



Full wwPDB X-ray Structure Validation Report i

Jul 24, 2023 – 04:07 PM EDT

PDB ID : 8EKT
Title : CYP51 from Acanthamoeba castellanii in complex with the tetrazole-based IND inhibitor VT-1161(VT1)
Authors : Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on : 2022-09-21
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i 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](#) i) 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 : 2.34
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 (Gargroove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

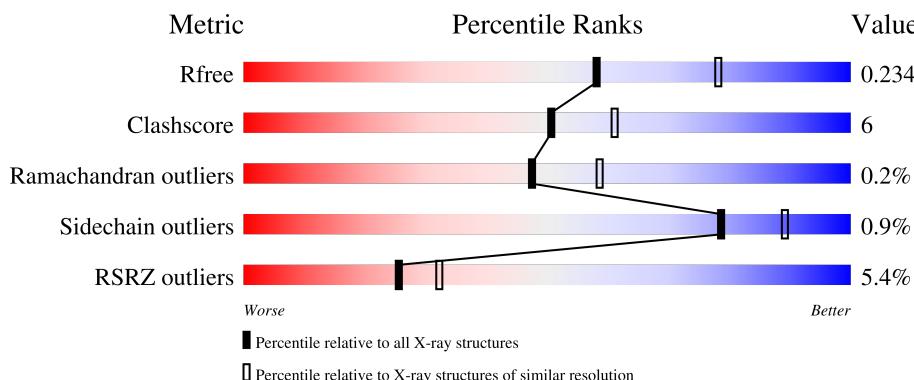
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain		
1	F	460	7%	81%	8% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20818 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 sterol 14a-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C 3336	N 2153	O 561	S 604	18	0	0
1	B	413	Total	C 3332	N 2150	O 560	S 604	18	0	0
1	C	413	Total	C 3324	N 2145	O 558	S 603	18	0	0
1	D	413	Total	C 3306	N 2134	O 554	S 600	18	0	0
1	E	413	Total	C 3300	N 2126	O 552	S 604	18	0	0
1	F	413	Total	C 3292	N 2125	O 548	S 601	18	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	initiating methionine	UNP L8GJB3
A	34	ALA	-	expression tag	UNP L8GJB3
A	35	LYS	-	expression tag	UNP L8GJB3
A	36	LYS	-	expression tag	UNP L8GJB3
A	37	THR	-	expression tag	UNP L8GJB3
A	38	SER	-	expression tag	UNP L8GJB3
A	39	SER	-	expression tag	UNP L8GJB3
A	40	LYS	-	expression tag	UNP L8GJB3
A	41	GLY	-	expression tag	UNP L8GJB3
A	42	LYS	-	expression tag	UNP L8GJB3
A	487	HIS	-	expression tag	UNP L8GJB3
A	488	HIS	-	expression tag	UNP L8GJB3
A	489	HIS	-	expression tag	UNP L8GJB3
A	490	HIS	-	expression tag	UNP L8GJB3
A	491	HIS	-	expression tag	UNP L8GJB3
A	492	HIS	-	expression tag	UNP L8GJB3
B	33	MET	-	initiating methionine	UNP L8GJB3

Continued on next page...

Continued from previous page...

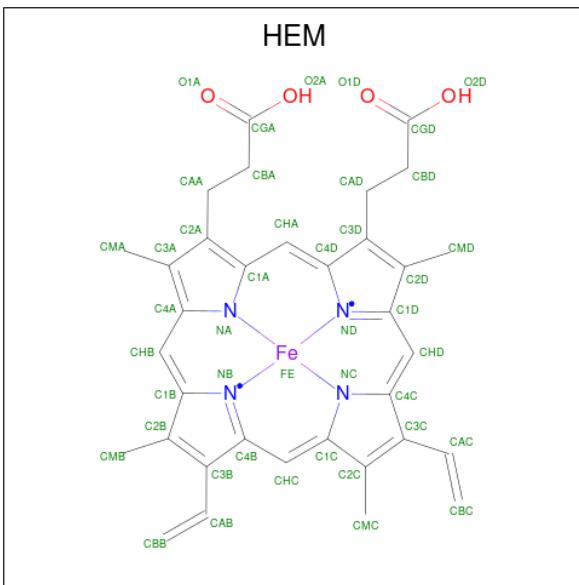
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
B	41	GLY	-	expression tag	UNP L8GJB3
B	42	LYS	-	expression tag	UNP L8GJB3
B	487	HIS	-	expression tag	UNP L8GJB3
B	488	HIS	-	expression tag	UNP L8GJB3
B	489	HIS	-	expression tag	UNP L8GJB3
B	490	HIS	-	expression tag	UNP L8GJB3
B	491	HIS	-	expression tag	UNP L8GJB3
B	492	HIS	-	expression tag	UNP L8GJB3
C	33	MET	-	initiating methionine	UNP L8GJB3
C	34	ALA	-	expression tag	UNP L8GJB3
C	35	LYS	-	expression tag	UNP L8GJB3
C	36	LYS	-	expression tag	UNP L8GJB3
C	37	THR	-	expression tag	UNP L8GJB3
C	38	SER	-	expression tag	UNP L8GJB3
C	39	SER	-	expression tag	UNP L8GJB3
C	40	LYS	-	expression tag	UNP L8GJB3
C	41	GLY	-	expression tag	UNP L8GJB3
C	42	LYS	-	expression tag	UNP L8GJB3
C	487	HIS	-	expression tag	UNP L8GJB3
C	488	HIS	-	expression tag	UNP L8GJB3
C	489	HIS	-	expression tag	UNP L8GJB3
C	490	HIS	-	expression tag	UNP L8GJB3
C	491	HIS	-	expression tag	UNP L8GJB3
C	492	HIS	-	expression tag	UNP L8GJB3
D	33	MET	-	initiating methionine	UNP L8GJB3
D	34	ALA	-	expression tag	UNP L8GJB3
D	35	LYS	-	expression tag	UNP L8GJB3
D	36	LYS	-	expression tag	UNP L8GJB3
D	37	THR	-	expression tag	UNP L8GJB3
D	38	SER	-	expression tag	UNP L8GJB3
D	39	SER	-	expression tag	UNP L8GJB3
D	40	LYS	-	expression tag	UNP L8GJB3
D	41	GLY	-	expression tag	UNP L8GJB3
D	42	LYS	-	expression tag	UNP L8GJB3
D	487	HIS	-	expression tag	UNP L8GJB3

Continued on next page...

Continued from previous page...

