



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 PM UTC

PDB ID : 6CSB / pdb\_00006csb  
Title : V308E mutant of cytochrome P450 2D6 complexed with thioridazine  
Authors : Yang, Y.T.; Fujita, K.; Wang, P.F.; Im, S.C.; Pearl, N.M.; Meagher, J.;  
Stuckey, J.; Waskell, L.  
Deposited on : 2018-03-20  
Resolution : 2.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

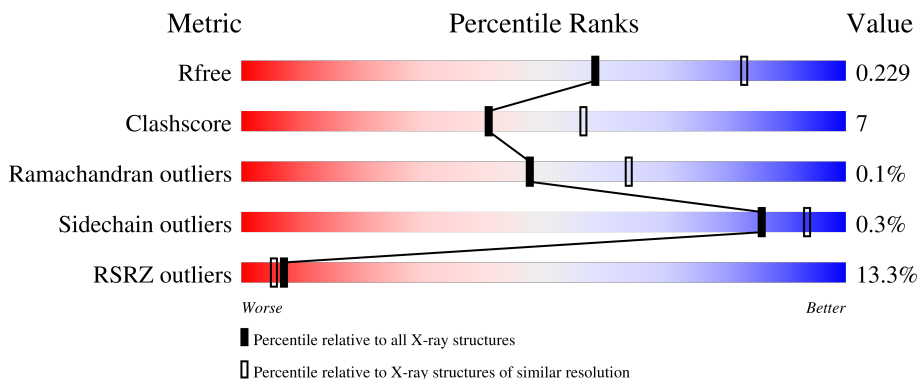
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	479	
1	B	479	
1	C	479	
1	D	479	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15058 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
			Total	C	N	O	S			
1	A	452	3527	2260	619	633	15	0	2	0
1	B	455	3550	2273	631	631	15	0	5	0
1	C	454	3519	2255	617	632	15	0	3	0
1	D	453	3501	2243	610	633	15	0	3	0

There are 64 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	308	GLU	VAL	engineered mutation	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

*Continued on next page...*

*Continued from previous page...*

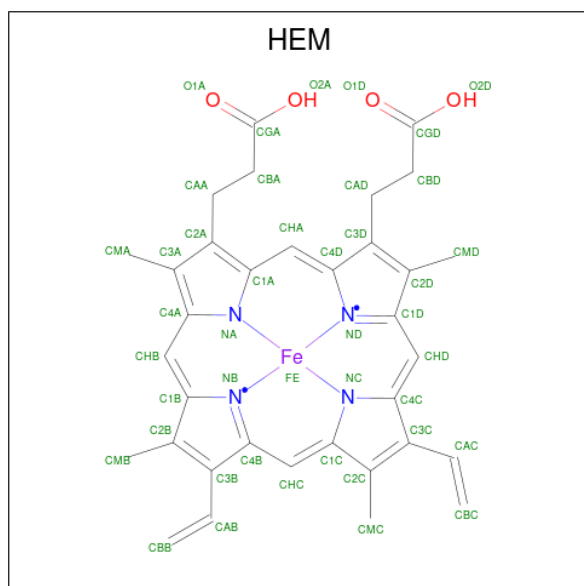
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	SER	-	expression tag	UNP P10635
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	308	GLU	VAL	engineered mutation	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	308	GLU	VAL	engineered mutation	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	308	GLU	VAL	engineered mutation	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635

*Continued on next page...*

Continued from previous page...

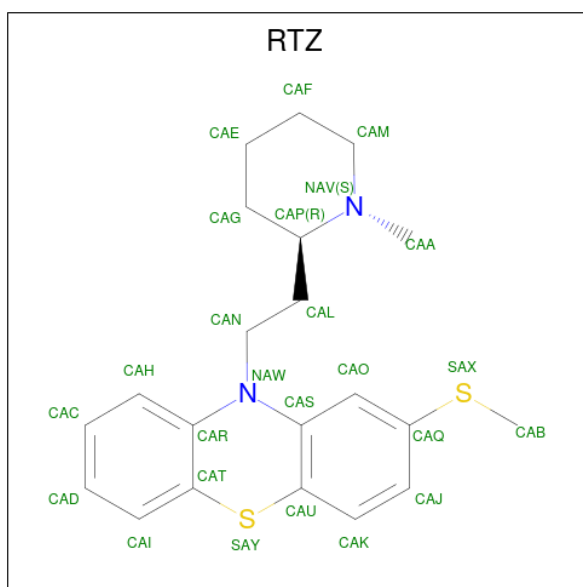
Chain	Residue	Modelled	Actual	Comment	Reference
D	501	HIS	-	expression tag	UNP P10635

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

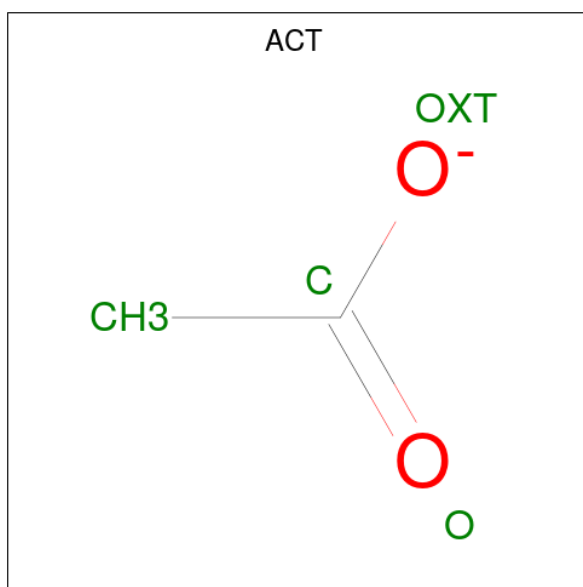
- Molecule 3 is 10-{2-[(2R)-1-methylpiperidin-2-yl]ethyl}-2-(methylsulfanyl)-10H-phenothiazine (CCD ID: RTZ) (formula:  $C_{21}H_{26}N_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
3	A	1	Total	C	N	S	0	0
			25	21	2	2		
3	A	1	Total	C	N	S	0	0
			25	21	2	2		
3	B	1	Total	C	N	S	0	0
			25	21	2	2		
3	B	1	Total	C	N	S	0	0
			25	21	2	2		
3	C	1	Total	C	N	S	0	0
			25	21	2	2		
3	C	1	Total	C	N	S	0	0
			25	21	2	2		
3	D	1	Total	C	N	S	0	0
			25	21	2	2		
3	D	1	Total	C	N	S	0	0
			25	21	2	2		

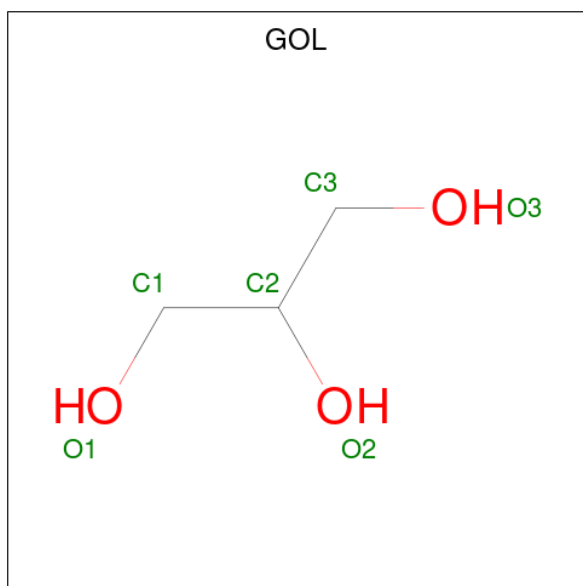
- Molecule 4 is HEGA-10 (CCD ID: 2CV) (formula: C<sub>18</sub>H<sub>37</sub>NO<sub>7</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	4	2	2	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	6	3	3	0	0

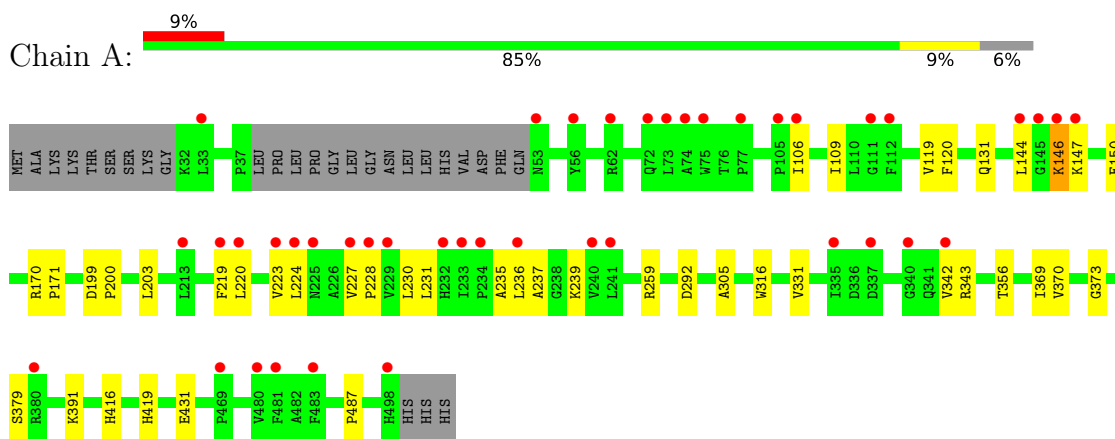
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	149	Total 149	O 149	0	0
8	B	178	Total 178	O 178	0	0
8	C	99	Total 99	O 99	0	0
8	D	120	Total 120	O 120	0	0

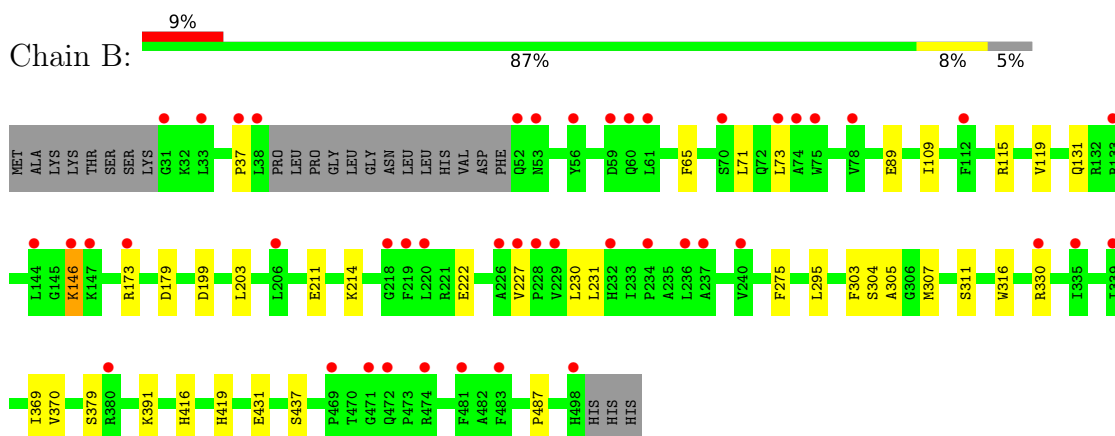
### 3 Residue-property plots [i](#)

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

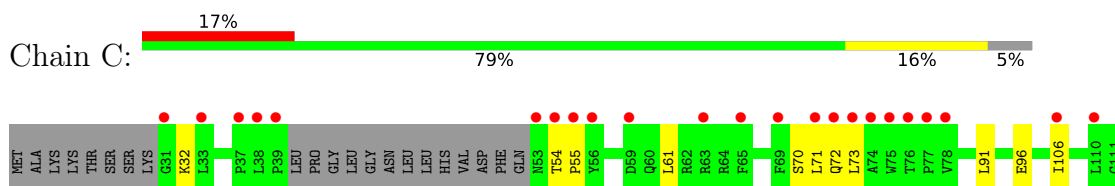
- Molecule 1: Cytochrome P450 2D6

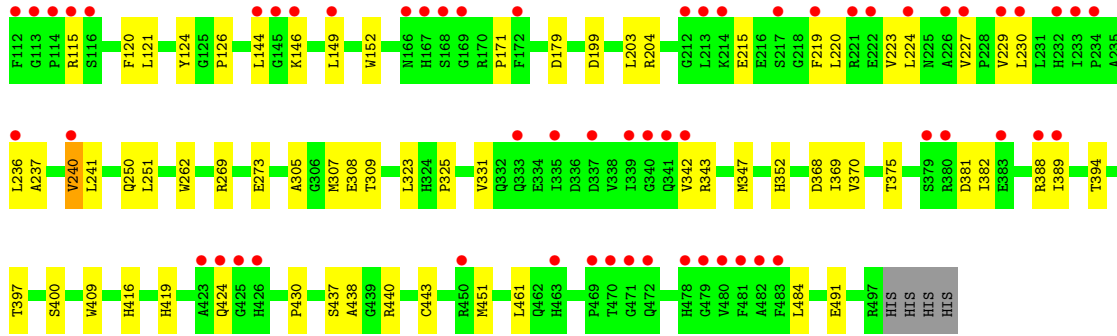


- Molecule 1: Cytochrome P450 2D6

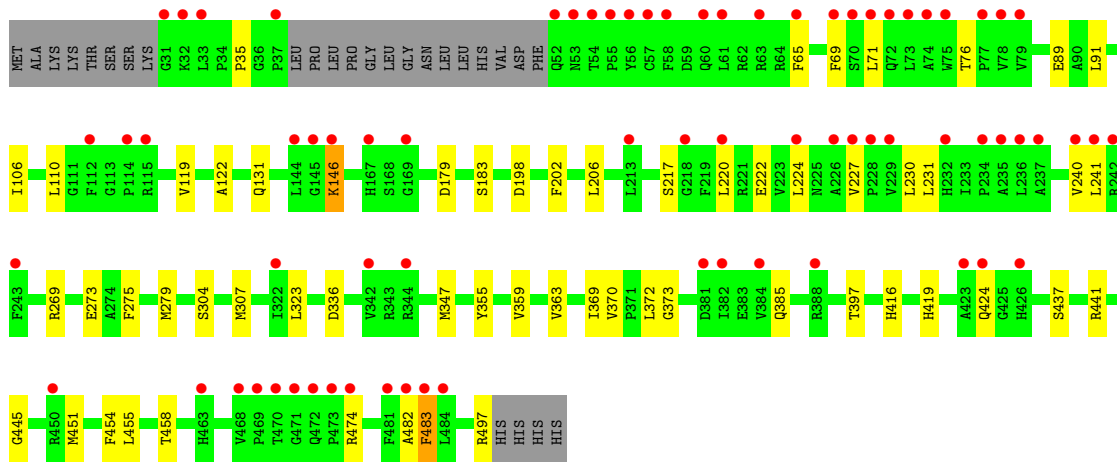
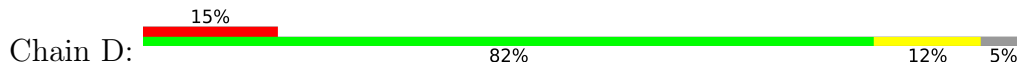


- Molecule 1: Cytochrome P450 2D6





● 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, $\alpha$ , $\beta$ , $\gamma$	57.74Å 192.00Å 250.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.39 48.47 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.47-2.39) 95.4 (48.47-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.193 , 0.229 0.192 , 0.229	Depositor DCC
$R_{free}$ test set	5234 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.460	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.65 % 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 8.2963e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, RTZ, ACT, 2CV, ZN, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/3626	0.56	0/4936
1	B	0.38	0/3658	0.56	0/4977
1	C	0.35	0/3620	0.56	0/4927
1	D	0.37	0/3601	0.57	0/4902
All	All	0.37	0/14505	0.56	0/19742

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	3527	0	3469	33	0
1	B	3550	0	3488	33	0
1	C	3519	0	3456	57	0
1	D	3501	0	3406	54	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
3	A	50	0	52	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	50	0	52	4	0
3	C	50	0	52	5	0
3	D	50	0	52	9	0
4	A	10	0	8	3	0
4	B	7	0	6	1	0
4	C	7	0	6	4	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	B	4	0	3	0	0
7	C	6	0	8	0	0
8	A	149	0	0	1	0
8	B	178	0	0	4	1
8	C	99	0	0	1	0
8	D	120	0	0	3	0
All	All	15058	0	14178	187	1

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 7.

