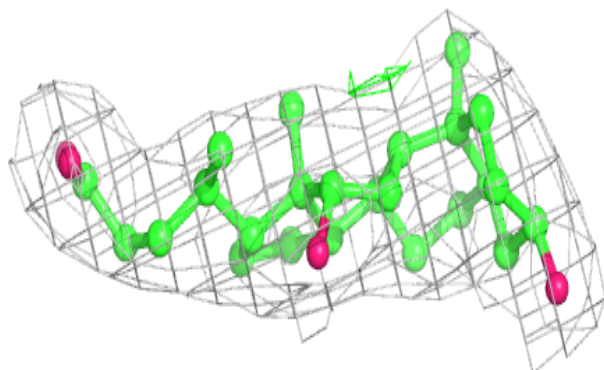
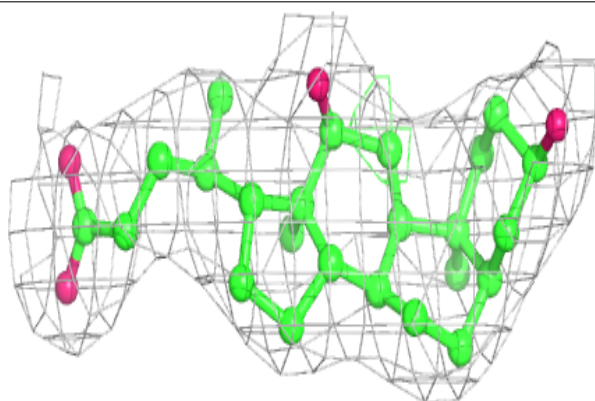


**Electron density around DXC A 607:**

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and green (positive)

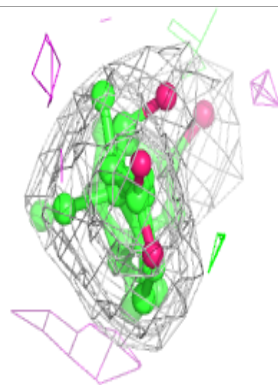
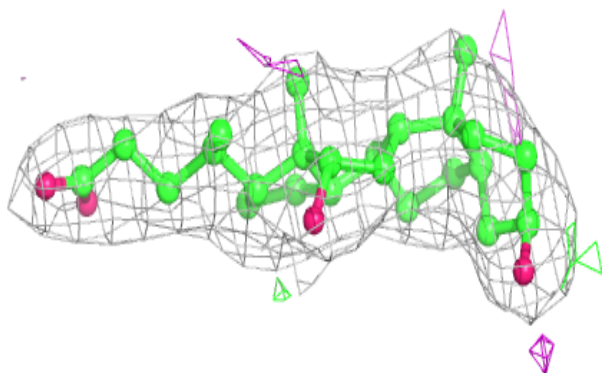
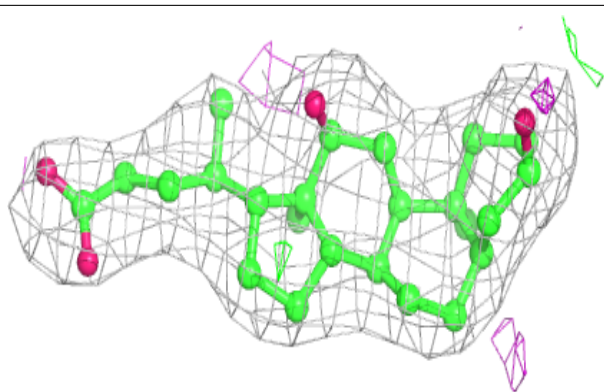
**Electron density around DXC A 604:**

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

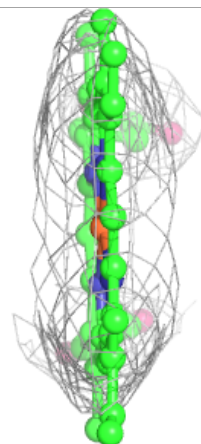
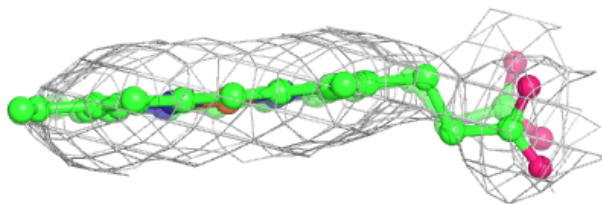
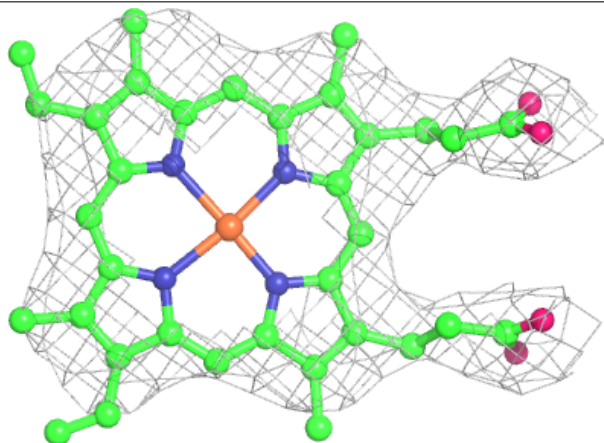


**Electron density around DXC A 605:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.