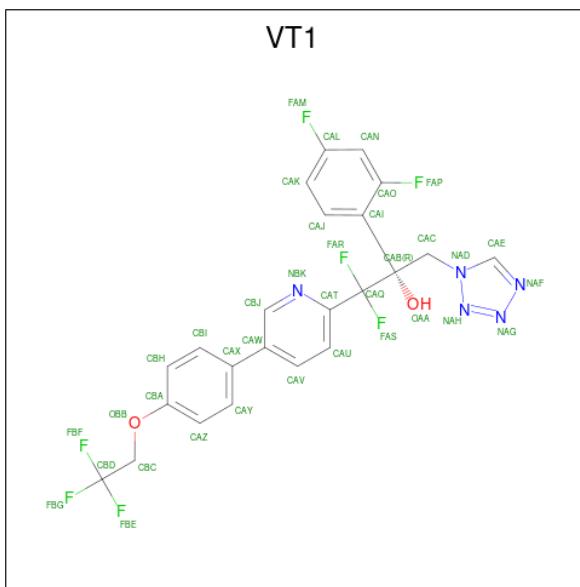
Chain	Residue	Modelled	Actual	Comment	Reference
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3
D	492	HIS	-	expression tag	UNP L8GJB3
E	33	MET	-	initiating methionine	UNP L8GJB3
E	34	ALA	-	expression tag	UNP L8GJB3
E	35	LYS	-	expression tag	UNP L8GJB3
E	36	LYS	-	expression tag	UNP L8GJB3
E	37	THR	-	expression tag	UNP L8GJB3
E	38	SER	-	expression tag	UNP L8GJB3
E	39	SER	-	expression tag	UNP L8GJB3
E	40	LYS	-	expression tag	UNP L8GJB3
E	41	GLY	-	expression tag	UNP L8GJB3
E	42	LYS	-	expression tag	UNP L8GJB3
E	487	HIS	-	expression tag	UNP L8GJB3
E	488	HIS	-	expression tag	UNP L8GJB3
E	489	HIS	-	expression tag	UNP L8GJB3
E	490	HIS	-	expression tag	UNP L8GJB3
E	491	HIS	-	expression tag	UNP L8GJB3
E	492	HIS	-	expression tag	UNP L8GJB3
F	33	MET	-	initiating methionine	UNP L8GJB3
F	34	ALA	-	expression tag	UNP L8GJB3
F	35	LYS	-	expression tag	UNP L8GJB3
F	36	LYS	-	expression tag	UNP L8GJB3
F	37	THR	-	expression tag	UNP L8GJB3
F	38	SER	-	expression tag	UNP L8GJB3
F	39	SER	-	expression tag	UNP L8GJB3
F	40	LYS	-	expression tag	UNP L8GJB3
F	41	GLY	-	expression tag	UNP L8GJB3
F	42	LYS	-	expression tag	UNP L8GJB3
F	487	HIS	-	expression tag	UNP L8GJB3
F	488	HIS	-	expression tag	UNP L8GJB3
F	489	HIS	-	expression tag	UNP L8GJB3
F	490	HIS	-	expression tag	UNP L8GJB3
F	491	HIS	-	expression tag	UNP L8GJB3
F	492	HIS	-	expression tag	UNP L8GJB3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is (R)-2-(2,4-Difluorophenyl)-1,1-difluoro-3-(1H-tetrazol-1-yl)-1-(5-(4-(2,2,2-trifluoroethoxy)phenyl)pyridin-2-yl)propan-2-ol (three-letter code: VT1) (formula: C₂₃H₁₆F₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			37	23	7	5	2		
3	B	1	Total	C	F	N	O	0	0
			37	23	7	5	2		
3	C	1	Total	C	F	N	O	0	0
			37	23	7	5	2		
3	D	1	Total	C	F	N	O	0	0
			37	23	7	5	2		
3	E	1	Total	C	F	N	O	0	0
			37	23	7	5	2		
3	F	1	Total	C	F	N	O	0	0
			37	23	7	5	2		

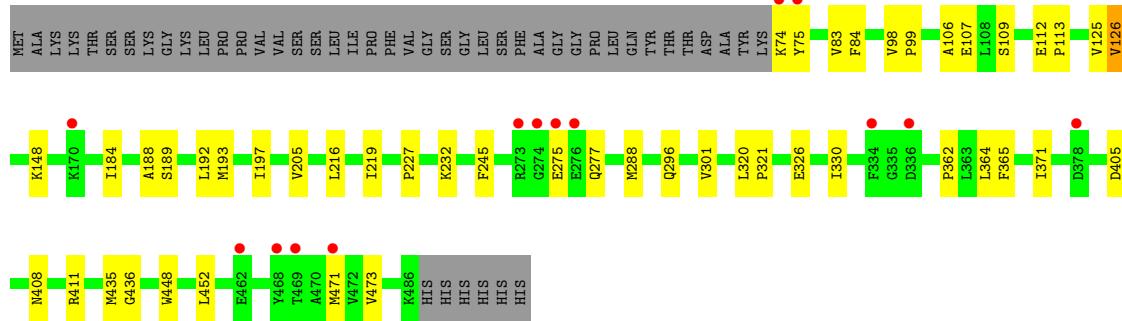
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	85	Total	O	0	0
			85	85		
4	C	79	Total	O	0	0
			79	79		
4	D	60	Total	O	0	0
			60	60		
4	E	53	Total	O	0	0
			53	53		
4	F	50	Total	O	0	0
			50	50		

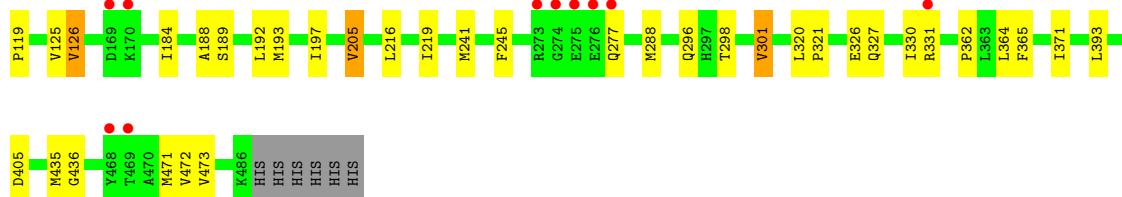
3 Residue-property plots

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.