All (187) 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:D:220:LEU:HD22	1:D:240:VAL:CG1	1.71	1.18
1:D:217:SER:HB3	1:D:483:PHE:HE1	1.34	0.92
1:D:220:LEU:HD22	1:D:240:VAL:HG12	1.58	0.83
1:D:220:LEU:HD22	1:D:240:VAL:HG13	1.60	0.83
3:D:603:RTZ:HAH	3:D:603:RTZ:HAA	1.62	0.82
1:C:54:THR:HG21	3:C:603:RTZ:HAI	1.63	0.81
1:D:220:LEU:CD2	1:D:240:VAL:CG1	2.57	0.78
1:B:222:GLU:CD	3:B:603:RTZ:HAAA	2.11	0.75
1:C:179:ASP:HA	1:C:307[B]:MET:HE1	1.69	0.74
1:D:416:HIS:ND1	8:D:701:HOH:O	2.20	0.74
1:C:124:TYR:OH	1:C:440:ARG:NH1	2.21	0.73
1:D:220:LEU:CD2	1:D:240:VAL:HG13	2.18	0.73
1:D:217:SER:HB3	1:D:483:PHE:CE1	2.22	0.72
1:A:230:LEU:HD12	1:A:230:LEU:H	1.54	0.70
1:A:224:LEU:H	1:A:224:LEU:HD12	1.57	0.70
1:D:122:ALA:O	1:D:441:ARG:NH2	2.22	0.69
1:A:219:PHE:O	1:A:223:VAL:HG23	1.94	0.68

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLY:O	3:A:603:RTZ:HAJ	1.95	0.67
2:B:601:HEM:HMB1	2:B:601:HEM:HBB2	1.76	0.65
1:C:342:VAL:HG23	1:C:343:ARG:H	1.61	0.65
1:D:220:LEU:HD23	1:D:224:LEU:HD13	1.79	0.64
3:D:603:RTZ:HAL	3:D:603:RTZ:CAH	2.27	0.64
1:A:235:ALA:O	1:A:239:LYS:HG2	1.98	0.64
3:D:603:RTZ:HAH	3:D:603:RTZ:CAA	2.28	0.63
1:D:224:LEU:HD22	1:D:240:VAL:HG11	1.81	0.63
1:B:222:GLU:OE2	3:B:603:RTZ:HAAA	2.00	0.62
1:D:323:LEU:O	1:D:474:ARG:NH2	2.33	0.62
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.82	0.61
1:C:381:ASP:OD2	1:C:388:ARG:NH1	2.35	0.59
1:D:76:THR:OG1	3:D:603:RTZ:HAEA	2.03	0.59
1:D:110:LEU:HD11	1:D:241:LEU:HD13	1.83	0.59
2:D:601:HEM:HMC1	2:D:601:HEM:HBC2	1.83	0.59
1:D:179:ASP:HA	1:D:307[B]:MET:HE1	1.85	0.58
1:C:115:ARG:HH12	1:C:126:PRO:HB2	1.69	0.58
1:B:89:GLU:OE1	8:B:701:HOH:O	2.17	0.57
1:A:230:LEU:HD12	1:A:230:LEU:N	2.19	0.57
1:A:224:LEU:HD21	1:A:236:LEU:HB3	1.87	0.56
1:C:224:LEU:HD12	1:C:224:LEU:H	1.69	0.56
1:C:54:THR:OG1	3:C:603:RTZ:HAD	2.05	0.56
1:A:119:VAL:HG22	1:A:131:GLN:HB3	1.88	0.55
1:C:96:GLU:CG	1:C:440:ARG:HH12	2.19	0.55
1:A:227:VAL:HG13	1:A:230:LEU:CD1	2.36	0.55
1:C:70:SER:O	1:C:71:LEU:HD12	2.06	0.55
1:C:424:GLN:N	1:C:424:GLN:OE1	2.40	0.53
1:C:220:LEU:O	1:C:224:LEU:HD12	2.08	0.53
1:A:259:ARG:NH2	1:A:292:ASP:OD1	2.38	0.53
1:D:217:SER:CB	1:D:483:PHE:HE1	2.14	0.53
1:B:227:VAL:HG13	1:B:230:LEU:CD1	2.38	0.53
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.89	0.53
1:A:199:ASP:O	1:A:203:LEU:HG	2.08	0.53
1:C:96:GLU:HG2	1:C:440:ARG:HH12	1.73	0.53
1:C:227:VAL:HG13	1:C:230:LEU:HG	1.91	0.53
1:A:227:VAL:HG13	1:A:230:LEU:HD11	1.91	0.52
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.91	0.52
1:B:227:VAL:HG13	1:B:230:LEU:HD13	1.91	0.52
1:B:379:SER:O	1:B:391:LYS:HD2	2.10	0.52
1:C:227:VAL:HG22	1:C:229:VAL:HG12	1.92	0.51
1:B:305:ALA:HA	4:B:605:2CV:H431	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLU:OE2	1:D:385:GLN:NE2	2.42	0.51
1:A:109:ILE:HD11	1:A:231:LEU:HD22	1.93	0.51
2:D:601:HEM:HMB2	2:D:601:HEM:HBB2	1.92	0.51
1:C:309:THR:HG21	4:C:605:2CV:H42	1.91	0.51
1:B:179:ASP:CB	1:B:307[B]:MET:HE1	2.40	0.51
1:B:109:ILE:HD11	1:B:231:LEU:HD22	1.93	0.50
1:A:106:ILE:HG22	1:A:231:LEU:HD11	1.94	0.49
1:B:71:LEU:HD13	1:B:73:LEU:HD11	1.93	0.49
1:B:71:LEU:HB3	1:B:73:LEU:HD21	1.92	0.49
1:C:106:ILE:HD11	1:C:240:VAL:HG11	1.94	0.49
1:B:330[B]:ARG:NH1	8:B:705:HOH:O	2.42	0.49
1:A:120:PHE:HE1	4:A:604:2CV:H432	1.77	0.49
1:D:372:LEU:HB2	3:D:603:RTZ:HAK	1.95	0.49
1:C:443:CYS:HB2	2:C:601:HEM:NA	2.26	0.48
1:D:230:LEU:H	1:D:230:LEU:HD12	1.76	0.48
1:B:179:ASP:OD1	1:B:311:SER:OG	2.31	0.48
1:C:120:PHE:HE1	4:C:605:2CV:H432	1.77	0.48
1:B:179:ASP:HB3	1:B:307[B]:MET:HE1	1.94	0.48
1:D:224:LEU:HD23	1:D:231:LEU:HD21	1.94	0.48
1:D:304:SER:HB3	3:D:602:RTZ:CAU	2.43	0.48
1:D:437:SER:HB3	2:D:601:HEM:HBA1	1.95	0.48
1:B:303:PHE:HB3	1:B:307[A]:MET:HE2	1.96	0.48
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.96	0.48
1:C:308:GLU:HG3	1:C:484:LEU:HD12	1.96	0.48
1:C:219:PHE:O	1:C:223:VAL:HG23	2.14	0.48
1:C:382:ILE:HG13	1:C:389:ILE:HB	1.96	0.48
1:A:170:ARG:HG3	1:A:171:PRO:HD2	1.96	0.48
1:A:239:LYS:HE3	1:A:239:LYS:HA	1.95	0.47
1:B:304:SER:HB3	3:B:602:RTZ:CAU	2.45	0.47
1:B:115:ARG:NH2	8:B:702:HOH:O	2.40	0.47
1:C:237:ALA:HA	1:C:240:VAL:HG23	1.95	0.47
1:C:331:VAL:HG11	1:C:461:LEU:HD12	1.96	0.47
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.97	0.47
1:D:445:GLY:HA3	2:D:601:HEM:C3C	2.50	0.46
1:B:199:ASP:O	1:B:203:LEU:HG	2.15	0.46
1:D:146[B]:LYS:HE3	1:D:146[B]:LYS:H	1.80	0.46
1:D:222:GLU:OE2	3:D:603:RTZ:HAM	2.16	0.46
1:B:275:PHE:CD2	1:B:295:LEU:HD13	2.51	0.46
1:B:431[A]:GLU:HG2	8:B:821:HOH:O	2.16	0.46
3:C:603:RTZ:HAA	3:C:603:RTZ:HAL	1.74	0.46
1:C:61:LEU:HD12	1:C:61:LEU:H	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:MET:HG3	1:C:451:MET:HE2	1.97	0.46
1:D:220:LEU:CD2	1:D:224:LEU:HD22	2.46	0.46
1:D:269:ARG:HG2	1:D:273:GLU:OE1	2.16	0.46
1:A:144:LEU:O	1:A:146[B]:LYS:HE3	2.16	0.45
1:C:368:ASP:OD2	1:C:400:SER:OG	2.23	0.45
1:D:336:ASP:OD2	1:D:497:ARG:NH2	2.48	0.45
1:D:220:LEU:HD22	1:D:240:VAL:HG11	1.81	0.45
1:C:236:LEU:HD23	1:C:236:LEU:HA	1.73	0.45
1:A:316:TRP:CD1	1:A:487:PRO:HD3	2.52	0.45
1:C:54:THR:HB	1:C:55:PRO:HD3	1.99	0.45
1:D:482:ALA:O	8:D:702:HOH:O	2.21	0.45
1:D:227:VAL:HB	1:D:230:LEU:CD1	2.47	0.44
1:B:71:LEU:HB3	1:B:73:LEU:CD2	2.48	0.44
1:B:173:ARG:HG2	1:B:173:ARG:HH11	1.82	0.44
1:C:424:GLN:O	1:D:424:GLN:HB3	2.17	0.44
1:A:147:LYS:HE3	1:A:150:GLU:OE2	2.17	0.44
1:C:96:GLU:HA	1:C:440:ARG:NH1	2.33	0.44
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.99	0.44
1:C:220:LEU:HG	1:C:224:LEU:HD11	1.99	0.44
1:D:35:PRO:HB2	1:D:65:PHE:CD2	2.53	0.44
1:B:211:GLU:O	1:B:214:LYS:HB2	2.18	0.43
1:D:222:GLU:CD	3:D:603:RTZ:HAM	2.43	0.43
1:D:275:PHE:HE2	1:D:279:MET:HE2	1.83	0.43
1:A:316:TRP:NE1	1:A:487:PRO:HD3	2.34	0.43
1:C:204:ARG:HG2	1:C:250:GLN:OE1	2.18	0.43
3:C:602:RTZ:HAI	4:C:605:2CV:C40	2.49	0.43
1:A:231:LEU:HD23	1:A:237:ALA:HA	1.99	0.43
1:D:347:MET:HG3	1:D:451:MET:HE2	2.00	0.43
1:B:37:PRO:HD3	1:B:65:PHE:CE1	2.54	0.43
1:B:179:ASP:CG	1:B:307[B]:MET:HE1	2.44	0.43
1:C:121:LEU:HD12	3:C:602:RTZ:HAAB	2.01	0.43
1:D:106:ILE:HD12	1:D:241:LEU:HD11	2.00	0.43
1:A:431:GLU:HG2	8:A:809:HOH:O	2.18	0.43
1:C:409:TRP:CZ3	1:C:430:PRO:HG2	2.53	0.43
1:C:215:GLU:OE1	1:C:241:LEU:HA	2.19	0.43
1:A:199:ASP:HA	1:A:200:PRO:HD3	1.91	0.43
1:B:316:TRP:CD1	1:B:487:PRO:HD3	2.54	0.43
1:D:69:PHE:HE1	1:D:71:LEU:HD23	1.83	0.43
1:D:359:VAL:O	1:D:363:VAL:HG23	2.18	0.43
1:D:373:GLY:O	3:D:603:RTZ:HAJ	2.18	0.43
1:D:183:SER:OG	1:D:307[B]:MET:HE3	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:LEU:HD11	1:C:397:THR:HG21	2.01	0.43
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.53	0.43
1:B:119:VAL:HG22	1:B:131:GLN:HB3	2.01	0.42
1:D:91:LEU:HD11	1:D:397:THR:HG21	2.01	0.42
1:D:227:VAL:O	1:D:230:LEU:HD12	2.19	0.42
1:C:375:THR:HG23	1:C:394:THR:HG23	2.01	0.42
1:C:437:SER:OG	1:C:438:ALA:N	2.49	0.42
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.54	0.42
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.84	0.42
1:C:220:LEU:O	1:C:223:VAL:N	2.52	0.42
1:C:437:SER:HB3	2:C:601:HEM:HBA1	2.01	0.42
1:D:198:ASP:OD2	1:D:198:ASP:N	2.47	0.42
1:D:119:VAL:HG13	1:D:131:GLN:HB3	2.01	0.42
1:D:275:PHE:CE2	1:D:279:MET:HE2	2.54	0.42
1:D:307[B]:MET:HG3	8:D:761:HOH:O	2.20	0.42
1:B:222:GLU:OE2	3:B:603:RTZ:CAA	2.67	0.42
1:A:220:LEU:O	1:A:224:LEU:HD12	2.19	0.42
1:C:416:HIS:HB3	1:C:419:HIS:CE1	2.54	0.42
2:C:601:HEM:HBC2	2:C:601:HEM:HMC2	2.01	0.42
1:C:305:ALA:HA	4:C:605:2CV:H431	2.01	0.42
1:C:152:TRP:HZ2	1:C:269[A]:ARG:HH22	1.67	0.42
1:C:323:LEU:C	1:C:325:PRO:HD3	2.44	0.42
1:A:224:LEU:O	1:A:228:PRO:HA	2.20	0.41
1:A:416:HIS:HB3	1:A:419:HIS:CE1	2.55	0.41
1:B:146[B]:LYS:H	1:B:146[B]:LYS:HG3	1.39	0.41
1:C:199:ASP:O	1:C:203:LEU:HG	2.20	0.41
1:A:342:VAL:HG13	1:A:343:ARG:H	1.85	0.41
1:C:352:HIS:HD2	8:C:756:HOH:O	2.02	0.41
1:B:316:TRP:NE1	1:B:487:PRO:HD3	2.35	0.41
1:C:32:LYS:HE2	1:C:32:LYS:HB3	1.75	0.41
1:C:72:GLN:C	1:C:73:LEU:HD23	2.44	0.41
1:D:454:PHE:CE2	1:D:458:THR:HG21	2.55	0.41
1:D:455:LEU:HD23	1:D:455:LEU:HA	1.85	0.41
1:A:120:PHE:CE1	4:A:604:2CV:H432	2.55	0.41
1:C:61:LEU:HD12	1:C:61:LEU:N	2.35	0.41
1:A:331:VAL:HG13	1:A:356:THR:OG1	2.21	0.41
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.49	0.41
1:C:171:PRO:HB2	1:C:491:GLU:OE2	2.21	0.41
1:C:342:VAL:HG23	1:C:343:ARG:N	2.33	0.41
1:D:355:TYR:O	1:D:359:VAL:HG23	2.21	0.41
1:A:379:SER:O	1:A:391:LYS:HD2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HD23	1:C:251:LEU:HA	1.87	0.41
1:D:202:PHE:O	1:D:206:LEU:HD13	2.20	0.41
1:A:305:ALA:HA	4:A:604:2CV:H431	2.03	0.40
1:D:227:VAL:HB	1:D:230:LEU:HD11	2.03	0.40
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.70	0.40
1:C:262:TRP:CD1	1:C:273:GLU:HG2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:702:HOH:O	8:B:769:HOH:O[4_545]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/479 (94%)	434 (96%)	16 (4%)	0	100	100
1	B	456/479 (95%)	441 (97%)	15 (3%)	0	100	100
1	C	453/479 (95%)	434 (96%)	18 (4%)	1 (0%)	43	58
1	D	452/479 (94%)	434 (96%)	17 (4%)	1 (0%)	43	58
All	All	1811/1916 (94%)	1743 (96%)	66 (4%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	483	PHE
1	C	240	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/409 (91%)	372 (100%)	2 (0%)	81	91
1	B	372/409 (91%)	370 (100%)	2 (0%)	81	91
1	C	371/409 (91%)	369 (100%)	2 (0%)	81	91
1	D	364/409 (89%)	362 (100%)	2 (0%)	81	91
All	All	1481/1636 (90%)	1473 (100%)	8 (0%)	86	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146[A]	LYS
1	A	146[B]	LYS
1	B	146[A]	LYS
1	B	146[B]	LYS
1	C	146[A]	LYS
1	C	146[B]	LYS
1	D	146[A]	LYS
1	D	146[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	131	GLN
1	A	210	GLN
1	B	463	HIS
1	C	167	HIS
1	C	324	HIS
1	C	350	GLN
1	D	424	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 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	1,8	50,50,50	1.61	9 (18%)	67,82,82	1.34	12 (17%)
4	2CV	C	605	2	6,6,25	0.42	0	7,7,30	0.60	0
2	HEM	A	601	4,1	50,50,50	1.67	11 (22%)	67,82,82	1.11	3 (4%)
3	RTZ	C	603	-	28,28,28	0.24	0	36,39,39	0.75	0
3	RTZ	D	603	-	28,28,28	0.27	0	36,39,39	1.46	1 (2%)
3	RTZ	B	602	-	28,28,28	0.28	0	36,39,39	0.51	0
4	2CV	B	605	2	6,6,25	0.42	0	7,7,30	1.06	1 (14%)
3	RTZ	A	602	-	28,28,28	0.28	0	36,39,39	0.49	0
6	ACT	B	604	-	3,3,3	1.37	1 (33%)	3,3,3	1.48	0
2	HEM	C	601	4,1	50,50,50	1.63	7 (14%)	67,82,82	1.14	5 (7%)
3	RTZ	B	603	-	28,28,28	0.20	0	36,39,39	0.78	1 (2%)
7	GOL	C	604	-	5,5,5	0.98	0	5,5,5	0.95	0
3	RTZ	A	603	-	28,28,28	0.25	0	36,39,39	0.96	2 (5%)
3	RTZ	D	602	-	28,28,28	0.29	0	36,39,39	0.46	0
2	HEM	B	601	4,1	50,50,50	1.77	10 (20%)	67,82,82	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RTZ	C	602	-	28,28,28	0.27	0	36,39,39	0.53	0
4	2CV	A	604	2	9,9,25	0.32	0	10,10,30	0.83	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	601	1,8	-	2/14/54/54	-
4	2CV	C	605	2	-	5/6/6/34	-
2	HEM	A	601	4,1	-	3/14/54/54	-
3	RTZ	C	603	-	-	2/7/30/30	0/4/4/4
3	RTZ	D	603	-	-	5/7/30/30	0/4/4/4
3	RTZ	B	602	-	-	4/7/30/30	0/4/4/4
4	2CV	B	605	2	-	0/6/6/34	-
3	RTZ	A	602	-	-	4/7/30/30	0/4/4/4
2	HEM	C	601	4,1	-	3/14/54/54	-
3	RTZ	B	603	-	-	3/7/30/30	0/4/4/4
7	GOL	C	604	-	-	2/4/4/4	-
3	RTZ	A	603	-	-	3/7/30/30	0/4/4/4
3	RTZ	D	602	-	-	4/7/30/30	0/4/4/4
2	HEM	B	601	4,1	-	3/14/54/54	-
3	RTZ	C	602	-	-	4/7/30/30	0/4/4/4
4	2CV	A	604	2	-	6/10/10/34	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	FE-NB	5.46	2.11	1.94
2	D	601	HEM	FE-NB	5.31	2.11	1.94
2	B	601	HEM	FE-ND	5.20	2.10	1.94
2	B	601	HEM	FE-NC	4.77	2.10	1.95
2	A	601	HEM	FE-NC	4.46	2.09	1.95
2	D	601	HEM	FE-ND	4.09	2.07	1.94
2	C	601	HEM	FE-ND	4.03	2.07	1.94
2	A	601	HEM	FE-NB	3.98	2.07	1.94
2	C	601	HEM	FE-NC	3.89	2.08	1.95
2	B	601	HEM	FE-NB	3.72	2.06	1.94