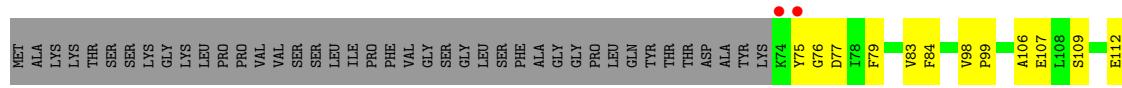
- Molecule 1: sterol 14a-demethylase

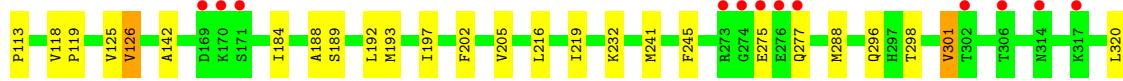


- Molecule 1: sterol 14a-demethylase

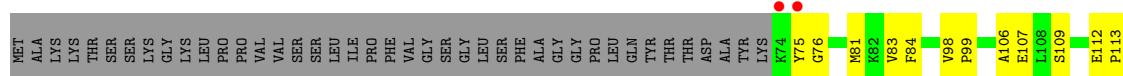
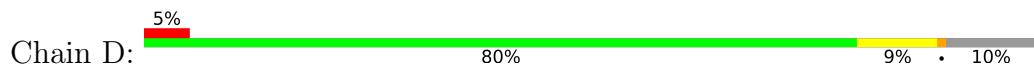


- Molecule 1: sterol 14a-demethylase

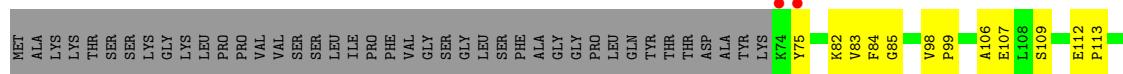
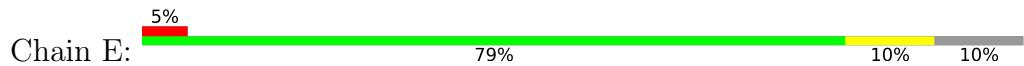




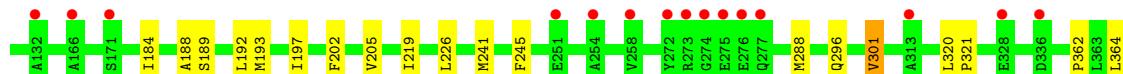
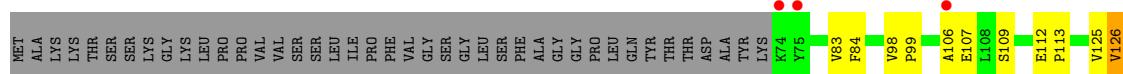
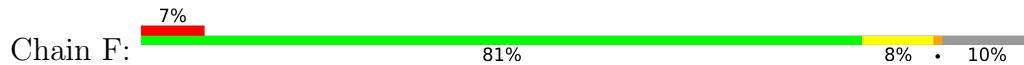
- Molecule 1: sterol 14a-demethylase



- Molecule 1: sterol 14a-demethylase



- Molecule 1: sterol 14a-demethylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.45 Å 99.30 Å 107.92 Å 81.22° 84.08° 60.08°	Depositor
Resolution (Å)	29.89 – 2.29 29.89 – 2.29	Depositor EDS
% Data completeness (in resolution range)	79.0 (29.89-2.29) 79.0 (29.89-2.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.68 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R , R_{free}	0.213 , 0.224 0.219 , 0.234	Depositor DCC
R_{free} test set	6103 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.0	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20818	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: VT1, 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	0.28	0/3416	0.49	0/4615
1	B	0.28	0/3412	0.48	0/4611
1	C	0.27	0/3404	0.47	0/4602
1	D	0.27	0/3386	0.48	0/4582
1	E	0.27	0/3379	0.47	0/4575
1	F	0.28	0/3372	0.48	0/4567
All	All	0.27	0/20369	0.48	0/27552

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	3336	0	3332	39	0
1	B	3332	0	3321	35	0
1	C	3324	0	3304	40	0
1	D	3306	0	3269	35	0
1	E	3300	0	3248	42	0
1	F	3292	0	3234	35	0
2	A	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	4	0
2	E	43	0	30	4	0
2	F	43	0	30	3	0
3	A	37	0	16	3	0
3	B	37	0	16	2	0
3	C	37	0	16	2	0
3	D	37	0	16	3	0
3	E	37	0	16	4	0
3	F	37	0	16	4	0
4	A	121	0	0	0	0
4	B	85	0	0	0	0
4	C	79	0	0	0	0
4	D	60	0	0	0	0
4	E	53	0	0	0	0
4	F	50	0	0	0	0
All	All	20818	0	19984	228	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 6.

All (228) 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:E:275:GLU:CD	1:E:277:GLN:HB2	1.94	0.88
1:B:219:ILE:HD12	1:B:219:ILE:H	1.41	0.86
1:A:219:ILE:H	1:A:219:ILE:HD12	1.42	0.85
1:C:219:ILE:HD12	1:C:219:ILE:H	1.43	0.83
1:F:219:ILE:HD12	1:F:219:ILE:H	1.43	0.83
1:E:219:ILE:HD12	1:E:219:ILE:H	1.43	0.82
1:A:301:VAL:HG21	1:A:362:PRO:HB3	1.62	0.81
1:D:219:ILE:HD12	1:D:219:ILE:H	1.48	0.78
1:A:232:LYS:HE3	1:F:405:ASP:OD1	1.86	0.75
1:A:301:VAL:CG2	1:A:362:PRO:HB3	2.19	0.71
1:D:106:ALA:HB3	1:D:107:GLU:OE1	1.93	0.69
1:F:106:ALA:HB3	1:F:107:GLU:OE1	1.93	0.68
1:A:365:PHE:HD2	3:A:502:VT1:HBC2	1.57	0.68
1:A:106:ALA:HB3	1:A:107:GLU:OE1	1.94	0.68
1:B:106:ALA:HB3	1:B:107:GLU:OE1	1.94	0.67
1:E:275:GLU:OE1	1:E:277:GLN:HB2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ALA:HB3	1:C:107:GLU:OE1	1.94	0.67
1:E:106:ALA:HB3	1:E:107:GLU:OE1	1.94	0.67
1:A:74:LYS:HD3	1:C:232:LYS:HA	1.80	0.64
1:E:202:PHE:O	1:E:205:VAL:HG12	1.98	0.63
1:E:367:MET:HE2	3:E:502:VT1:HBI	1.81	0.62
1:F:202:PHE:O	1:F:205:VAL:HG12	1.99	0.62
1:E:219:ILE:HD12	1:E:219:ILE:N	2.14	0.60
1:F:219:ILE:HD12	1:F:219:ILE:N	2.14	0.60
1:C:219:ILE:HD12	1:C:219:ILE:N	2.15	0.60
1:A:219:ILE:HD12	1:A:219:ILE:N	2.13	0.60
1:A:219:ILE:H	1:A:219:ILE:CD1	2.15	0.60
1:B:219:ILE:HD12	1:B:219:ILE:N	2.14	0.59
1:A:188:ALA:O	1:A:192:LEU:HB2	2.02	0.59
1:B:327:GLN:O	1:B:331:ARG:HG3	2.03	0.59
1:C:202:PHE:O	1:C:205:VAL:HG12	2.03	0.59
1:C:79:PHE:CZ	1:F:226:LEU:HD11	2.38	0.59
1:E:188:ALA:O	1:E:192:LEU:HB2	2.02	0.59
1:C:188:ALA:O	1:C:192:LEU:HB2	2.02	0.59
1:D:219:ILE:HD12	1:D:219:ILE:N	2.16	0.58
1:F:188:ALA:O	1:F:192:LEU:HB2	2.02	0.58
1:F:364:LEU:HG	1:F:473:VAL:CG2	2.34	0.58
1:E:219:ILE:H	1:E:219:ILE:CD1	2.16	0.58
1:B:188:ALA:O	1:B:192:LEU:HB2	2.04	0.57
1:D:333:GLU:O	1:D:333:GLU:HG2	2.03	0.57
1:E:435:MET:CE	2:E:501:HEM:HMD1	2.35	0.57
1:E:365:PHE:HD2	3:E:502:VT1:HBC2	1.70	0.57
1:A:232:LYS:CE	1:F:405:ASP:OD1	2.53	0.56
1:A:275:GLU:OE1	1:A:277:GLN:HB2	2.05	0.56
1:D:188:ALA:O	1:D:192:LEU:HB2	2.04	0.56
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.87	0.56
1:B:365:PHE:HD2	3:B:502:VT1:HBC2	1.70	0.56
1:A:197:ILE:HD13	1:A:245:PHE:CE1	2.41	0.56
1:A:365:PHE:CD2	3:A:502:VT1:HBC2	2.40	0.56
1:B:245:PHE:CE1	1:B:288:MET:HE1	2.41	0.55
1:C:365:PHE:O	3:C:502:VT1:HAY	2.07	0.55
1:C:219:ILE:H	1:C:219:ILE:CD1	2.16	0.55
1:E:82:LYS:HE3	1:E:85:GLY:HA2	1.88	0.54
1:A:245:PHE:CE1	1:A:288:MET:HE1	2.42	0.53
1:C:79:PHE:CZ	1:F:226:LEU:CD1	2.92	0.53
2:D:501:HEM:HBD1	2:D:501:HEM:HHA	1.90	0.53
1:D:219:ILE:H	1:D:219:ILE:CD1	2.20	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:LEU:HG	1:F:473:VAL:HG23	1.89	0.53
1:C:75:TYR:O	1:C:76:GLY:C	2.48	0.52
1:F:219:ILE:H	1:F:219:ILE:CD1	2.16	0.52
1:E:197:ILE:HD13	1:E:245:PHE:CE1	2.44	0.52
1:C:364:LEU:HG	1:C:473:VAL:CG2	2.40	0.52
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.40	0.52
1:F:301:VAL:CG2	1:F:362:PRO:HB3	2.40	0.52
3:F:502:VT1:HAC2	3:F:502:VT1:FAP	2.01	0.51
1:A:216:LEU:HG	1:A:471:MET:HG3	1.93	0.51
1:F:471:MET:CE	3:F:502:VT1:HBC1	2.41	0.51
1:A:227:PRO:HG2	1:F:393:LEU:HD12	1.93	0.51
1:B:216:LEU:HG	1:B:471:MET:HG3	1.92	0.51
1:B:364:LEU:HG	1:B:473:VAL:CG2	2.41	0.50
1:D:470:ALA:C	1:D:472:VAL:H	2.13	0.50
1:E:320:LEU:N	1:E:321:PRO:CD	2.74	0.50
1:B:219:ILE:H	1:B:219:ILE:CD1	2.15	0.50
1:E:275:GLU:C	1:E:277:GLN:H	2.14	0.50
1:A:275:GLU:CD	1:A:277:GLN:HB2	2.31	0.50
1:B:320:LEU:N	1:B:321:PRO:CD	2.75	0.50
1:B:436:GLY:HA3	2:B:501:HEM:C3C	2.47	0.50
1:C:125:VAL:HG13	1:C:126:VAL:HG23	1.94	0.50
1:A:364:LEU:HG	1:A:473:VAL:CG2	2.42	0.49
1:A:245:PHE:CE1	1:A:288:MET:CE	2.95	0.49
1:C:301:VAL:CG2	1:C:362:PRO:HB3	2.43	0.49
1:C:197:ILE:HD13	1:C:245:PHE:CE1	2.47	0.49
1:C:216:LEU:HG	1:C:471:MET:HG3	1.94	0.49
1:F:197:ILE:HD13	1:F:245:PHE:CE1	2.48	0.49
1:A:197:ILE:CD1	1:A:245:PHE:CE1	2.95	0.49
1:B:245:PHE:CE1	1:B:288:MET:CE	2.96	0.49
1:D:320:LEU:N	1:D:321:PRO:CD	2.76	0.49
1:E:125:VAL:HG13	1:E:126:VAL:HG23	1.94	0.49
1:F:320:LEU:N	1:F:321:PRO:CD	2.75	0.49
1:A:320:LEU:N	1:A:321:PRO:CD	2.76	0.49
1:A:74:LYS:CD	1:C:232:LYS:HA	2.42	0.48
1:D:125:VAL:HG13	1:D:126:VAL:HG23	1.95	0.48
1:E:301:VAL:CG2	1:E:362:PRO:HB3	2.43	0.48
1:C:275:GLU:CD	1:C:277:GLN:CB	2.82	0.48
1:C:320:LEU:N	1:C:321:PRO:CD	2.76	0.48
1:A:326:GLU:O	1:A:330:ILE:HG12	2.14	0.48
1:B:326:GLU:O	1:B:330:ILE:HG12	2.14	0.48
1:D:364:LEU:HG	1:D:473:VAL:CG2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:HG13	1:B:126:VAL:HG23	1.95	0.48
1:F:125:VAL:HG13	1:F:126:VAL:HG23	1.96	0.48
1:C:245:PHE:CE1	1:C:288:MET:CE	2.96	0.48
1:E:205:VAL:HG23	1:E:241:MET:HE2	1.94	0.48
1:D:76:GLY:H	1:E:225:TYR:HB3	1.78	0.48
1:D:301:VAL:CG2	1:D:362:PRO:HB3	2.43	0.48
1:D:467:ASP:OD1	1:D:469:THR:HG23	2.13	0.48
2:F:501:HEM:HHA	2:F:501:HEM:HBD1	1.94	0.48
1:F:245:PHE:CE1	1:F:288:MET:CE	2.97	0.48
1:B:301:VAL:CG2	1:B:362:PRO:HB3	2.44	0.47
1:B:197:ILE:HD13	1:B:245:PHE:CE1	2.49	0.47
1:E:367:MET:CE	3:E:502:VT1:HBI	2.43	0.47
1:A:75:TYR:O	1:A:75:TYR:CG	2.67	0.47
1:F:365:PHE:O	3:F:502:VT1:HAY	2.15	0.47
1:D:245:PHE:CE1	1:D:288:MET:HE1	2.49	0.47
3:D:502:VT1:HBH	3:D:502:VT1:HBC2	1.66	0.47
1:E:83:VAL:HG12	1:E:84:PHE:CD2	2.50	0.47
1:F:112:GLU:HB2	1:F:113:PRO:HD3	1.96	0.47
1:C:109:SER:HB2	1:C:371:ILE:HD11	1.96	0.47
1:D:109:SER:HB2	1:D:371:ILE:HD11	1.97	0.47
1:F:83:VAL:HG12	1:F:84:PHE:CD2	2.50	0.47
1:F:205:VAL:HG23	1:F:241:MET:HE2	1.96	0.47
1:D:365:PHE:H	3:D:502:VT1:HAZ	1.79	0.47
3:D:502:VT1:HAC2	3:D:502:VT1:FAP	2.05	0.47
1:E:197:ILE:CD1	1:E:245:PHE:CE1	2.98	0.47