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	CAC-C3C	3.56	1.56	1.47
2	A	601	HEM	CAC-C3C	3.54	1.56	1.47
2	D	601	HEM	CAC-C3C	3.45	1.56	1.47
2	B	601	HEM	CAC-C3C	3.37	1.56	1.47
2	D	601	HEM	FE-NA	3.31	2.06	1.95
2	D	601	HEM	FE-NC	3.30	2.06	1.95
2	A	601	HEM	CAB-C3B	3.07	1.55	1.47
2	A	601	HEM	CMD-C2D	3.07	1.57	1.50
2	B	601	HEM	CMD-C2D	3.06	1.57	1.50
2	B	601	HEM	CAB-C3B	3.01	1.55	1.47
2	A	601	HEM	FE-ND	3.00	2.04	1.94
2	B	601	HEM	CMB-C2B	3.00	1.56	1.50
2	A	601	HEM	FE-NA	2.94	2.04	1.95
2	C	601	HEM	CAB-C3B	2.75	1.54	1.47
2	B	601	HEM	FE-NA	2.71	2.04	1.95
2	C	601	HEM	CMC-C2C	2.68	1.56	1.50
2	D	601	HEM	CAB-C3B	2.65	1.54	1.47
2	A	601	HEM	CMB-C2B	2.60	1.56	1.50
2	D	601	HEM	CMB-C2B	2.52	1.55	1.50
2	B	601	HEM	CMC-C2C	2.47	1.55	1.50
2	A	601	HEM	CMC-C2C	2.29	1.55	1.50
2	B	601	HEM	CMA-C3A	2.25	1.55	1.50
2	A	601	HEM	CMA-C3A	2.18	1.55	1.50
2	C	601	HEM	CMA-C3A	2.17	1.55	1.50
2	A	601	HEM	C1B-NB	-2.10	1.36	1.40
6	B	604	ACT	CH3-C	2.10	1.57	1.49
2	D	601	HEM	CMC-C2C	2.09	1.55	1.50
2	D	601	HEM	CMD-C2D	2.08	1.55	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	RTZ	CAL-CAP-CAG	-7.30	101.57	112.65
2	D	601	HEM	C4D-ND-C1D	3.34	109.17	105.21
2	D	601	HEM	C3B-C4B-NB	-3.06	107.27	109.47
2	B	601	HEM	C3B-C4B-NB	-2.99	107.32	109.47
2	B	601	HEM	C1B-NB-C4B	2.98	108.73	105.21
2	D	601	HEM	C3D-C4D-ND	-2.92	106.97	110.17
2	C	601	HEM	C1B-NB-C4B	2.80	108.52	105.21
2	D	601	HEM	C1B-NB-C4B	2.79	108.51	105.21
2	D	601	HEM	C2A-C1A-NA	-2.77	107.08	110.15
2	B	601	HEM	C2A-C1A-NA	-2.75	107.10	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	C4D-ND-C1D	2.68	108.38	105.21
2	A	601	HEM	C3B-C4B-NB	-2.64	107.57	109.47
2	D	601	HEM	O2D-CGD-CBD	2.61	122.25	114.00
2	C	601	HEM	CHD-C4C-NC	2.47	127.14	124.45
2	B	601	HEM	CAA-CBA-CGA	-2.46	107.13	113.67
2	A	601	HEM	C4D-ND-C1D	2.42	108.07	105.21
2	C	601	HEM	C4D-ND-C1D	2.40	108.04	105.21
3	B	603	RTZ	CAF-CAM-NAV	-2.33	107.71	111.36
2	D	601	HEM	CAA-CBA-CGA	-2.33	107.50	113.67
2	C	601	HEM	C3B-C4B-NB	-2.32	107.81	109.47
2	D	601	HEM	CHD-C4C-NC	2.26	126.91	124.45
4	B	605	2CV	O44-C43-C42	2.26	115.90	111.16
2	B	601	HEM	CHC-C4B-NB	2.25	126.85	124.42
2	A	601	HEM	C1B-NB-C4B	2.24	107.86	105.21
3	A	603	RTZ	CAG-CAP-NAV	-2.13	106.07	110.86
2	D	601	HEM	O2A-CGA-CBA	2.13	120.73	114.00
3	A	603	RTZ	CAF-CAM-NAV	-2.08	108.11	111.36
2	D	601	HEM	CBD-CAD-C3D	-2.05	106.87	112.53
2	D	601	HEM	CHC-C4B-NB	2.05	126.63	124.42
2	D	601	HEM	C4A-NA-C1A	2.04	109.14	105.82
2	C	601	HEM	CMB-C2B-C1B	-2.03	121.86	125.03

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	RTZ	CAN-CAL-CAP-CAG
3	A	602	RTZ	CAN-CAL-CAP-NAV
3	A	603	RTZ	CAN-CAL-CAP-CAG
3	A	603	RTZ	CAN-CAL-CAP-NAV
3	B	602	RTZ	CAN-CAL-CAP-CAG
3	B	602	RTZ	CAN-CAL-CAP-NAV
3	B	603	RTZ	CAP-CAL-CAN-NAW
3	B	603	RTZ	CAN-CAL-CAP-CAG
3	B	603	RTZ	CAN-CAL-CAP-NAV
3	C	602	RTZ	CAN-CAL-CAP-CAG
3	C	602	RTZ	CAN-CAL-CAP-NAV
3	C	603	RTZ	CAP-CAL-CAN-NAW
3	D	602	RTZ	CAP-CAL-CAN-NAW
3	D	602	RTZ	CAN-CAL-CAP-CAG
3	D	602	RTZ	CAN-CAL-CAP-NAV
3	D	603	RTZ	CAP-CAL-CAN-NAW

Continued on next page...

*Continued from previous page...*

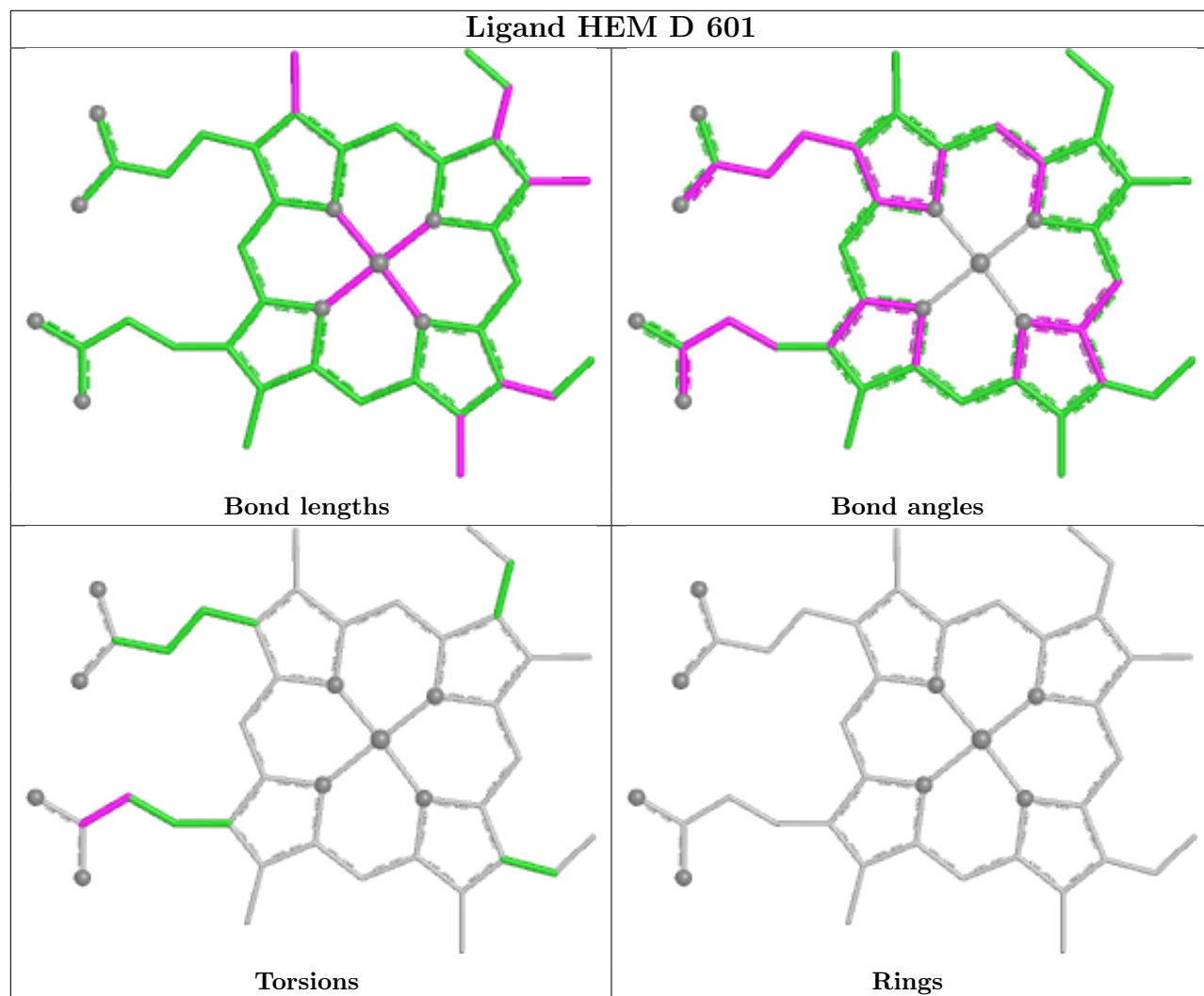
Mol	Chain	Res	Type	Atoms
3	D	603	RTZ	CAN-CAL-CAP-CAG
3	D	603	RTZ	CAN-CAL-CAP-NAV
3	D	603	RTZ	CAL-CAN-NAW-CAR
3	D	603	RTZ	CAL-CAN-NAW-CAS
4	C	605	2CV	C40-C41-C42-C43
7	C	604	GOL	O1-C1-C2-C3
4	A	604	2CV	C37-C40-C41-O51
7	C	604	GOL	O1-C1-C2-O2
4	A	604	2CV	C36-C37-C40-C41
4	A	604	2CV	O53-C42-C43-O44
4	C	605	2CV	C40-C41-C42-O53
4	A	604	2CV	C37-C40-C41-C42
4	A	604	2CV	N33-C36-C37-C40
4	A	604	2CV	C41-C42-C43-O44
4	C	605	2CV	O51-C41-C42-C43
3	A	602	RTZ	CAP-CAL-CAN-NAW
3	B	602	RTZ	CAP-CAL-CAN-NAW
3	C	602	RTZ	CAP-CAL-CAN-NAW
4	C	605	2CV	O53-C42-C43-O44
3	D	602	RTZ	CAL-CAN-NAW-CAS
2	A	601	HEM	CAA-CBA-CGA-O1A
4	C	605	2CV	C41-C42-C43-O44
2	A	601	HEM	CAA-CBA-CGA-O2A
3	A	602	RTZ	CAL-CAN-NAW-CAS
2	D	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O1A
3	C	602	RTZ	CAL-CAN-NAW-CAR
2	A	601	HEM	CAD-CBD-CGD-O2D
3	A	603	RTZ	CAP-CAL-CAN-NAW
3	B	602	RTZ	CAL-CAN-NAW-CAS
3	C	603	RTZ	CAL-CAN-NAW-CAS
2	C	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O2D

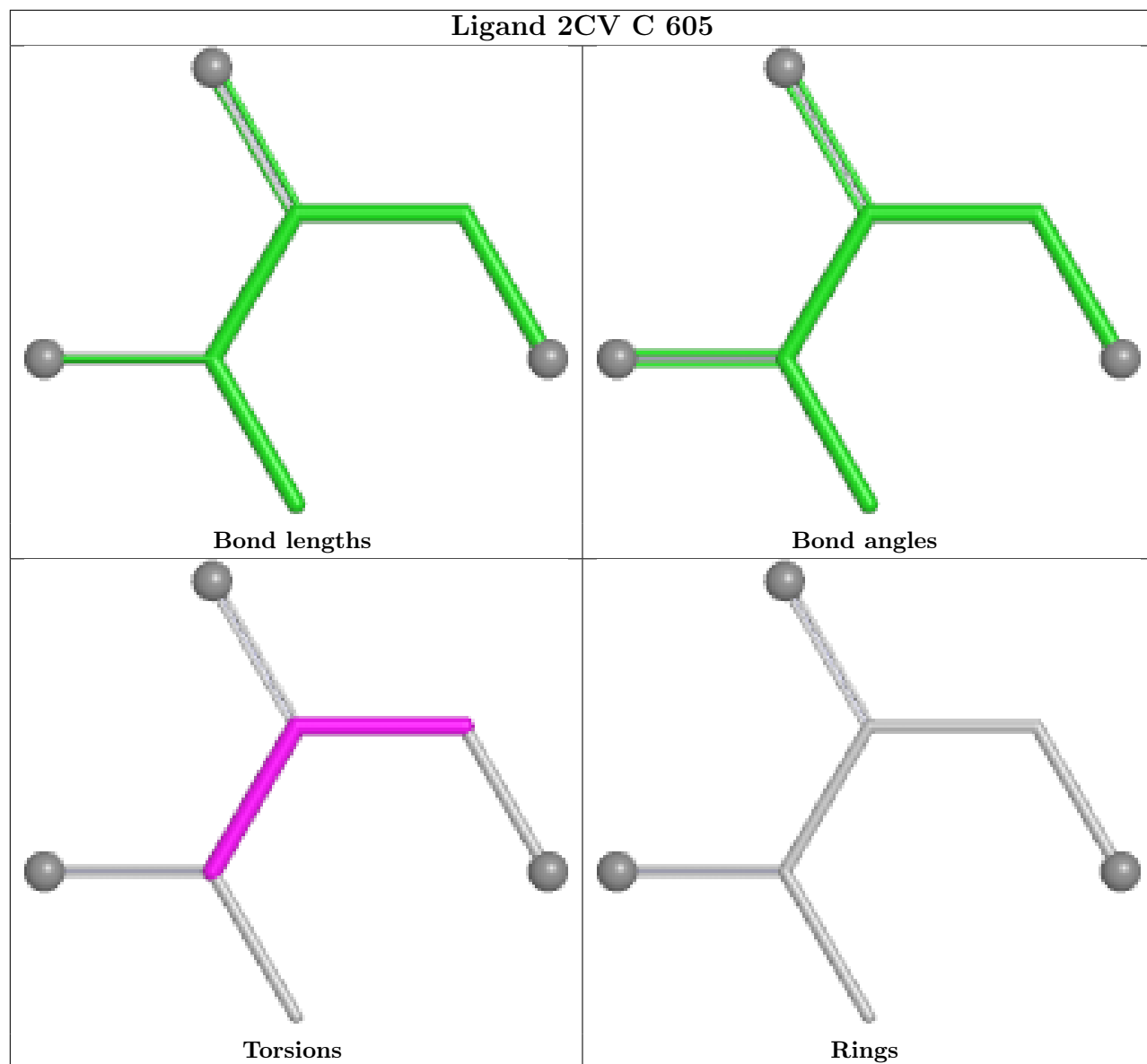
There are no ring outliers.

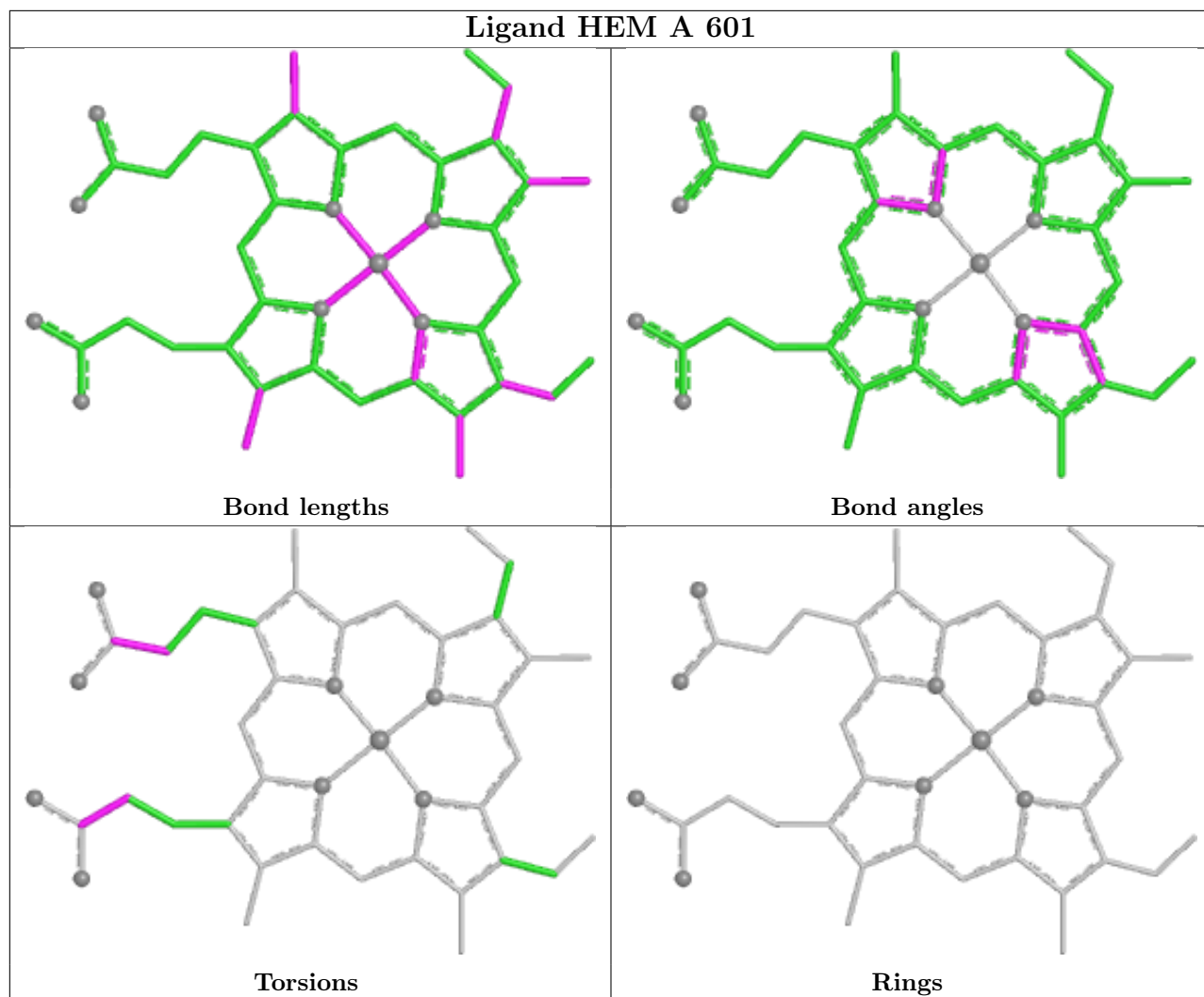
13 monomers are involved in 37 short contacts:

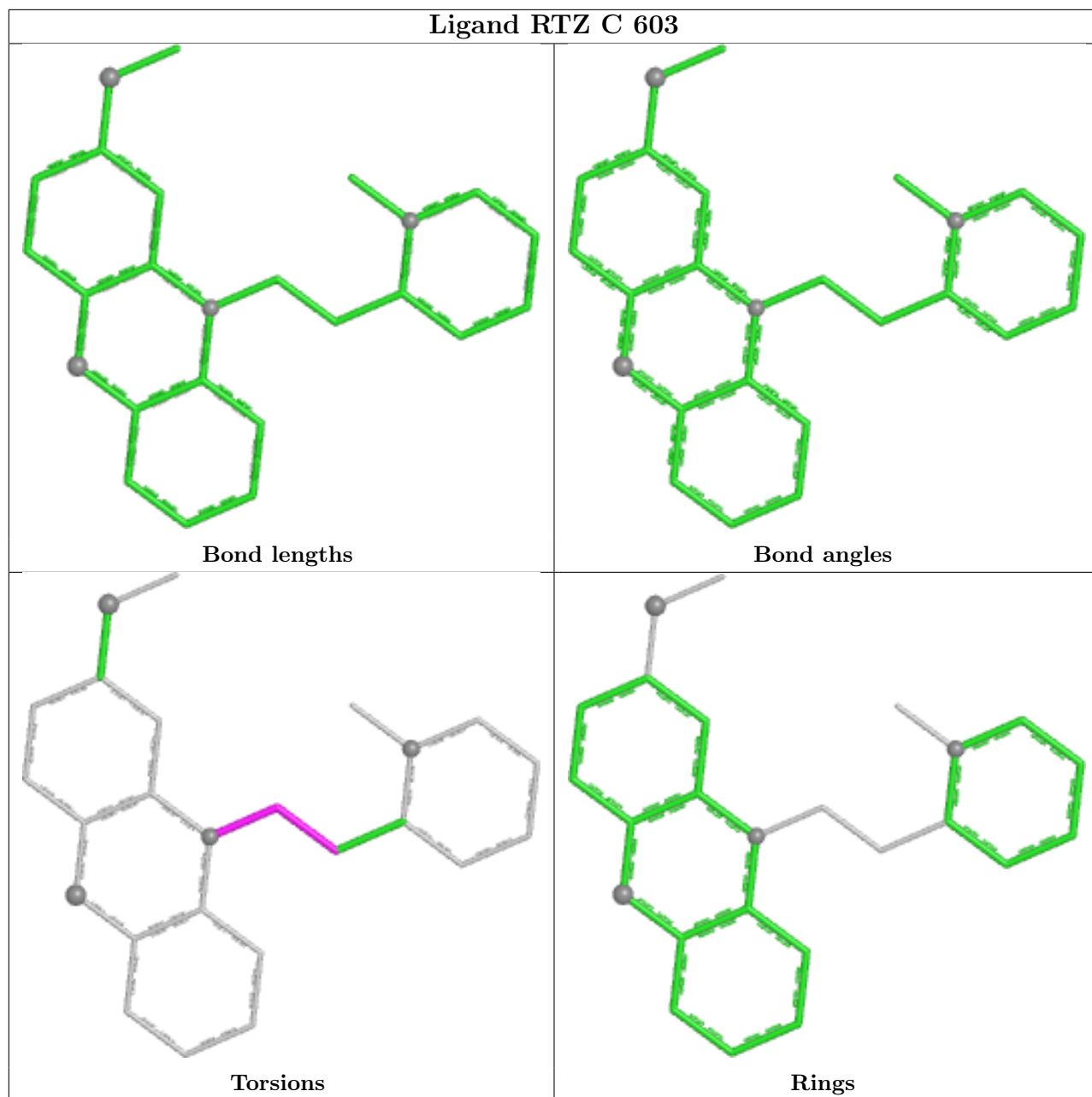
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	4	0
4	C	605	2CV	4	0
3	C	603	RTZ	3	0
3	D	603	RTZ	8	0
3	B	602	RTZ	1	0
4	B	605	2CV	1	0
2	C	601	HEM	4	0
3	B	603	RTZ	3	0
3	A	603	RTZ	1	0
3	D	602	RTZ	1	0
2	B	601	HEM	3	0
3	C	602	RTZ	2	0
4	A	604	2CV	3	0

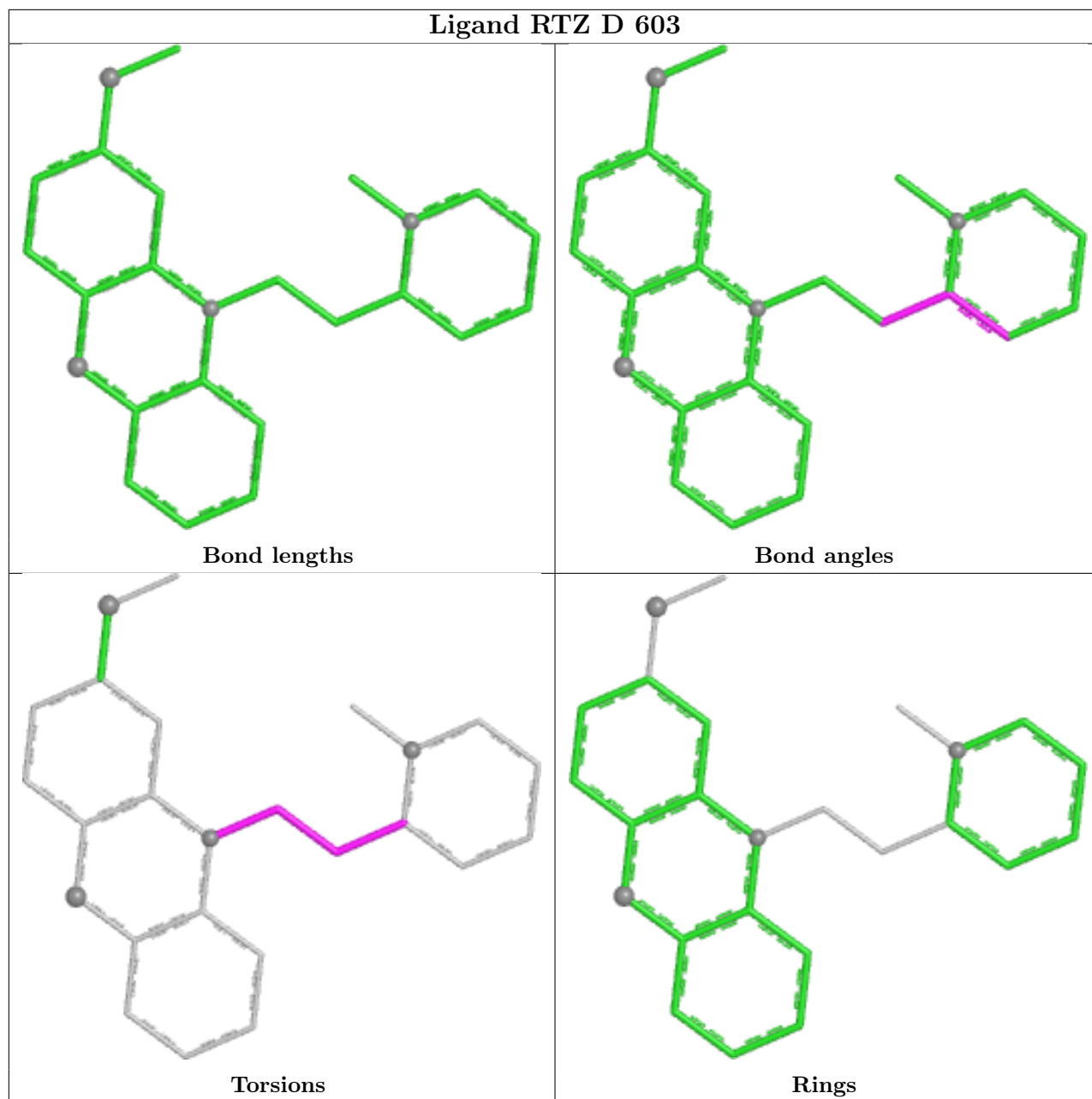
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

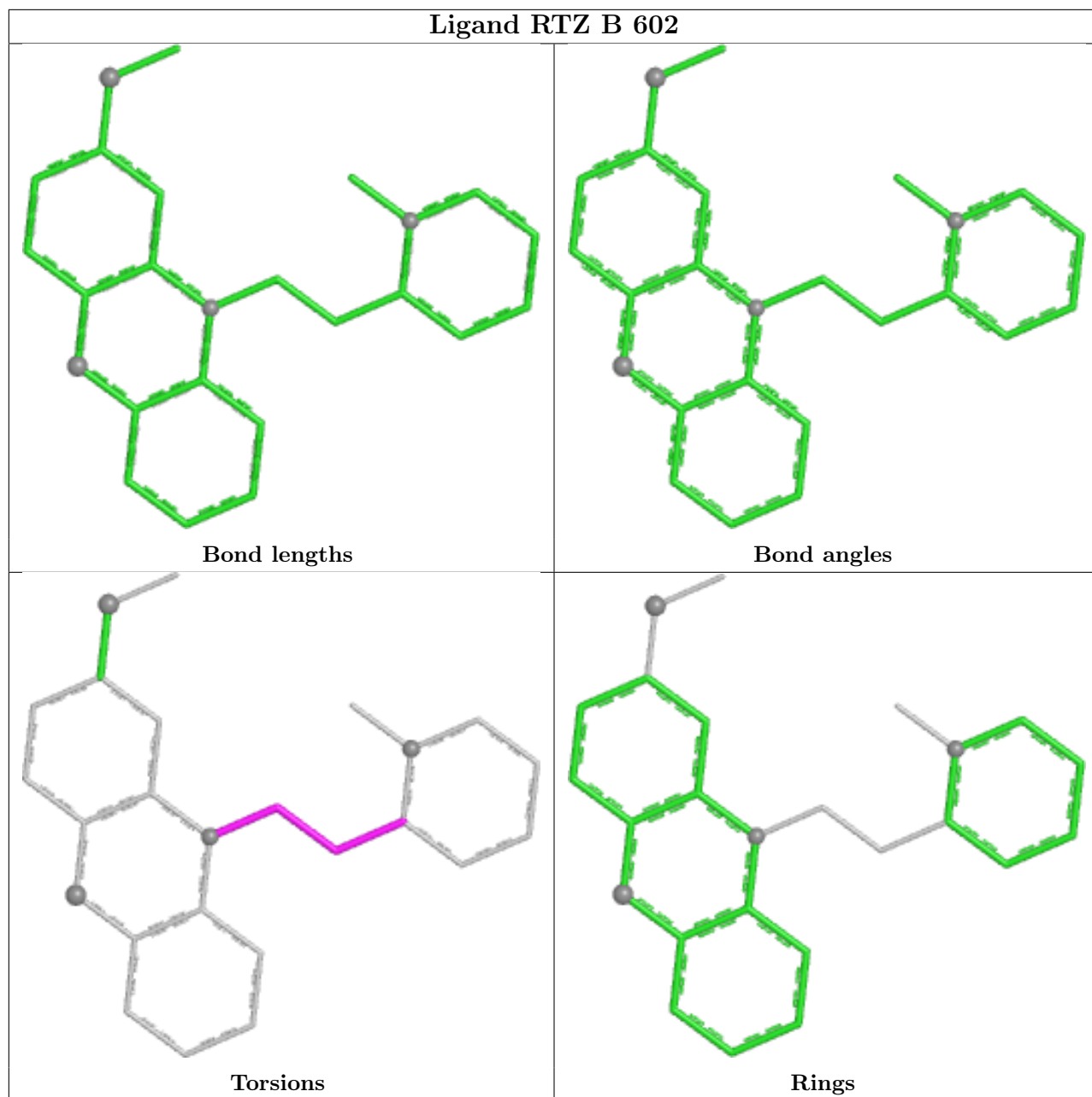


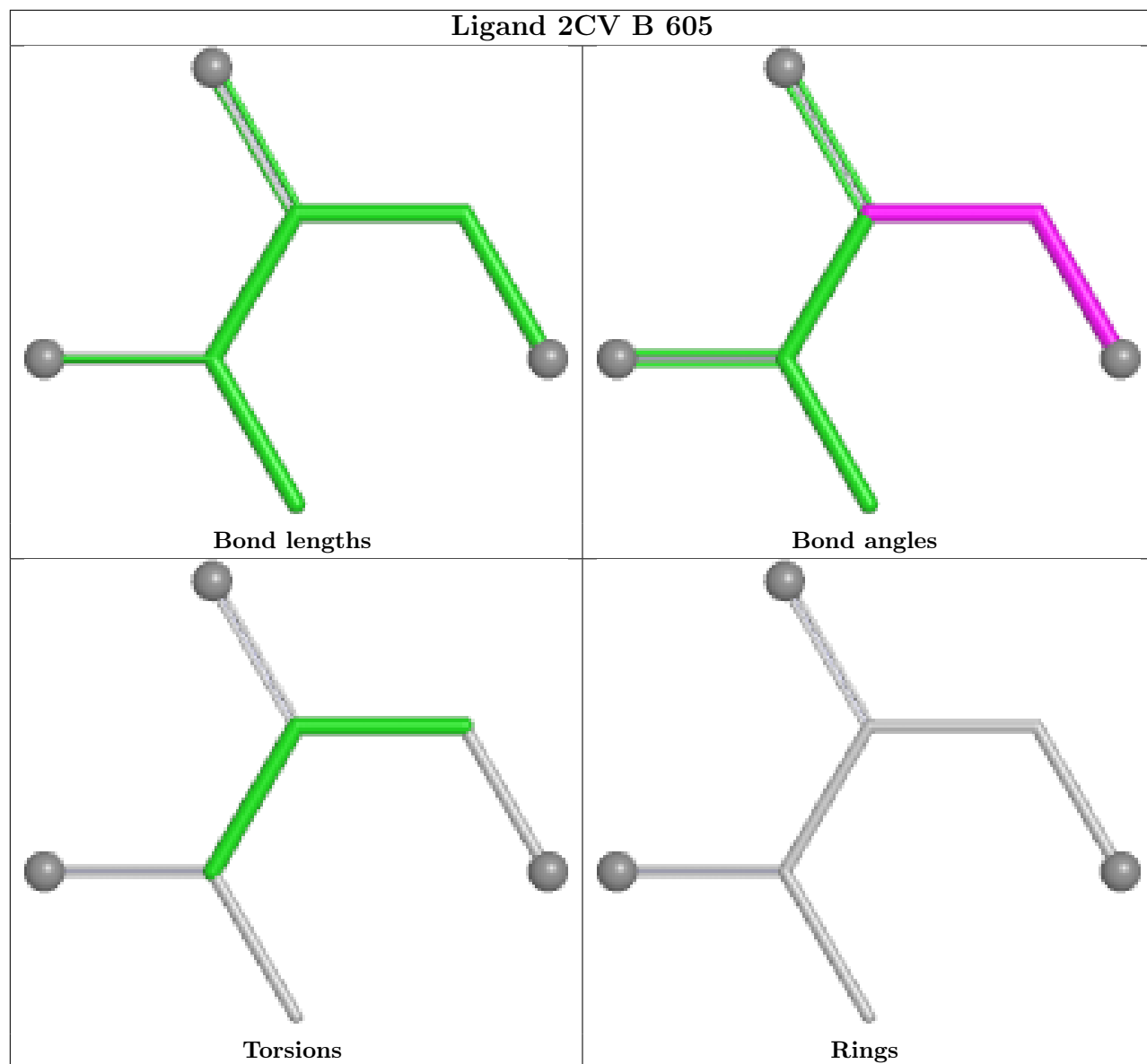


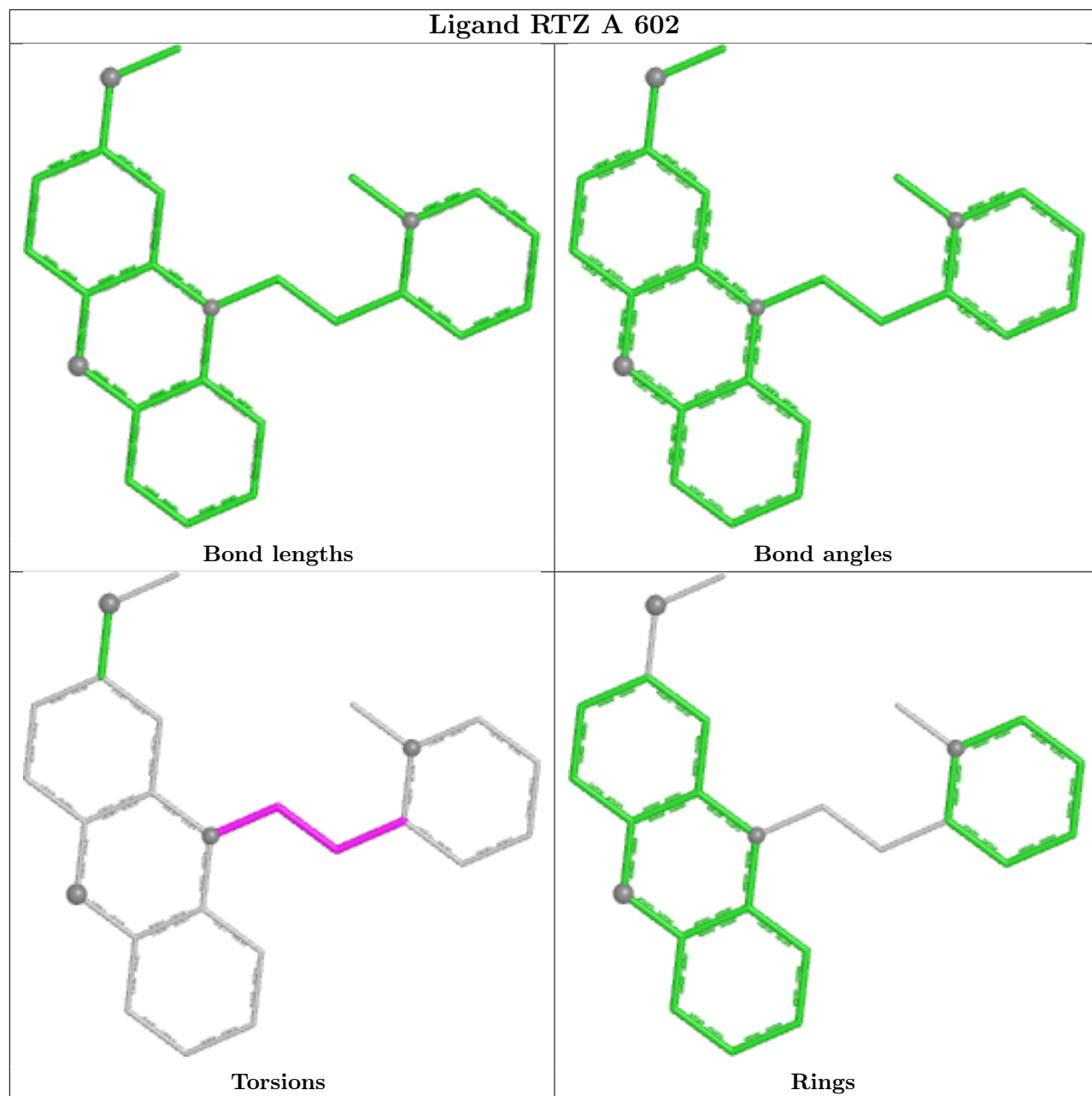


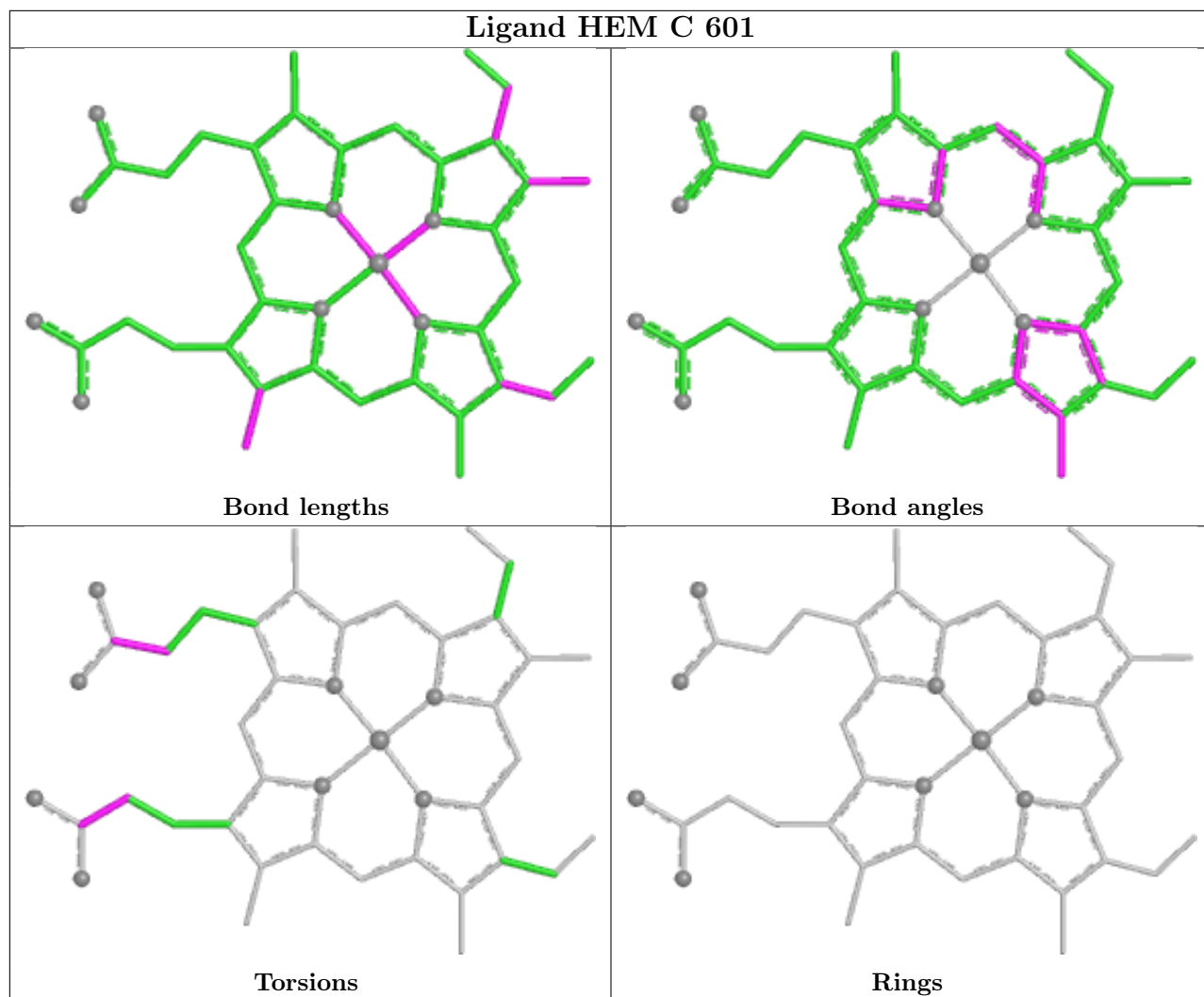


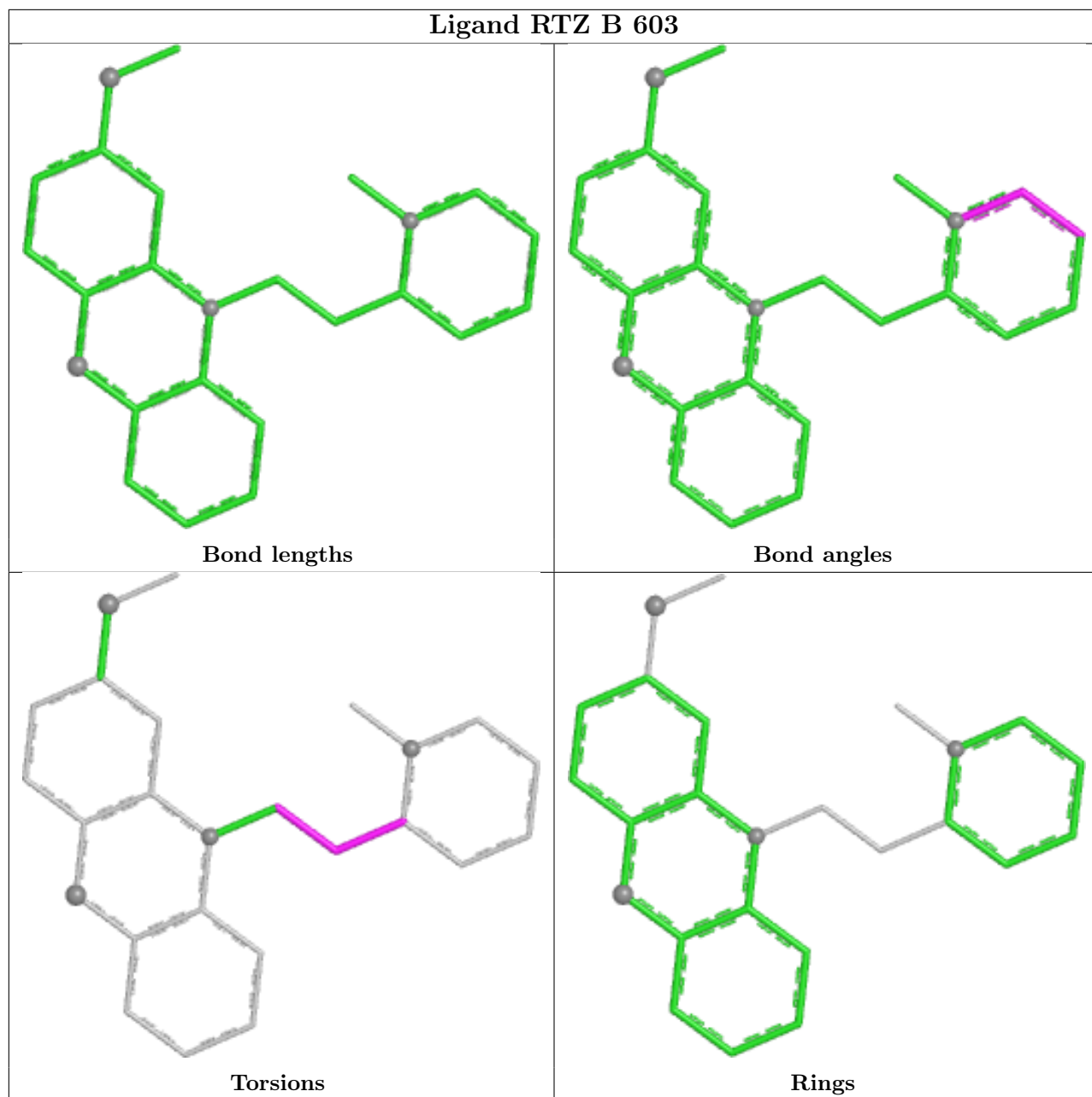


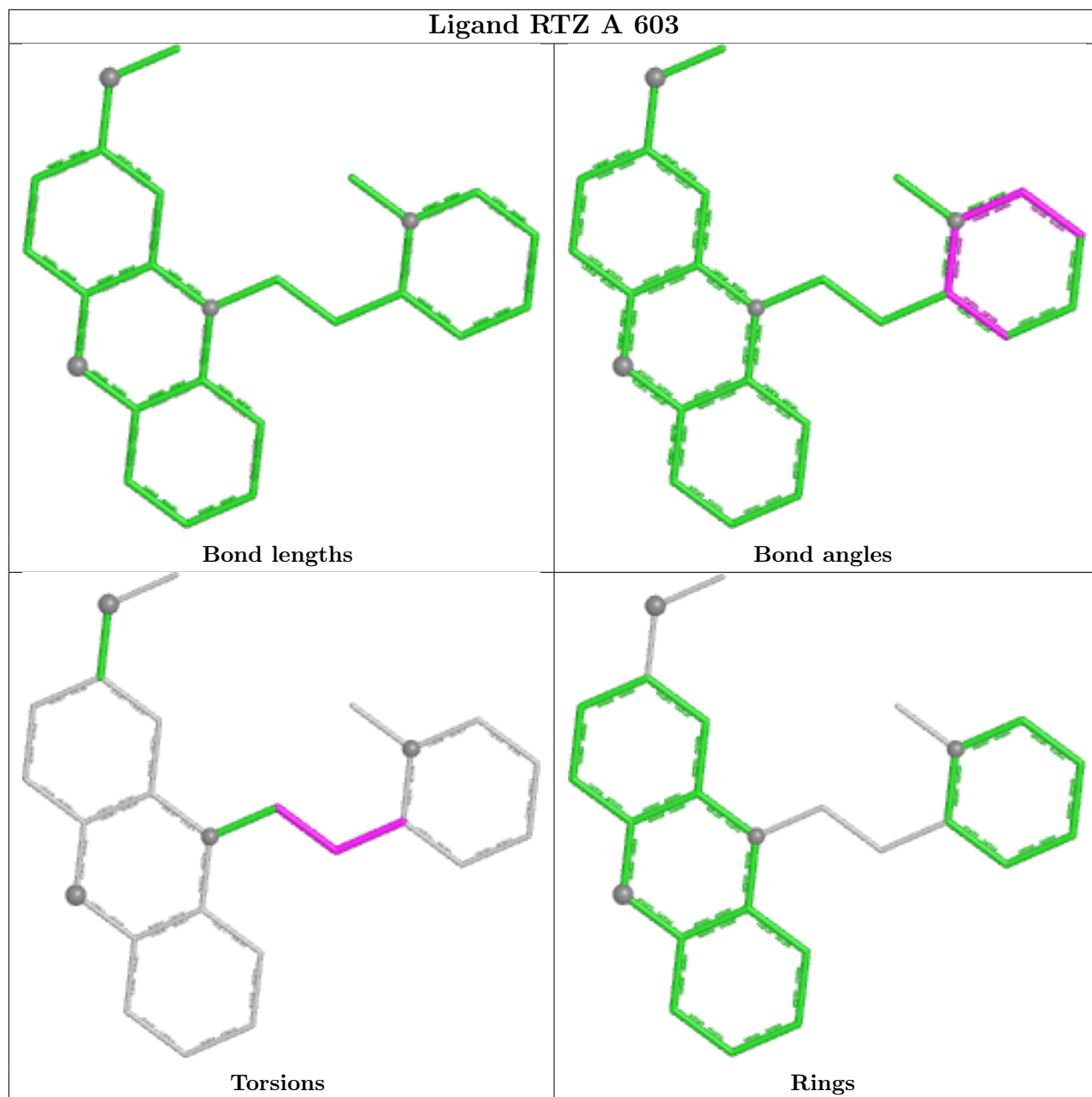


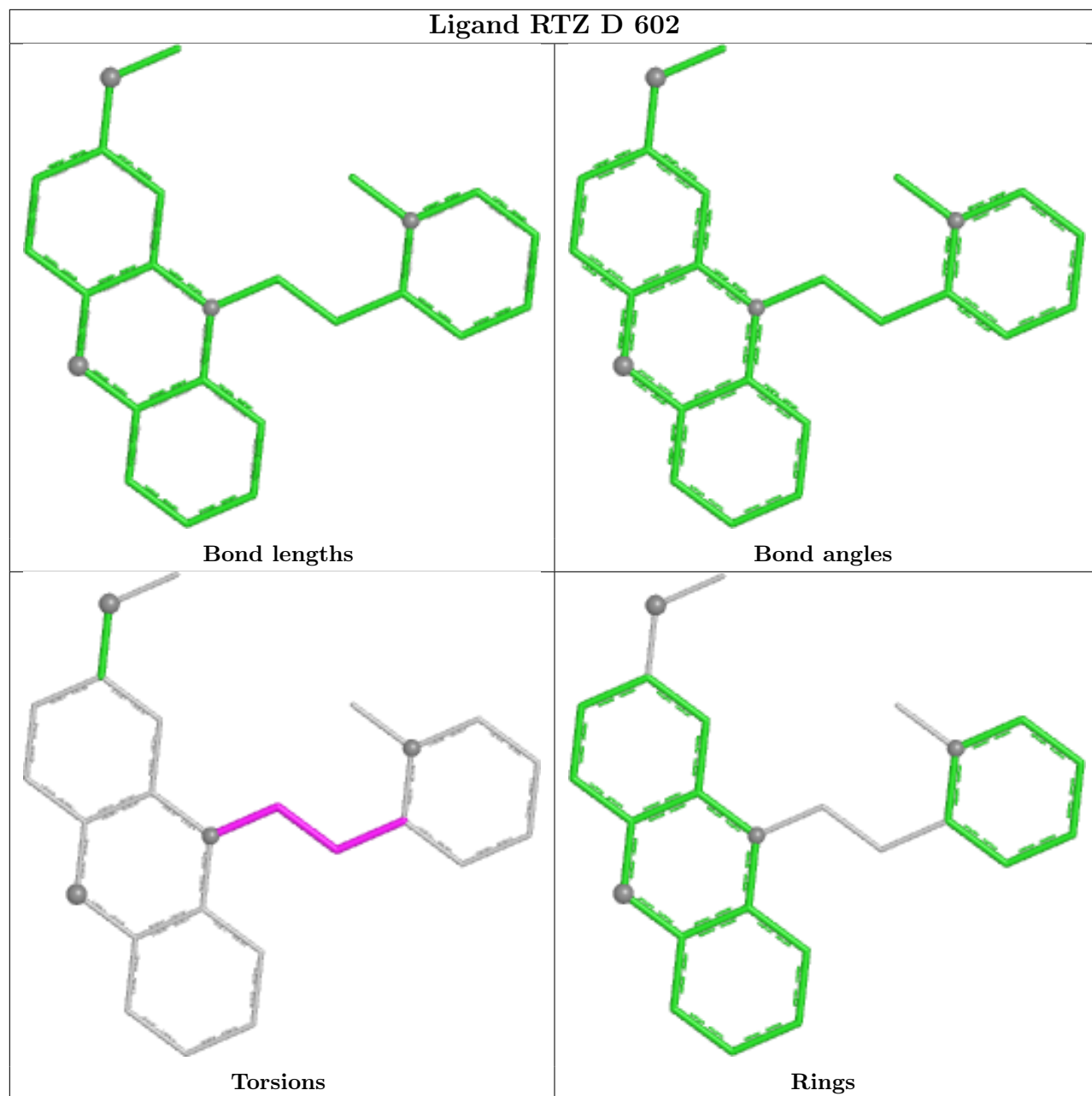


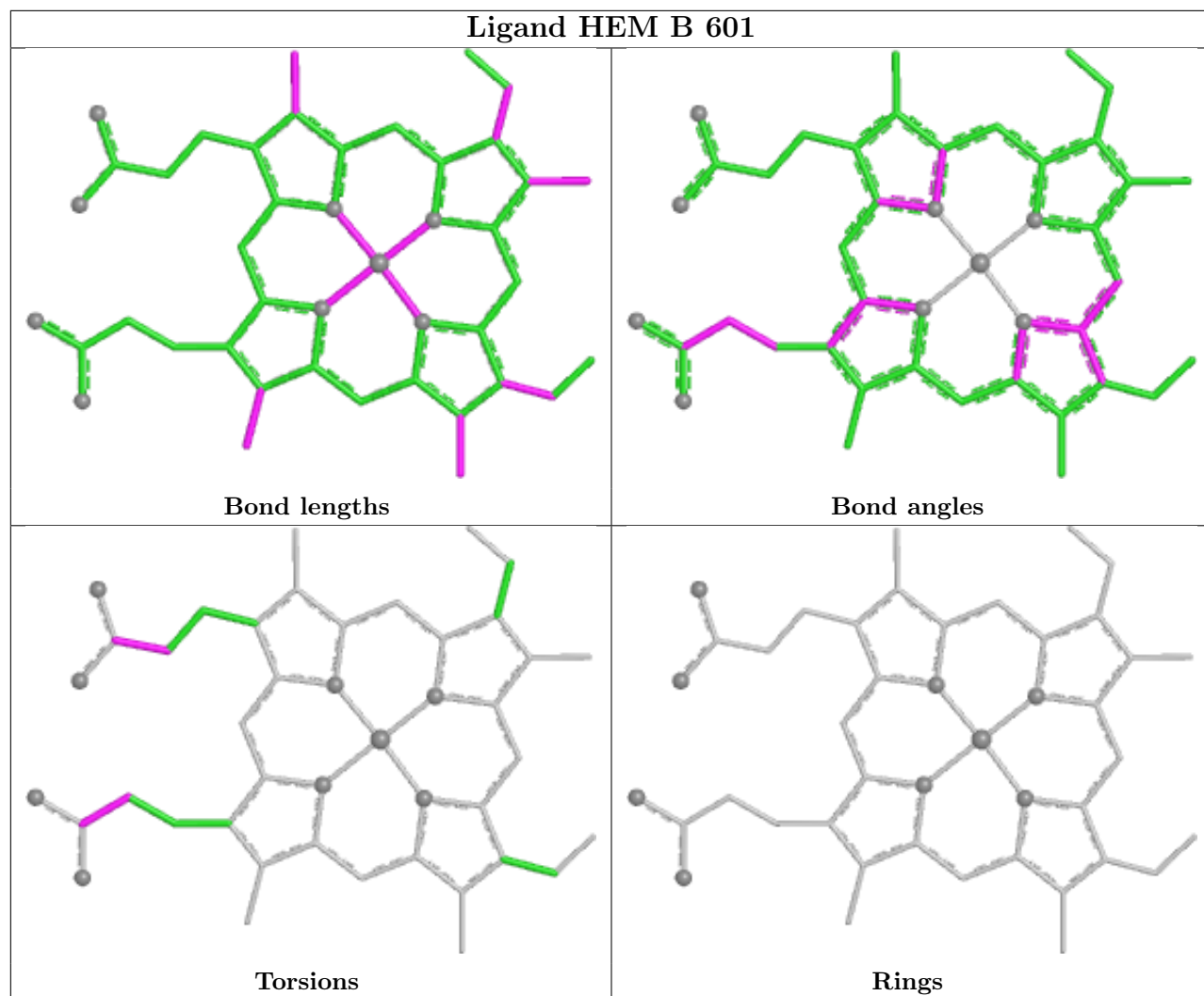


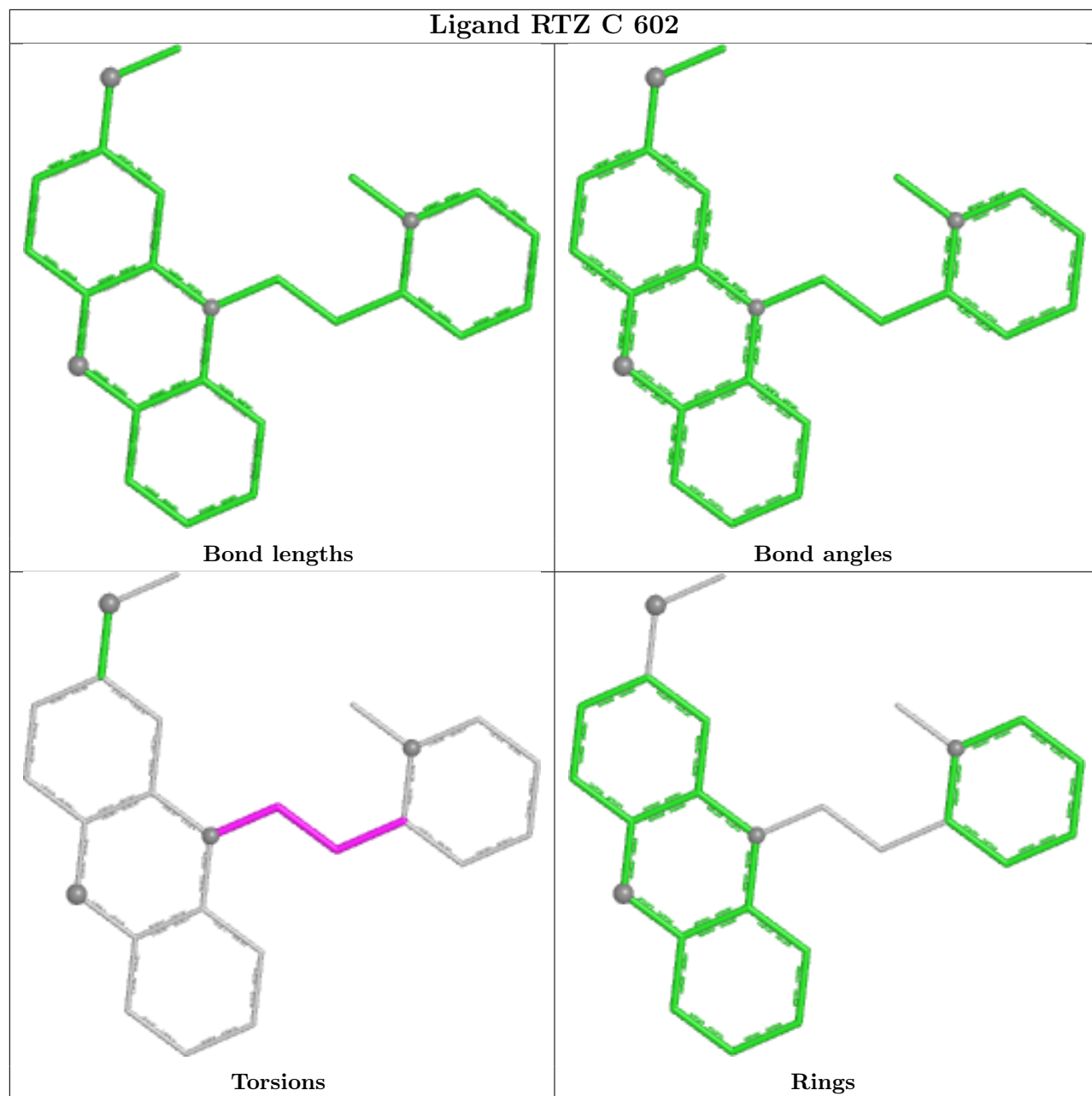


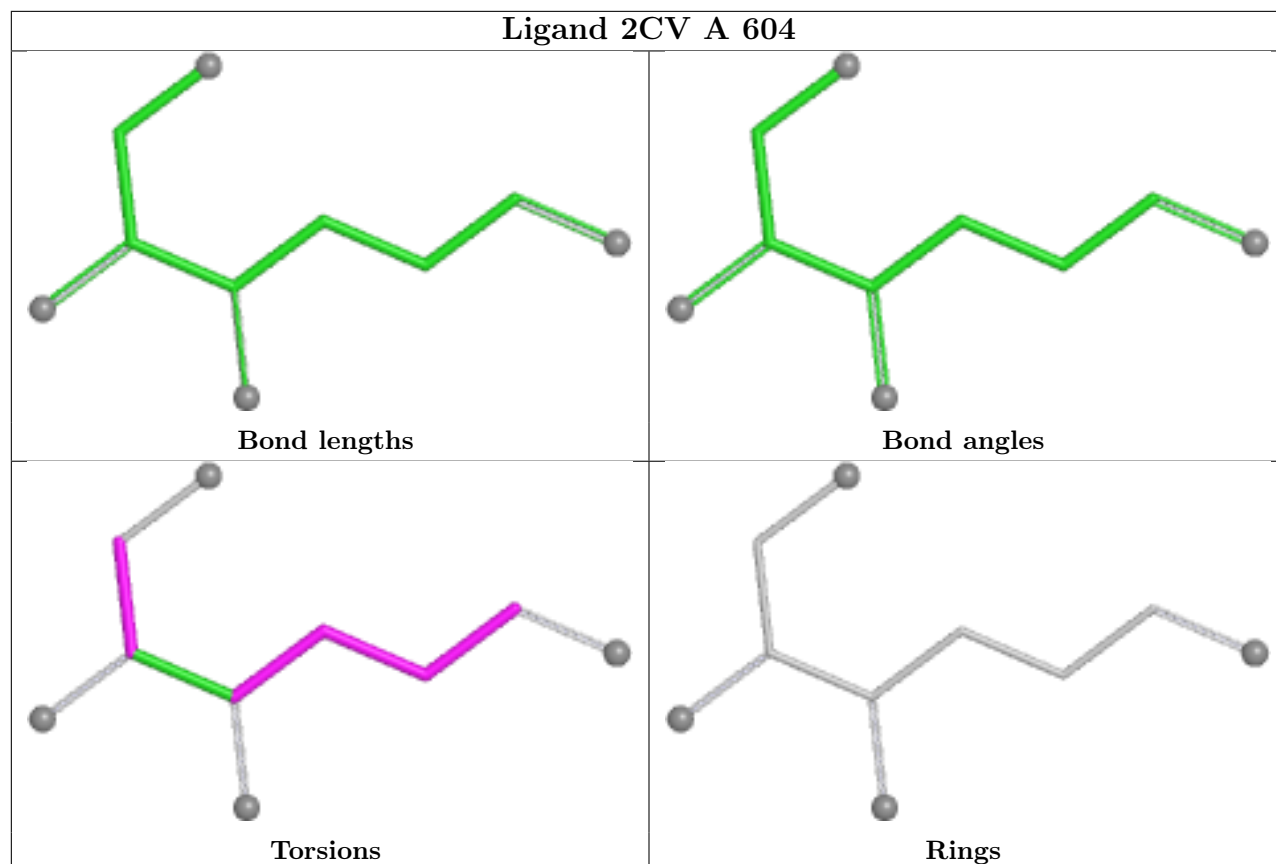












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	452/479 (94%)	0.52	42 (9%) 14 11	20, 43, 90, 111	2 (0%)
1	B	455/479 (94%)	0.55	45 (9%) 13 9	19, 43, 85, 113	5 (1%)
1	C	454/479 (94%)	0.95	82 (18%) 3 3	22, 51, 97, 135	3 (0%)
1	D	453/479 (94%)	0.88	73 (16%) 4 4	23, 49, 98, 124	3 (0%)
All	All	1814/1916 (94%)	0.72	242 (13%) 7 5	19, 46, 93, 135	13 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	PRO	6.4
1	C	483	PHE	6.4
1	D	74	ALA	5.7
1	D	481	PHE	5.6
1	C	112	PHE	5.4
1	D	483	PHE	5.2
1	C	56	TYR	5.2
1	C	481	PHE	5.2
1	D	240	VAL	5.1
1	D	472	GLN	5.0
1	A	74	ALA	4.8
1	D	146[A]	LYS	4.7
1	D	213	LEU	4.6
1	D	482	ALA	4.5
1	C	38	LEU	4.4
1	A	227	VAL	4.4
1	B	74	ALA	4.4
1	D	56	TYR	4.4
1	C	53	ASN	4.3
1	A	144	LEU	4.3
1	D	55	PRO	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	146[A]	LYS	4.2
1	B	52	GLN	4.2
1	B	75	TRP	4.2
1	C	77	PRO	4.2
1	C	213	LEU	4.1
1	C	55	PRO	4.1
1	B	38	LEU	4.1
1	C	78	VAL	4.0
1	A	228	PRO	4.0
1	D	463	HIS	3.9
1	D	54	THR	3.9
1	B	146[A]	LYS	3.9
1	C	219	PHE	3.8
1	D	33	LEU	3.8
1	D	220	LEU	3.8
1	D	37	PRO	3.8
1	A	213	LEU	3.8
1	C	342	VAL	3.8
1	C	74	ALA	3.7
1	C	169	GLY	3.7
1	C	229	VAL	3.7
1	C	424	GLN	3.7
1	C	482	ALA	3.7
1	D	423	ALA	3.7
1	D	169	GLY	3.6
1	A	229	VAL	3.6
1	C	479	GLY	3.6
1	C	471	GLY	3.6
1	A	233	ILE	3.6
1	A	75	TRP	3.6
1	D	469	PRO	3.5
1	B	472	GLN	3.5
1	C	65	PHE	3.5
1	D	77	PRO	3.4
1	B	70	SER	3.4
1	C	463	HIS	3.4
1	C	145	GLY	3.4
1	D	73	LEU	3.4
1	B	483	PHE	3.4
1	C	337	ASP	3.4
1	A	234	PRO	3.4
1	C	73	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	112	PHE	3.3
1	B	56	TYR	3.3
1	D	229	VAL	3.3
1	D	471	GLY	3.3
1	B	33	LEU	3.3
1	A	483	PHE	3.3
1	D	470	THR	3.3
1	A	337	ASP	3.3
1	C	75	TRP	3.3
1	B	240	VAL	3.3
1	C	31	GLY	3.2
1	B	234	PRO	3.2
1	C	426	HIS	3.2
1	D	424	GLN	3.2
1	C	33	LEU	3.2
1	B	469	PRO	3.2
1	A	342	VAL	3.2
1	A	145	GLY	3.2
1	A	33	LEU	3.2
1	B	219	PHE	3.1
1	C	146[A]	LYS	3.1
1	C	144	LEU	3.1
1	D	388	ARG	3.1
1	D	57	CYS	3.1
1	C	240	VAL	3.1
1	D	70	SER	3.0
1	D	65	PHE	3.0
1	B	144	LEU	3.0
1	D	71	LEU	3.0
1	D	78	VAL	3.0
1	D	344	ARG	3.0
1	D	61	LEU	3.0
1	D	426	HIS	3.0
1	D	218	GLY	3.0
1	D	144	LEU	2.9
1	D	145	GLY	2.9
1	D	72	GLN	2.9
1	A	232	HIS	2.9