1:C:205:VAL:HG23	1:C:241:MET:HE2	1.97	0.46
1:C:197:ILE:CD1	1:C:245:PHE:CE1	2.97	0.46
1:D:245:PHE:CE1	1:D:288:MET:CE	2.98	0.46
1:B:109:SER:HB2	1:B:371:ILE:HD11	1.97	0.46
1:B:365:PHE:CD2	3:B:502:VT1:HBC2	2.50	0.46
1:D:75:TYR:CG	1:D:75:TYR:O	2.69	0.46
1:A:125:VAL:HG13	1:A:126:VAL:HG23	1.97	0.46
1:B:184:ILE:HG22	1:B:296:GLN:HE22	1.80	0.46
1:D:184:ILE:HG22	1:D:296:GLN:HE22	1.80	0.46
1:F:197:ILE:CD1	1:F:245:PHE:CE1	2.99	0.46
1:F:245:PHE:CE1	1:F:288:MET:HE1	2.51	0.46
1:B:197:ILE:CD1	1:B:245:PHE:CE1	2.98	0.46
1:D:197:ILE:HD13	1:D:245:PHE:CE1	2.51	0.46
1:A:112:GLU:HB2	1:A:113:PRO:HD3	1.97	0.46
1:D:197:ILE:CD1	1:D:245:PHE:CE1	2.99	0.46
1:E:75:TYR:O	1:E:75:TYR:CD2	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:LEU:HG	1:E:473:VAL:CG2	2.45	0.46
1:F:109:SER:HB2	1:F:371:ILE:HD11	1.97	0.46
1:A:436:GLY:HA3	2:A:501:HEM:C3C	2.52	0.45
1:A:435:MET:CE	2:A:501:HEM:HMD1	2.46	0.45
1:D:83:VAL:HG12	1:D:84:PHE:CD2	2.50	0.45
1:B:112:GLU:HB2	1:B:113:PRO:HD3	1.98	0.45
1:F:98:VAL:N	1:F:99:PRO:HD2	2.31	0.45
1:E:435:MET:HE3	2:E:501:HEM:HMD1	1.98	0.45
1:C:189:SER:O	1:C:193:MET:HB2	2.17	0.45
1:C:245:PHE:CE1	1:C:288:MET:HE1	2.52	0.45
1:D:434:CYS:HB2	2:D:501:HEM:NA	2.31	0.45
2:A:501:HEM:HHA	2:A:501:HEM:HBD1	1.97	0.45
1:C:301:VAL:HG21	1:C:362:PRO:HB3	1.98	0.45
1:A:189:SER:O	1:A:193:MET:HB2	2.17	0.45
1:E:112:GLU:HB2	1:E:113:PRO:HD3	1.98	0.45
1:A:109:SER:HB2	1:A:371:ILE:HD11	1.99	0.45
1:C:184:ILE:HG22	1:C:296:GLN:HE22	1.81	0.45
1:C:365:PHE:H	3:C:502:VT1:HAZ	1.81	0.45
1:D:468:TYR:CD1	1:D:468:TYR:N	2.84	0.45
1:A:83:VAL:HG12	1:A:84:PHE:CD2	2.52	0.45
1:D:112:GLU:HB2	1:D:113:PRO:HD3	1.99	0.45
1:E:109:SER:HB2	1:E:371:ILE:HD11	1.99	0.45
1:A:98:VAL:N	1:A:99:PRO:HD2	2.32	0.45
1:C:112:GLU:HB2	1:C:113:PRO:HD3	1.98	0.45
1:E:75:TYR:O	1:E:75:TYR:CG	2.69	0.44
1:D:301:VAL:HG21	1:D:362:PRO:HB3	1.98	0.44
1:E:301:VAL:HG21	1:E:362:PRO:HB3	1.99	0.44
2:F:501:HEM:HBC2	2:F:501:HEM:HMC1	1.98	0.44
1:E:189:SER:O	1:E:193:MET:HB2	2.17	0.44
1:B:189:SER:O	1:B:193:MET:HB2	2.16	0.44
1:B:98:VAL:N	1:B:99:PRO:HD2	2.33	0.44
1:C:98:VAL:N	1:C:99:PRO:HD2	2.33	0.44
1:F:189:SER:O	1:F:193:MET:HB2	2.18	0.44
1:F:301:VAL:HG21	1:F:362:PRO:HB3	1.99	0.44
1:B:75:TYR:CG	1:B:75:TYR:O	2.70	0.44
1:C:83:VAL:HG12	1:C:84:PHE:CD2	2.53	0.44
1:D:189:SER:O	1:D:193:MET:HB2	2.18	0.44
1:F:320:LEU:N	1:F:321:PRO:HD2	2.33	0.44
1:A:184:ILE:HG22	1:A:296:GLN:HE22	1.82	0.43
1:F:184:ILE:HG22	1:F:296:GLN:HE22	1.82	0.43
1:B:205:VAL:HG22	1:B:241:MET:CE	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:VAL:N	1:E:99:PRO:HD2	2.33	0.43
1:F:408:ASN:O	1:F:411:ARG:HG2	2.18	0.43
1:B:83:VAL:HG12	1:B:84:PHE:CD2	2.52	0.43
1:D:98:VAL:N	1:D:99:PRO:HD2	2.32	0.43
1:D:75:TYR:O	1:D:75:TYR:CD2	2.71	0.43
1:E:159:LYS:HE3	1:F:482:ARG:HD3	2.01	0.43
1:E:184:ILE:HG22	1:E:296:GLN:HE22	1.84	0.43
3:E:502:VT1:HAC2	3:E:502:VT1:FAP	2.09	0.43
2:F:501:HEM:HBC2	2:F:501:HEM:CMC	2.48	0.43
1:B:301:VAL:HG21	1:B:362:PRO:HB3	2.00	0.43
1:C:435:MET:CE	2:C:501:HEM:HMD1	2.48	0.43
1:C:75:TYR:O	1:C:75:TYR:CG	2.72	0.42
1:E:408:ASN:O	1:E:411:ARG:HG2	2.19	0.42
1:E:435:MET:HE2	2:E:501:HEM:HMD1	2.01	0.42
1:C:298:THR:HB	2:C:501:HEM:C3B	2.55	0.42
1:E:275:GLU:CD	1:E:277:GLN:CB	2.77	0.42
1:B:435:MET:CE	2:B:501:HEM:HMD1	2.50	0.42
1:C:142:ALA:HB2	1:C:435:MET:SD	2.60	0.42
3:A:502:VT1:HAC2	3:A:502:VT1:FAP	2.10	0.41
1:C:118:VAL:N	1:C:119:PRO:HD2	2.35	0.41
1:E:205:VAL:HG23	1:E:241:MET:CE	2.50	0.41
1:E:436:GLY:HA3	2:E:501:HEM:C3C	2.55	0.41
1:A:408:ASN:O	1:A:411:ARG:HG2	2.20	0.41
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.91	0.41
1:A:364:LEU:HG	1:A:473:VAL:HG23	2.02	0.41
1:A:448:TRP:O	1:A:452:LEU:HG	2.21	0.41
1:B:245:PHE:CD1	1:B:288:MET:HE1	2.56	0.41
1:C:77:ASP:OD2	1:C:376:TYR:OH	2.22	0.41
1:D:142:ALA:HB2	1:D:435:MET:SD	2.60	0.41
1:B:393:LEU:CD1	1:D:228:ILE:HG22	2.51	0.41
1:D:81:MET:HG2	1:E:223:PHE:HZ	1.85	0.41
1:D:118:VAL:N	1:D:119:PRO:HD2	2.36	0.41
1:F:301:VAL:HG22	1:F:362:PRO:HB3	2.02	0.41
1:B:112:GLU:N	1:B:113:PRO:CD	2.84	0.41
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.90	0.41
1:E:112:GLU:N	1:E:113:PRO:CD	2.84	0.41
1:C:364:LEU:HG	1:C:473:VAL:HG23	2.03	0.40
1:B:118:VAL:N	1:B:119:PRO:HD2	2.37	0.40
1:F:205:VAL:HG23	1:F:241:MET:CE	2.51	0.40
3:F:502:VT1:FAP	3:F:502:VT1:CAC	2.59	0.40
1:A:112:GLU:N	1:A:113:PRO:CD	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HD2	1:A:148:LYS:HA	1.80	0.40
1:E:118:VAL:N	1:E:119:PRO:HD2	2.36	0.40
1:E:320:LEU:N	1:E:321:PRO:HD2	2.36	0.40
1:C:408:ASN:O	1:C:411:ARG:HG2	2.21	0.40
1:B:205:VAL:HG22	1:B:241:MET:HE2	2.03	0.40
1:B:298:THR:HB	2:B:501:HEM:C3B	2.57	0.40
1:D:364:LEU:HG	1:D:473:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	411/460 (89%)	403 (98%)	7 (2%)	1 (0%)	47 58
1	B	411/460 (89%)	401 (98%)	9 (2%)	1 (0%)	47 58
1	C	411/460 (89%)	402 (98%)	8 (2%)	1 (0%)	47 58
1	D	411/460 (89%)	401 (98%)	9 (2%)	1 (0%)	47 58
1	E	411/460 (89%)	401 (98%)	9 (2%)	1 (0%)	47 58
1	F	411/460 (89%)	403 (98%)	7 (2%)	1 (0%)	47 58
All	All	2466/2760 (89%)	2411 (98%)	49 (2%)	6 (0%)	47 58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	B	126	VAL
1	C	126	VAL
1	D	126	VAL
1	E	126	VAL
1	F	126	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	358/397 (90%)	356 (99%)	2 (1%)	86 94
1	B	357/397 (90%)	352 (99%)	5 (1%)	67 81
1	C	355/397 (89%)	353 (99%)	2 (1%)	86 94
1	D	351/397 (88%)	348 (99%)	3 (1%)	78 89
1	E	350/397 (88%)	347 (99%)	3 (1%)	78 89
1	F	348/397 (88%)	344 (99%)	4 (1%)	73 86
All	All	2119/2382 (89%)	2100 (99%)	19 (1%)	78 89