1	B	229	VAL	2.9
1	D	342	VAL	2.9
1	C	389	ILE	2.9
1	A	147	LYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	242	ARG	2.9
1	A	72	GLN	2.9
1	C	423	ALA	2.9
1	C	472	GLN	2.9
1	A	480	VAL	2.9
1	C	227	VAL	2.9
1	C	54	THR	2.9
1	C	335	ILE	2.9
1	D	236	LEU	2.8
1	D	237	ALA	2.8
1	A	240	VAL	2.8
1	A	481	PHE	2.8
1	B	226	ALA	2.8
1	D	226	ALA	2.8
1	D	32	LYS	2.8
1	C	450	ARG	2.8
1	B	335	ILE	2.8
1	A	112	PHE	2.8
1	D	112	PHE	2.8
1	A	236	LEU	2.7
1	B	237	ALA	2.7
1	C	234	PRO	2.7
1	C	388	ARG	2.7
1	B	498	HIS	2.7
1	C	212	GLY	2.7
1	D	473	PRO	2.7
1	C	115	ARG	2.7
1	C	59	ASP	2.7
1	C	217	SER	2.7
1	C	379	SER	2.7
1	B	218	GLY	2.6
1	B	330[A]	ARG	2.6
1	D	69	PHE	2.6
1	A	469	PRO	2.6
1	C	339	ILE	2.6
1	D	52	GLN	2.6
1	B	481	PHE	2.6
1	A	73	LEU	2.6
1	B	73	LEU	2.6
1	C	425	GLY	2.6
1	B	61	LEU	2.5
1	C	470	THR	2.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	167	HIS	2.5
1	A	219	PHE	2.5
1	C	110	LEU	2.5
1	C	114	PRO	2.5
1	D	234	PRO	2.5
1	B	227	VAL	2.5
1	D	115	ARG	2.5
1	A	220	LEU	2.5
1	A	241	LEU	2.5
1	B	220	LEU	2.5
1	C	478	HIS	2.5
1	D	232	HIS	2.5
1	C	37	PRO	2.5
1	C	333	GLN	2.5
1	C	469	PRO	2.5
1	D	450	ARG	2.4
1	C	71	LEU	2.4
1	D	484	LEU	2.4
1	D	60	GLN	2.4
1	C	340	GLY	2.4
1	C	168	SER	2.4
1	D	75	TRP	2.4
1	A	56	TYR	2.4
1	D	79	VAL	2.4
1	B	380	ARG	2.4
1	A	225	ASN	2.4
1	C	383	GLU	2.4
1	C	113	GLY	2.4
1	A	223	VAL	2.4
1	D	227	VAL	2.4
1	C	380	ARG	2.4
1	C	341	GLN	2.4
1	C	222	GLU	2.4
1	A	340	GLY	2.3
1	B	31	GLY	2.3
1	D	235	ALA	2.3
1	B	474	ARG	2.3
1	A	53	ASN	2.3
1	D	228	PRO	2.3
1	A	335	ILE	2.3
1	B	339	ILE	2.3
1	B	78	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	147	LYS	2.3
1	D	53	ASN	2.3
1	B	37	PRO	2.3
1	B	133	ARG	2.3
1	B	232	HIS	2.3
1	C	232	HIS	2.3
1	C	72	GLN	2.3
1	C	69	PHE	2.2
1	C	224	LEU	2.2
1	D	224	LEU	2.2
1	A	224	LEU	2.2
1	C	480	VAL	2.2
1	D	241	LEU	2.2
1	D	243	PHE	2.2
1	A	77	PRO	2.2
1	D	63	ARG	2.2
1	B	471	GLY	2.2
1	C	226	ALA	2.2
1	C	149	LEU	2.2
1	C	233	ILE	2.2
1	D	468	VAL	2.2
1	B	228	PRO	2.2
1	D	31	GLY	2.2
1	C	76	THR	2.2
1	C	63	ARG	2.1
1	B	206	LEU	2.1
1	B	236	LEU	2.1
1	C	106	ILE	2.1
1	C	166	ASN	2.1
1	C	221	ARG	2.1
1	C	214	LYS	2.1
1	C	236	LEU	2.1
1	D	114	PRO	2.1
1	B	173	ARG	2.1
1	C	116	SER	2.1
1	B	59	ASP	2.1
1	B	60	GLN	2.1
1	C	167	HIS	2.1
1	A	105	PRO	2.1
1	D	58	PHE	2.1
1	A	498	HIS	2.0
1	B	53	ASN	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	230	LEU	2.0
1	D	382	ILE	2.0
1	A	380	ARG	2.0
1	D	384	VAL	2.0
1	D	474	ARG	2.0
1	A	111	GLY	2.0
1	C	172	PHE	2.0
1	D	381	ASP	2.0
1	A	62	ARG	2.0
1	A	106	ILE	2.0
1	D	322	ILE	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 oligosaccharides 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.