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	405	ASP
1	B	205	VAL
1	B	277	GLN
1	B	301	VAL
1	B	405	ASP
1	B	472	VAL
1	C	301	VAL
1	C	405	ASP
1	D	301	VAL
1	D	405	ASP
1	D	472	VAL
1	E	301	VAL
1	E	393	LEU
1	E	405	ASP
1	F	301	VAL
1	F	393	LEU
1	F	405	ASP
1	F	472	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	296	GLN
1	A	297	HIS
1	B	115	GLN
1	B	296	GLN
1	B	297	HIS
1	C	115	GLN
1	C	296	GLN
1	C	297	HIS
1	D	115	GLN
1	D	265	GLN
1	D	296	GLN
1	D	297	HIS
1	E	115	GLN
1	E	296	GLN
1	E	297	HIS
1	F	115	GLN
1	F	296	GLN
1	F	297	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

12 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
3	VT1	C	502	2	36,40,40	0.39	0	46,60,60	0.46	0
2	HEM	E	501	1,3	41,50,50	1.41	5 (12%)	45,82,82	2.04	11 (24%)
3	VT1	D	502	2	36,40,40	0.37	0	46,60,60	0.47	0
3	VT1	E	502	2	36,40,40	0.37	0	46,60,60	0.49	0
2	HEM	B	501	1,3	41,50,50	1.43	6 (14%)	45,82,82	2.04	13 (28%)
2	HEM	A	501	1,3	41,50,50	1.37	5 (12%)	45,82,82	1.86	9 (20%)
3	VT1	B	502	2	36,40,40	0.37	0	46,60,60	0.43	0
3	VT1	F	502	2	36,40,40	0.34	0	46,60,60	0.47	0
3	VT1	A	502	2	36,40,40	0.34	0	46,60,60	0.55	0
2	HEM	D	501	1,3	41,50,50	1.29	5 (12%)	45,82,82	2.22	13 (28%)
2	HEM	F	501	1,3	41,50,50	1.42	6 (14%)	45,82,82	2.21	12 (26%)
2	HEM	C	501	1,3	41,50,50	1.39	7 (17%)	45,82,82	1.99	11 (24%)