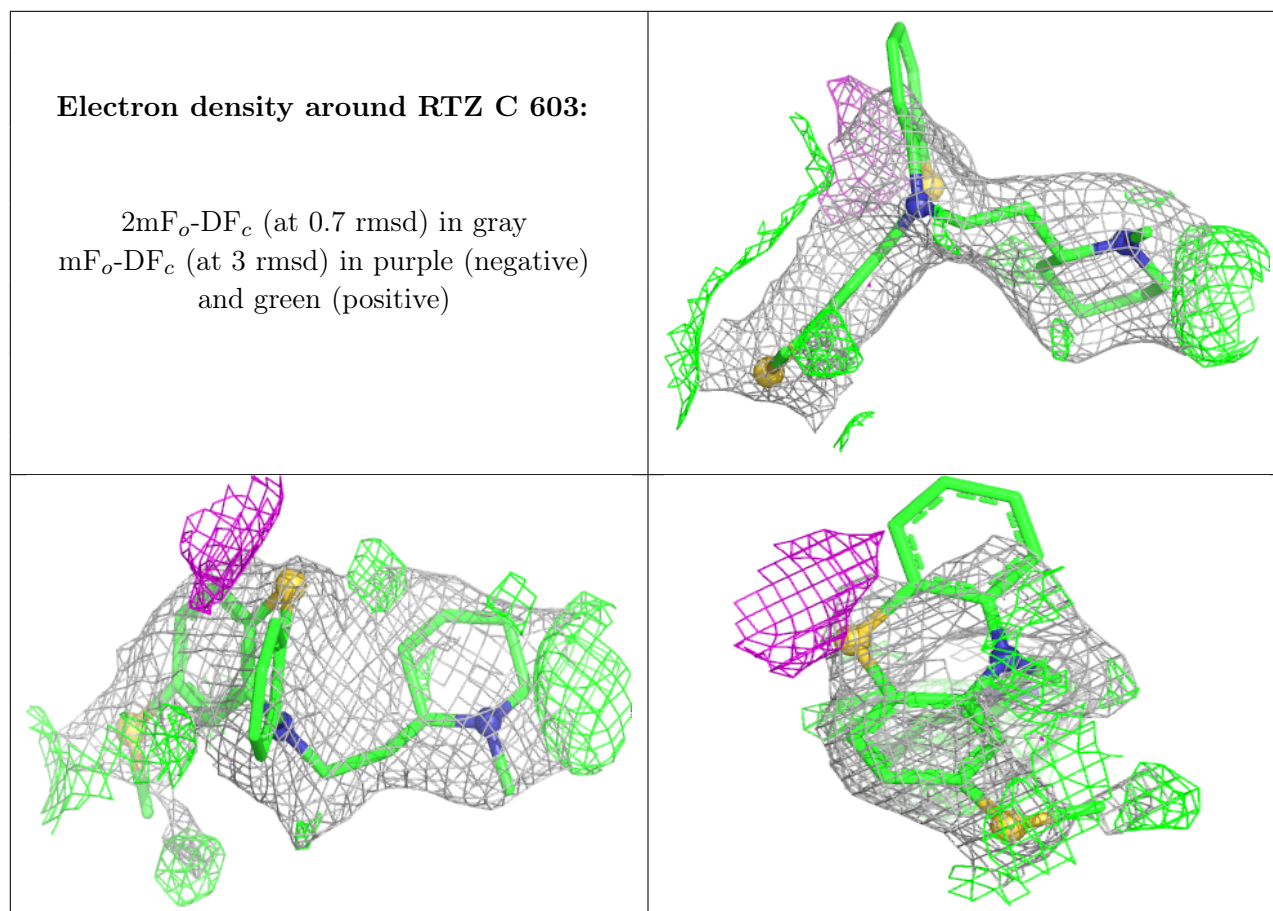
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	RTZ	C	603	25/25	0.66	0.31	73,118,134,151	0
5	ZN	C	607	1/1	0.68	0.16	139,139,139,139	0
3	RTZ	D	603	25/25	0.71	0.38	87,124,166,168	0
6	ACT	B	604	4/4	0.72	0.30	60,68,74,98	0
3	RTZ	A	603	25/25	0.76	0.30	72,98,136,163	0
4	2CV	C	605	7/26	0.79	0.22	41,68,80,81	0
3	RTZ	B	603	25/25	0.81	0.23	67,89,117,127	0
5	ZN	B	608	1/1	0.83	0.11	121,121,121,121	0
4	2CV	B	605	7/26	0.85	0.28	37,93,115,125	0
3	RTZ	D	602	25/25	0.87	0.17	54,74,92,95	0
3	RTZ	C	602	25/25	0.88	0.19	58,87,113,122	0
7	GOL	C	604	6/6	0.88	0.15	55,75,78,82	0

*Continued on next page...*

Continued from previous page...

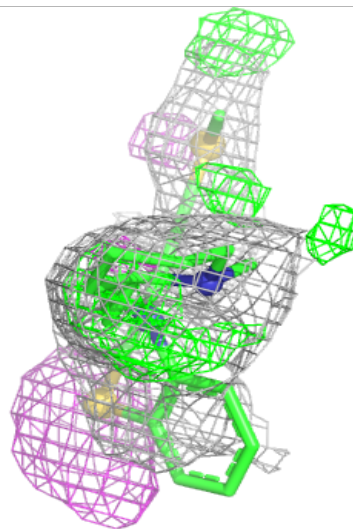
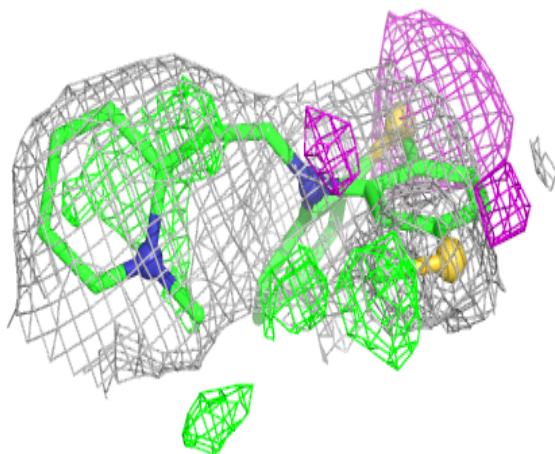
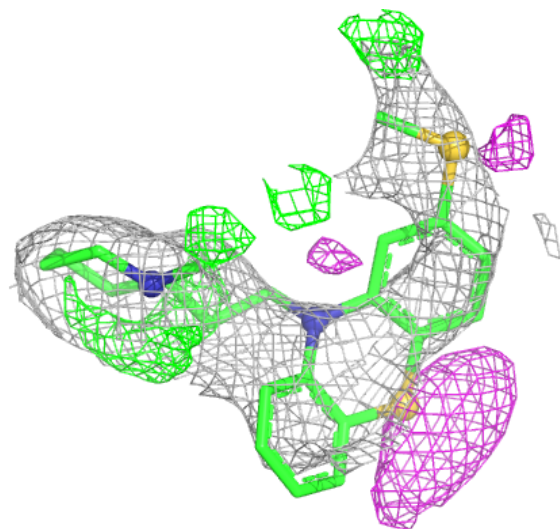
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	RTZ	A	602	25/25	0.90	0.16	55,72,85,102	0
3	RTZ	B	602	25/25	0.91	0.13	44,59,70,75	0
4	2CV	A	604	10/26	0.91	0.22	39,75,98,105	0
5	ZN	A	607	1/1	0.93	0.10	104,104,104,104	0
5	ZN	B	607	1/1	0.93	0.12	110,110,110,110	0
2	HEM	B	601	43/43	0.98	0.08	18,25,30,34	0
2	HEM	C	601	43/43	0.98	0.07	23,31,36,44	0
2	HEM	D	601	43/43	0.98	0.07	18,28,32,34	0
2	HEM	A	601	43/43	0.98	0.07	18,26,29,32	0
5	ZN	A	606	1/1	0.99	0.04	46,46,46,46	0
5	ZN	D	604	1/1	0.99	0.03	37,37,37,37	0
5	ZN	B	606	1/1	1.00	0.03	38,38,38,38	0
5	ZN	C	606	1/1	1.00	0.01	36,36,36,36	0
5	ZN	A	605	1/1	1.00	0.04	38,38,38,38	0

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



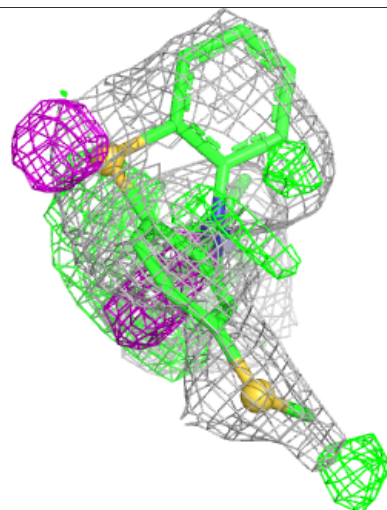
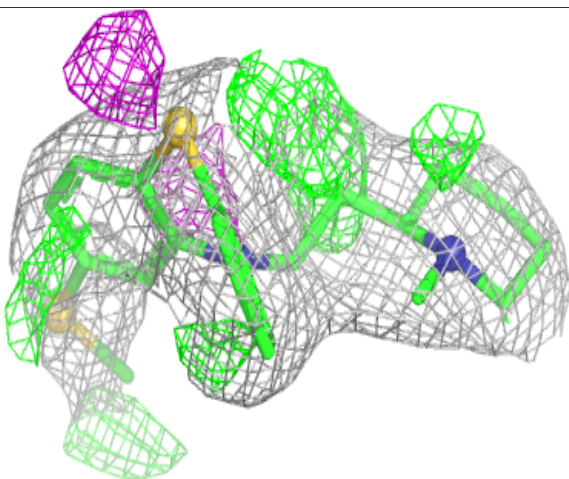
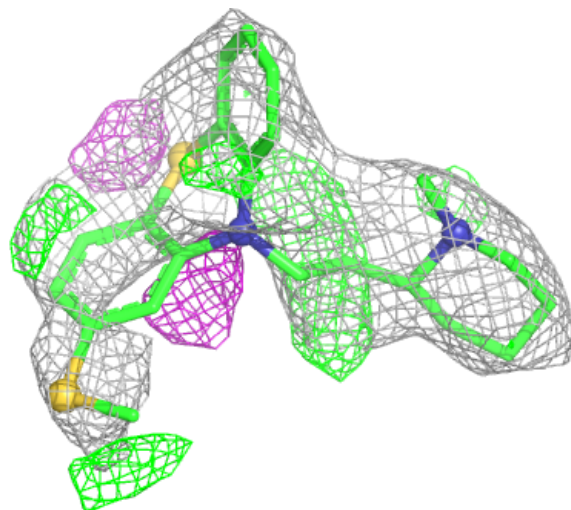
**Electron density around RTZ D 603:**

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



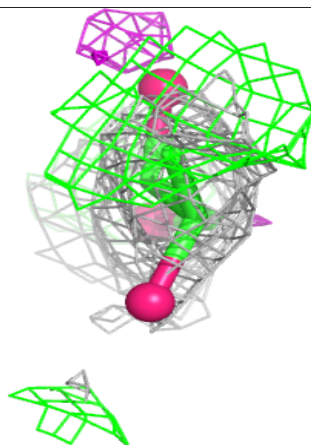
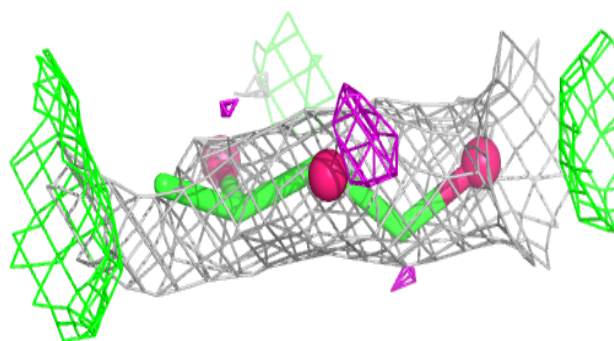
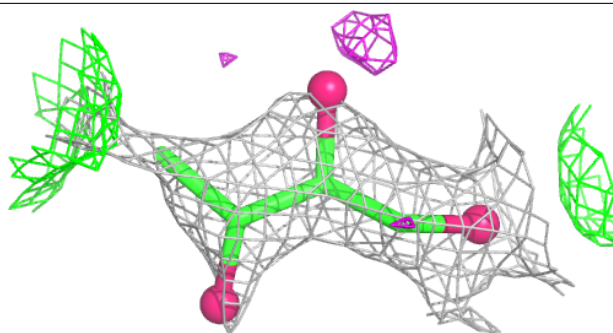
**Electron density around RTZ A 603:**

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



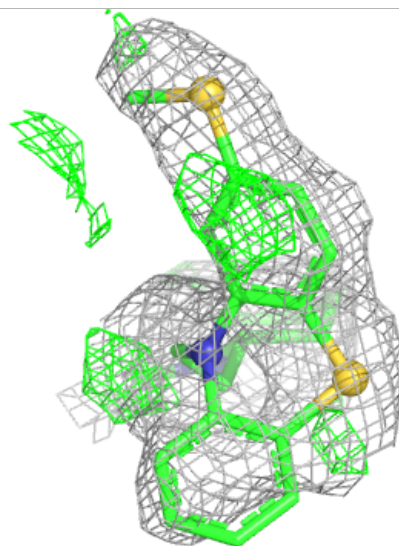
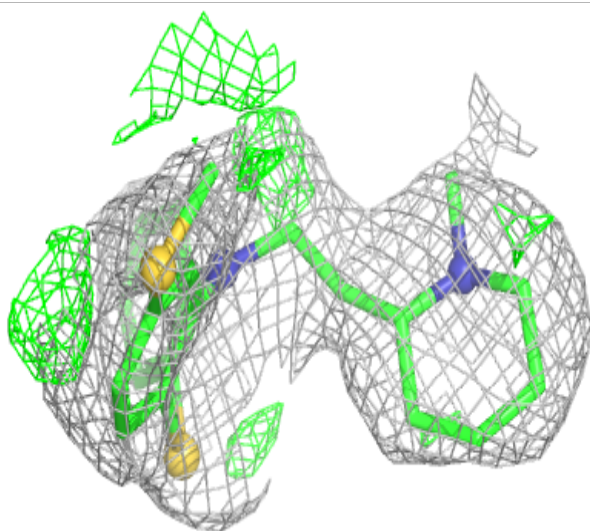
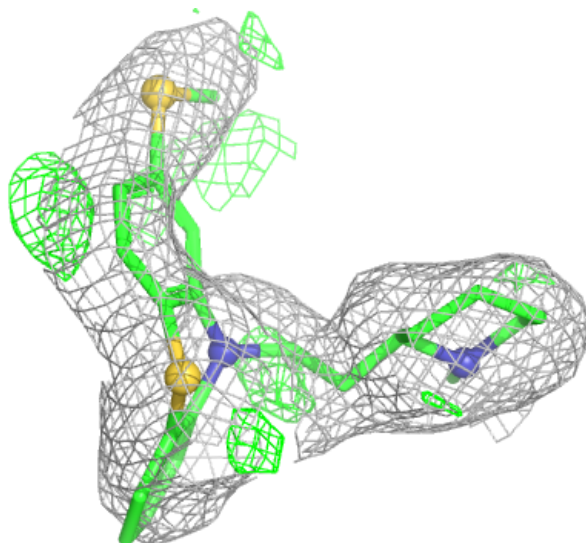
**Electron density around 2CV C 605:**

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



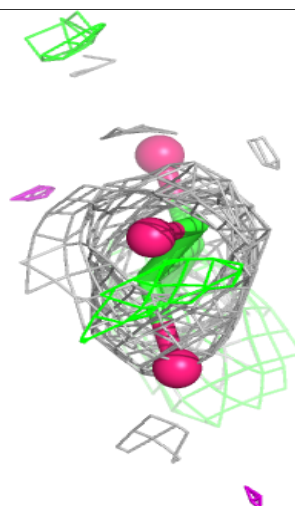
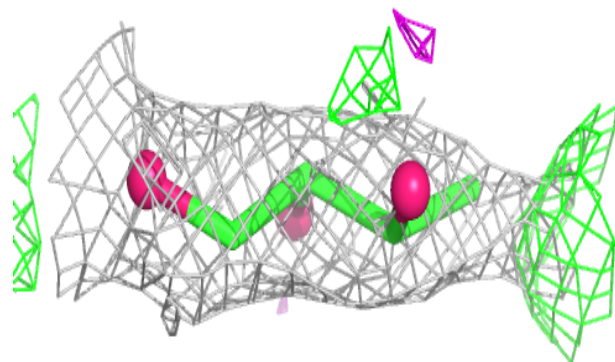
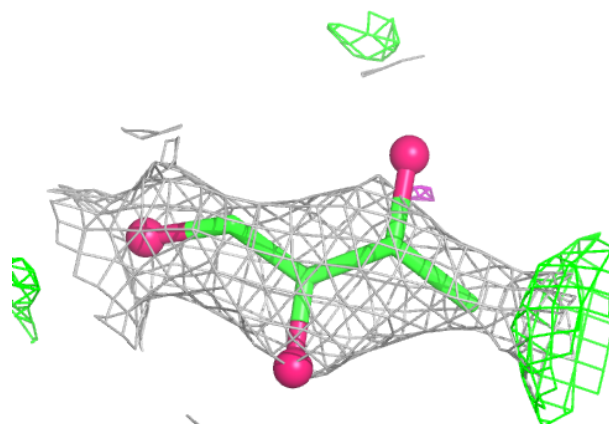
**Electron density around RTZ B 603:**

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



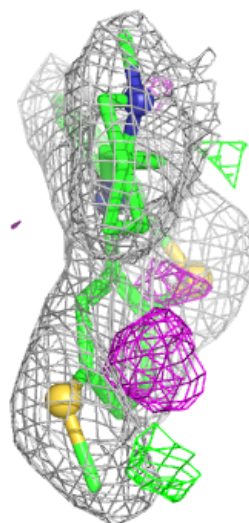
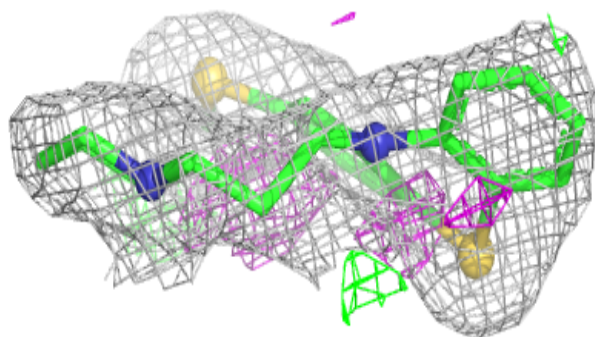
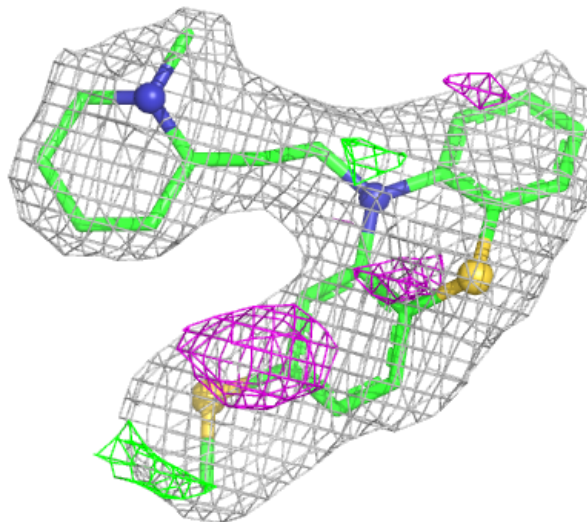
**Electron density around 2CV B 605:**