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
3	VT1	C	502	2	-	4/33/36/36	0/4/4/4
2	HEM	E	501	1,3	-	4/12/54/54	-
3	VT1	D	502	2	-	6/33/36/36	0/4/4/4
3	VT1	E	502	2	-	9/33/36/36	0/4/4/4
2	HEM	B	501	1,3	-	4/12/54/54	-
2	HEM	A	501	1,3	-	6/12/54/54	-
3	VT1	B	502	2	-	7/33/36/36	0/4/4/4
3	VT1	F	502	2	-	6/33/36/36	0/4/4/4
3	VT1	A	502	2	-	12/33/36/36	0/4/4/4
2	HEM	D	501	1,3	-	4/12/54/54	-
2	HEM	F	501	1,3	-	5/12/54/54	-
2	HEM	C	501	1,3	-	3/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	HEM	C1B-NB	-4.15	1.33	1.40
2	B	501	HEM	C1B-NB	-3.92	1.33	1.40
2	C	501	HEM	C1B-NB	-3.90	1.33	1.40
2	E	501	HEM	C1B-NB	-3.83	1.33	1.40
2	A	501	HEM	C1B-NB	-3.73	1.33	1.40
2	B	501	HEM	C4D-ND	-3.50	1.34	1.40
2	E	501	HEM	C4D-ND	-3.40	1.34	1.40
2	D	501	HEM	C1B-NB	-3.36	1.34	1.40
2	C	501	HEM	C4D-ND	-3.25	1.34	1.40
2	F	501	HEM	C4D-ND	-3.17	1.34	1.40
2	A	501	HEM	C4D-ND	-3.10	1.35	1.40
2	D	501	HEM	FE-NB	3.04	2.11	1.96
2	A	501	HEM	FE-NB	2.93	2.11	1.96
2	E	501	HEM	FE-NB	2.92	2.11	1.96
2	C	501	HEM	FE-NB	2.86	2.11	1.96
2	B	501	HEM	FE-NB	2.84	2.10	1.96
2	F	501	HEM	FE-NB	2.79	2.10	1.96
2	D	501	HEM	C4D-ND	-2.60	1.35	1.40
2	B	501	HEM	C4B-NB	-2.55	1.33	1.38
2	A	501	HEM	C4B-NB	-2.43	1.33	1.38
2	F	501	HEM	C4B-NB	-2.42	1.33	1.38
2	B	501	HEM	C1D-ND	-2.42	1.33	1.38
2	E	501	HEM	C1D-ND	-2.40	1.33	1.38
2	E	501	HEM	C4B-NB	-2.38	1.33	1.38
2	F	501	HEM	C1D-ND	-2.30	1.34	1.38
2	A	501	HEM	C1D-ND	-2.27	1.34	1.38
2	D	501	HEM	C4D-C3D	2.23	1.48	1.45
2	C	501	HEM	C1D-ND	-2.21	1.34	1.38
2	B	501	HEM	FE-ND	-2.15	1.86	1.96
2	C	501	HEM	C4B-NB	-2.14	1.34	1.38
2	D	501	HEM	CHB-C1B	2.13	1.40	1.35
2	F	501	HEM	CHB-C1B	2.11	1.40	1.35
2	C	501	HEM	O2A-CGA	-2.03	1.23	1.30
2	C	501	HEM	CHB-C1B	2.02	1.40	1.35

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHD-C1D-ND	5.73	130.66	124.43
2	D	501	HEM	CHC-C4B-NB	5.62	130.54	124.43
2	B	501	HEM	CHC-C4B-NB	5.30	130.19	124.43
2	F	501	HEM	CHC-C4B-NB	5.28	130.17	124.43
2	D	501	HEM	CAD-C3D-C4D	5.23	133.79	124.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	HEM	CHD-C1D-ND	5.18	130.06	124.43
2	E	501	HEM	CHC-C4B-NB	5.17	130.04	124.43
2	B	501	HEM	CHD-C1D-ND	5.16	130.04	124.43
2	E	501	HEM	CHD-C1D-ND	5.05	129.91	124.43
2	F	501	HEM	C1B-NB-C4B	4.98	110.22	105.07
2	A	501	HEM	CHC-C4B-NB	4.98	129.84	124.43
2	C	501	HEM	CHC-C4B-NB	4.96	129.81	124.43
2	C	501	HEM	CHD-C1D-ND	4.87	129.72	124.43
2	F	501	HEM	CAD-CBD-CGD	-4.76	103.35	113.60
2	C	501	HEM	CAD-CBD-CGD	-4.59	103.72	113.60
2	A	501	HEM	CHD-C1D-ND	4.56	129.38	124.43
2	C	501	HEM	C1B-NB-C4B	4.45	109.67	105.07
2	F	501	HEM	CAD-C3D-C4D	4.34	132.23	124.66
2	D	501	HEM	CAD-C3D-C2D	-4.28	119.90	127.88
2	E	501	HEM	CAD-CBD-CGD	-4.27	104.41	113.60
2	D	501	HEM	CAD-CBD-CGD	-4.16	104.64	113.60
2	A	501	HEM	C1B-NB-C4B	4.11	109.31	105.07
2	E	501	HEM	C1B-NB-C4B	4.06	109.27	105.07
2	B	501	HEM	C1B-NB-C4B	4.04	109.25	105.07
2	B	501	HEM	CAD-CBD-CGD	-3.89	105.22	113.60
2	F	501	HEM	CHD-C1D-C2D	-3.89	118.90	124.98
2	D	501	HEM	CHD-C1D-C2D	-3.84	118.98	124.98
2	D	501	HEM	C1B-NB-C4B	3.69	108.89	105.07
2	F	501	HEM	CAD-C3D-C2D	-3.69	121.01	127.88
2	F	501	HEM	CHB-C1B-NB	3.41	128.59	124.38
2	C	501	HEM	CHD-C1D-C2D	-3.40	119.67	124.98
2	C	501	HEM	CAD-C3D-C4D	3.35	130.52	124.66
2	B	501	HEM	CHD-C1D-C2D	-3.33	119.78	124.98
2	E	501	HEM	CHB-C1B-NB	3.24	128.38	124.38
2	E	501	HEM	CHA-C4D-ND	3.21	128.35	124.38
2	E	501	HEM	CAD-C3D-C4D	3.18	130.22	124.66
2	B	501	HEM	CAD-C3D-C4D	3.15	130.16	124.66
2	E	501	HEM	CHD-C1D-C2D	-3.14	120.07	124.98
2	B	501	HEM	CHA-C4D-ND	3.14	128.26	124.38
2	A	501	HEM	CHD-C1D-C2D	-3.14	120.08	124.98
2	B	501	HEM	CHB-C1B-NB	3.12	128.24	124.38
2	A	501	HEM	CHB-C1B-NB	3.03	128.12	124.38
2	A	501	HEM	CAD-CBD-CGD	-2.97	107.22	113.60
2	C	501	HEM	CHB-C1B-NB	2.82	127.86	124.38
2	A	501	HEM	CHA-C4D-ND	2.72	127.75	124.38
2	D	501	HEM	CHB-C1B-NB	2.68	127.70	124.38
2	F	501	HEM	CHA-C4D-ND	2.67	127.69	124.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	C4D-ND-C1D	2.64	107.80	105.07
2	E	501	HEM	CAD-C3D-C2D	-2.61	123.02	127.88
2	A	501	HEM	CAD-C3D-C4D	2.54	129.09	124.66
2	B	501	HEM	CAD-C3D-C2D	-2.47	123.28	127.88
2	D	501	HEM	C4D-ND-C1D	2.45	107.60	105.07
2	B	501	HEM	C4D-ND-C1D	2.43	107.59	105.07
2	D	501	HEM	CBD-CAD-C3D	2.40	119.28	112.63
2	B	501	HEM	O2D-CGD-CBD	2.33	121.53	114.03
2	F	501	HEM	O2D-CGD-CBD	2.31	121.46	114.03
2	D	501	HEM	CHA-C4D-ND	2.30	127.22	124.38
2	C	501	HEM	CAD-C3D-C2D	-2.29	123.61	127.88
2	C	501	HEM	CHA-C4D-ND	2.29	127.21	124.38
2	D	501	HEM	CHC-C4B-C3B	-2.27	121.09	124.57
2	A	501	HEM	O2D-CGD-CBD	2.24	121.22	114.03
2	C	501	HEM	CBD-CAD-C3D	2.20	118.73	112.63
2	B	501	HEM	O2A-CGA-CBA	2.14	120.90	114.03
2	D	501	HEM	CMC-C2C-C3C	2.10	128.60	124.68
2	C	501	HEM	O2D-CGD-CBD	2.07	120.69	114.03
2	F	501	HEM	O2A-CGA-O1A	-2.04	118.22	123.30
2	B	501	HEM	C4B-C3B-C2B	-2.02	105.51	107.11
2	E	501	HEM	O2D-CGD-CBD	2.01	120.47	114.03
2	F	501	HEM	O2A-CGA-CBA	2.00	120.46	114.03