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



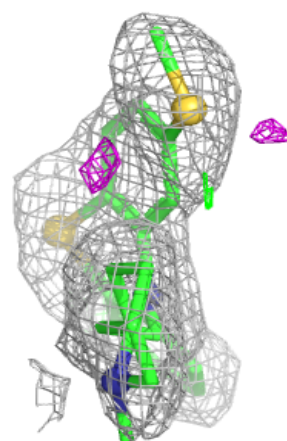
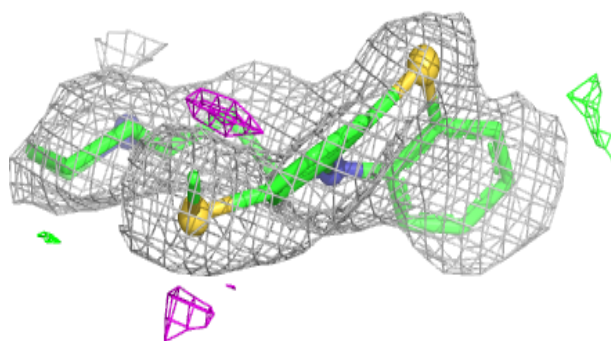
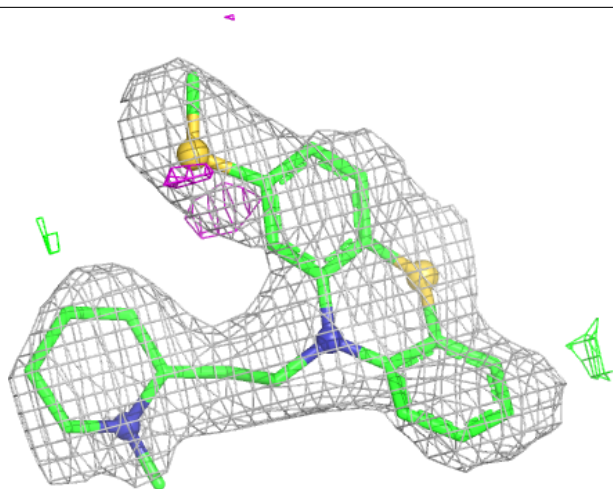
**Electron density around RTZ D 602:**

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



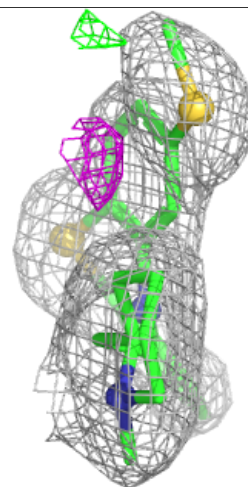
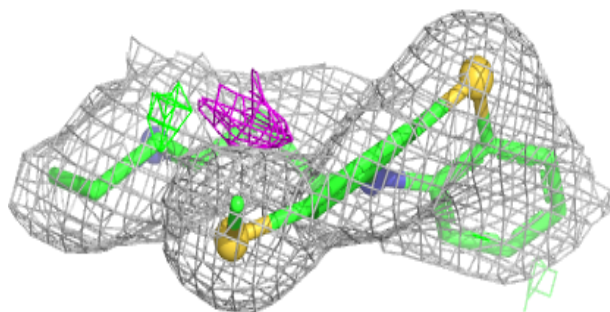
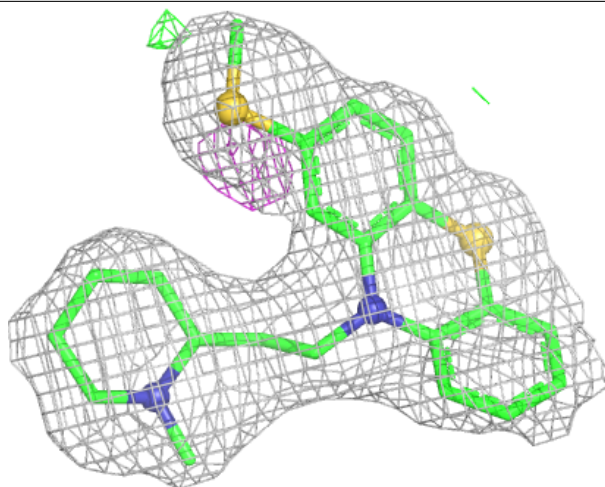
**Electron density around RTZ C 602:**

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



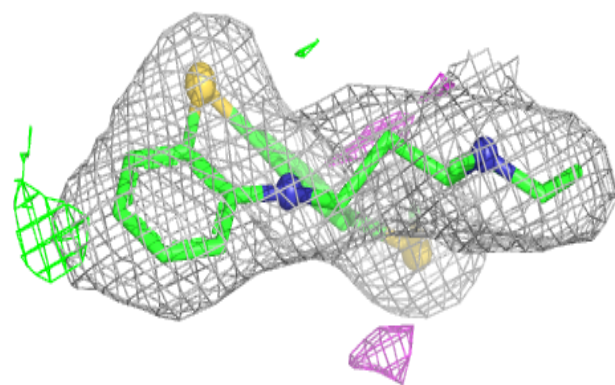
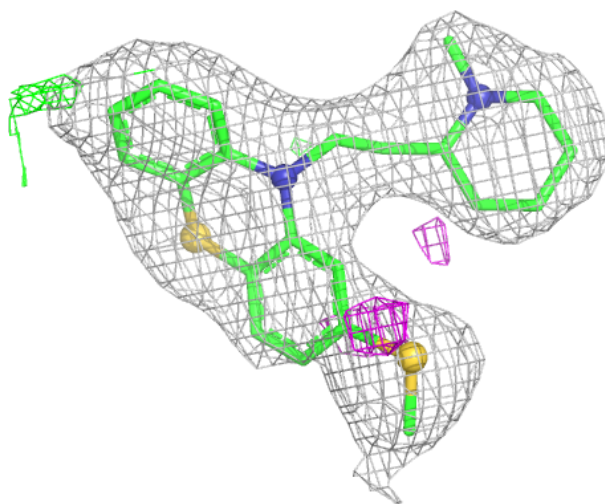
**Electron density around RTZ A 602:**

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



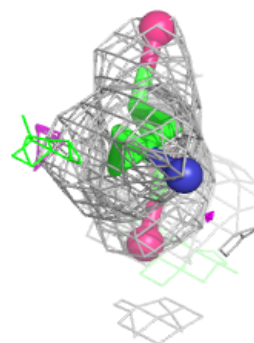
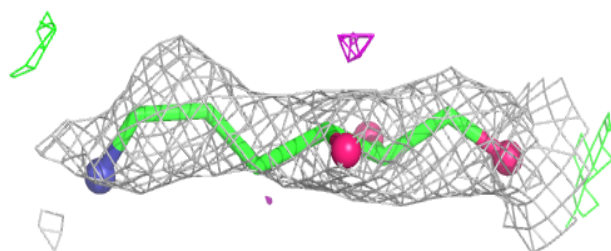
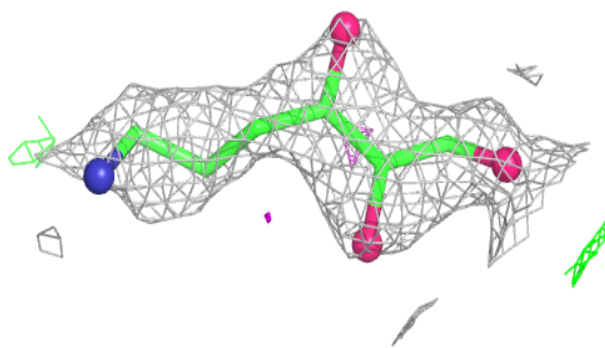
**Electron density around RTZ B 602:**

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



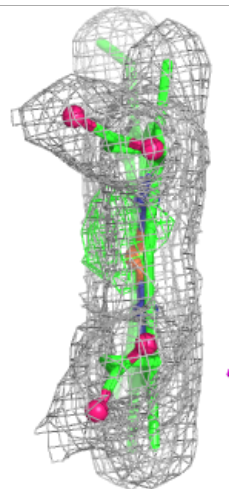
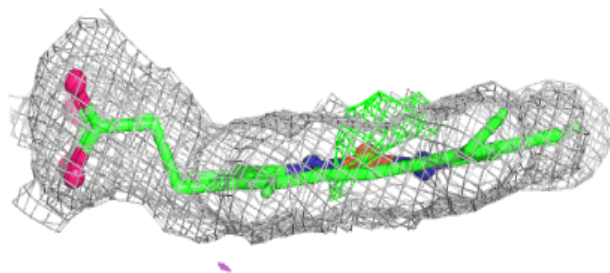
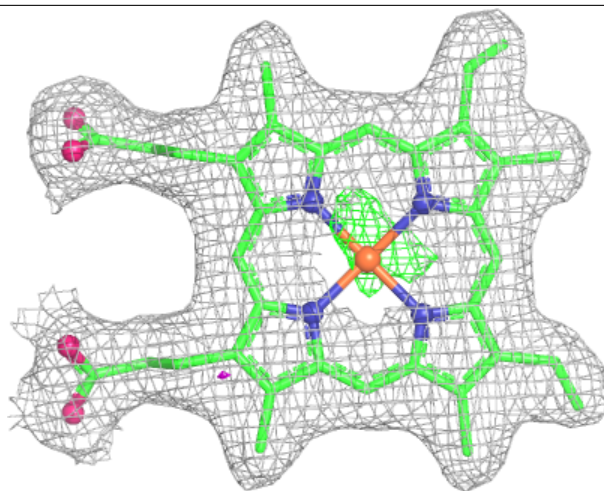
**Electron density around 2CV A 604:**

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



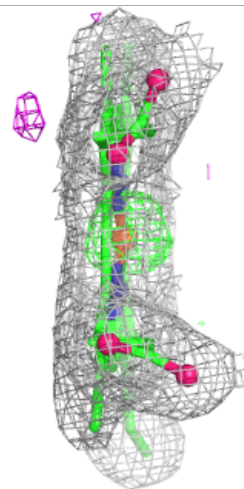
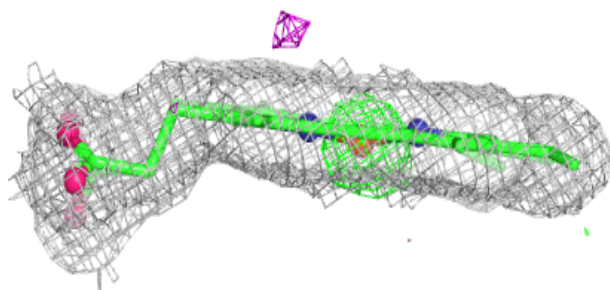
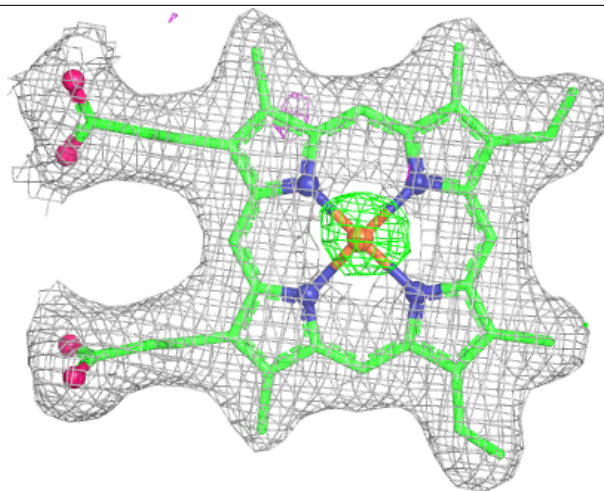
**Electron density around HEM B 601:**

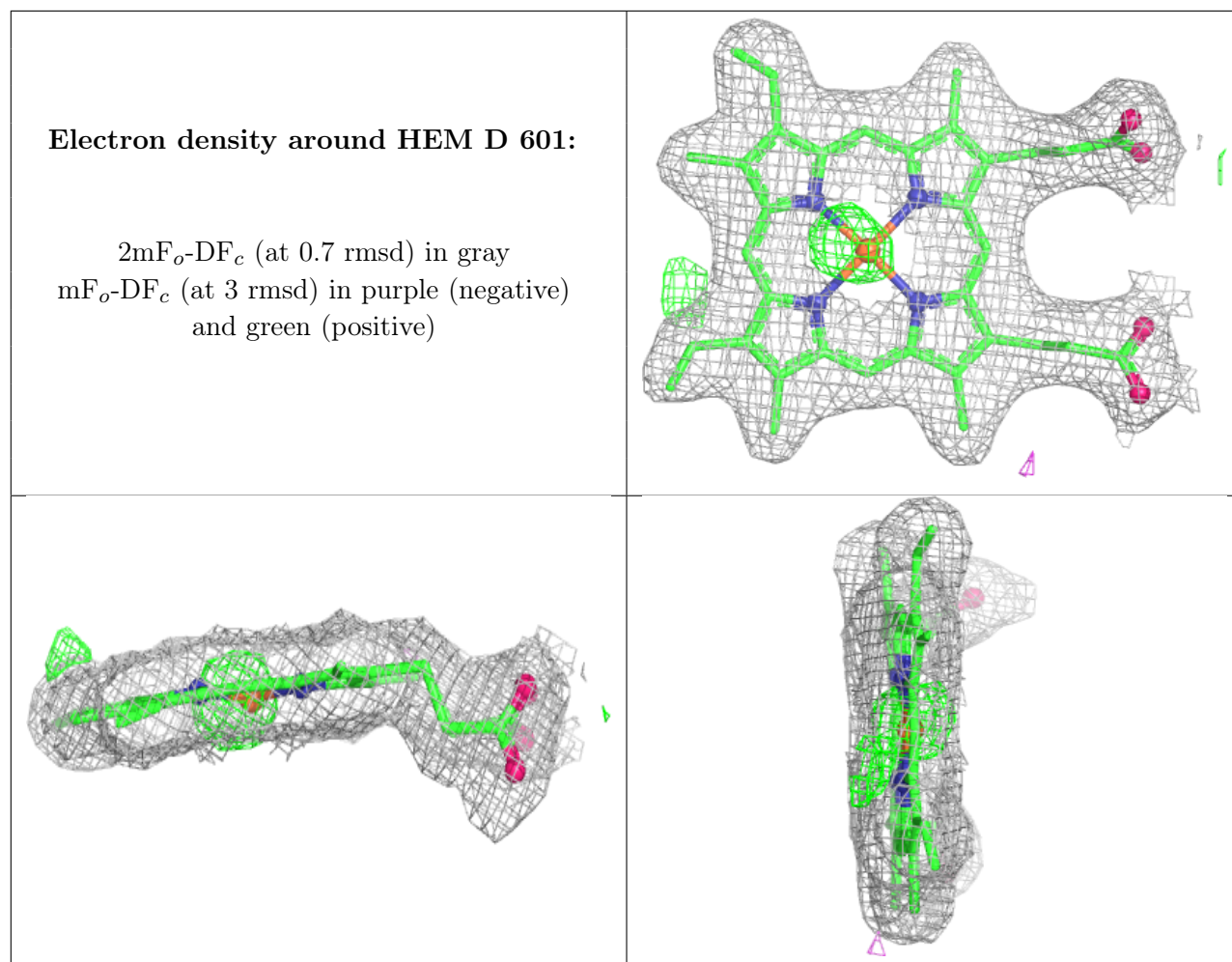
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

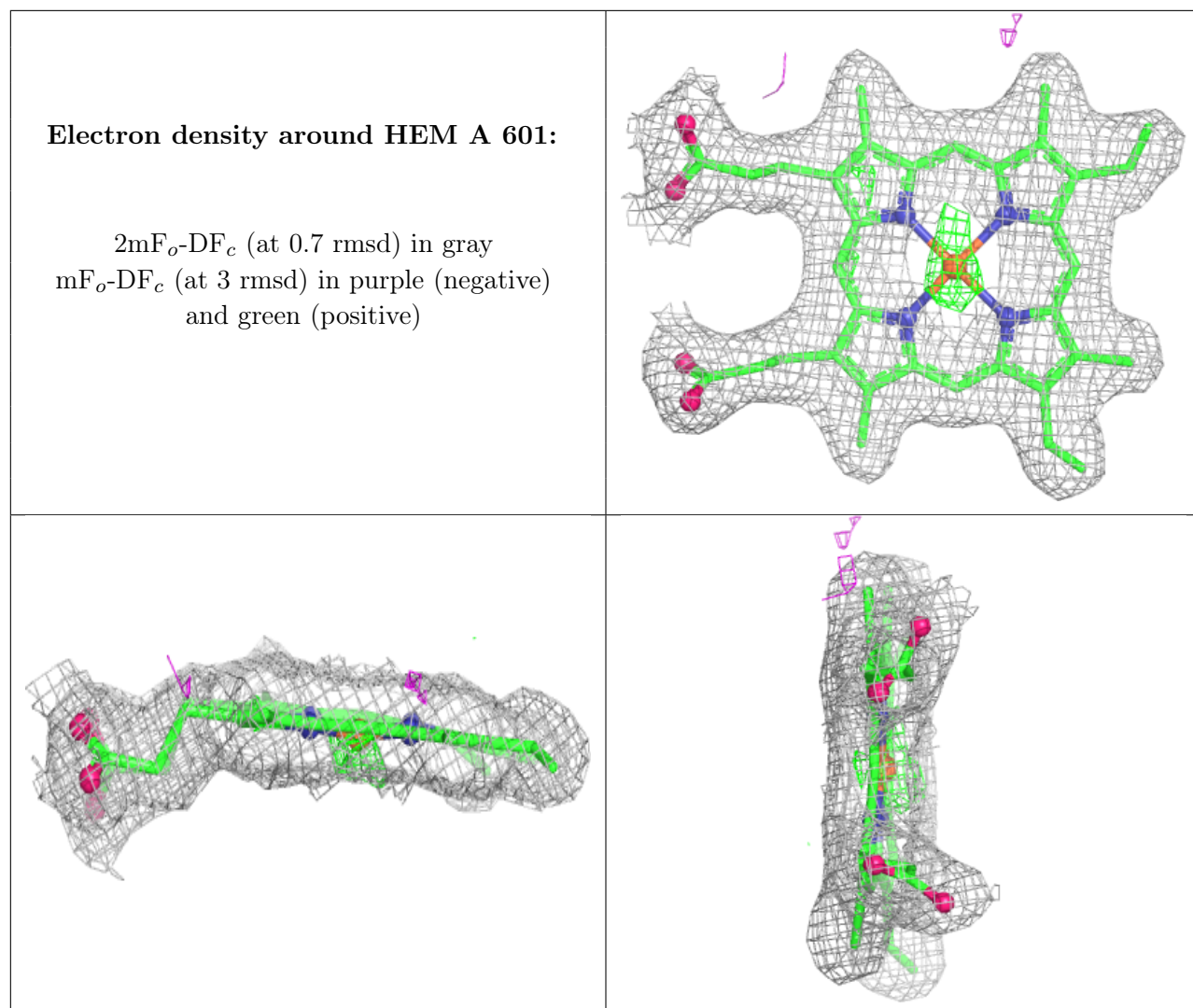


**Electron density around HEM C 601:**

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







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.