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	C4D-C3D-CAD-CBD
3	A	502	VT1	CAB-CAC-NAD-NAH
3	A	502	VT1	CAB-CAC-NAD-CAE
3	B	502	VT1	CAB-CAC-NAD-NAH
3	B	502	VT1	CAB-CAC-NAD-CAE
3	C	502	VT1	CAB-CAC-NAD-NAH
3	C	502	VT1	CAB-CAC-NAD-CAE
3	D	502	VT1	CAB-CAC-NAD-NAH
3	D	502	VT1	CAB-CAC-NAD-CAE
3	E	502	VT1	CAB-CAC-NAD-NAH
3	E	502	VT1	CAB-CAC-NAD-CAE
3	F	502	VT1	CAB-CAC-NAD-NAH
3	F	502	VT1	CAB-CAC-NAD-CAE
3	A	502	VT1	CBJ-CAW-CAX-CBI

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	502	VT1	CBJ-CAW-CAX-CBI
3	D	502	VT1	CBJ-CAW-CAX-CAY
3	B	502	VT1	CAV-CAW-CAX-CBI
3	B	502	VT1	CAV-CAW-CAX-CAY
3	D	502	VT1	CAV-CAW-CAX-CBI
3	D	502	VT1	CAV-CAW-CAX-CAY
3	B	502	VT1	CBJ-CAW-CAX-CAY
3	A	502	VT1	CAV-CAW-CAX-CBI
3	A	502	VT1	CAV-CAW-CAX-CAY
3	D	502	VT1	CBJ-CAW-CAX-CBI
3	A	502	VT1	CBJ-CAW-CAX-CAY
2	F	501	HEM	C4D-C3D-CAD-CBD
2	F	501	HEM	C2D-C3D-CAD-CBD
3	A	502	VT1	OAA-CAB-CAI-CAO
2	A	501	HEM	C4D-C3D-CAD-CBD
2	B	501	HEM	C4D-C3D-CAD-CBD
3	A	502	VT1	CAZ-CBA-OBB-CBC
3	E	502	VT1	OAA-CAB-CAI-CAO
3	F	502	VT1	OAA-CAB-CAI-CAO
2	B	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	C2D-C3D-CAD-CBD
3	A	502	VT1	CBH-CBA-OBB-CBC
3	A	502	VT1	CAC-CAB-CAI-CAO
3	F	502	VT1	CAC-CAB-CAI-CAO
3	E	502	VT1	OBB-CBC-CBD-FBG
2	E	501	HEM	C2D-C3D-CAD-CBD
3	E	502	VT1	OBB-CBC-CBD-FBE
3	E	502	VT1	CAC-CAB-CAI-CAO
3	E	502	VT1	OBB-CBC-CBD-FBF
3	E	502	VT1	CAZ-CBA-OBB-CBC
2	B	501	HEM	CAD-CBD-CGD-O1D
3	C	502	VT1	CAV-CAW-CAX-CBI
2	A	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAD-CBD-CGD-O1D
3	C	502	VT1	CAV-CAW-CAX-CAY
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	E	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	501	HEM	C4D-C3D-CAD-CBD
3	A	502	VT1	OBB-CBC-CBD-FBF
3	E	502	VT1	CBH-CBA-OBB-CBC
3	A	502	VT1	OBB-CBC-CBD-FBE
2	C	501	HEM	CAD-CBD-CGD-O1D
3	F	502	VT1	CAV-CAW-CAX-CBI
2	A	501	HEM	C2B-C3B-CAB-CBB
3	B	502	VT1	OAA-CAB-CAI-CAO
2	A	501	HEM	C4B-C3B-CAB-CBB
2	F	501	HEM	C4B-C3B-CAB-CBB
2	E	501	HEM	CAD-CBD-CGD-O2D
3	F	502	VT1	CAV-CAW-CAX-CAY
2	C	501	HEM	CAD-CBD-CGD-O2D

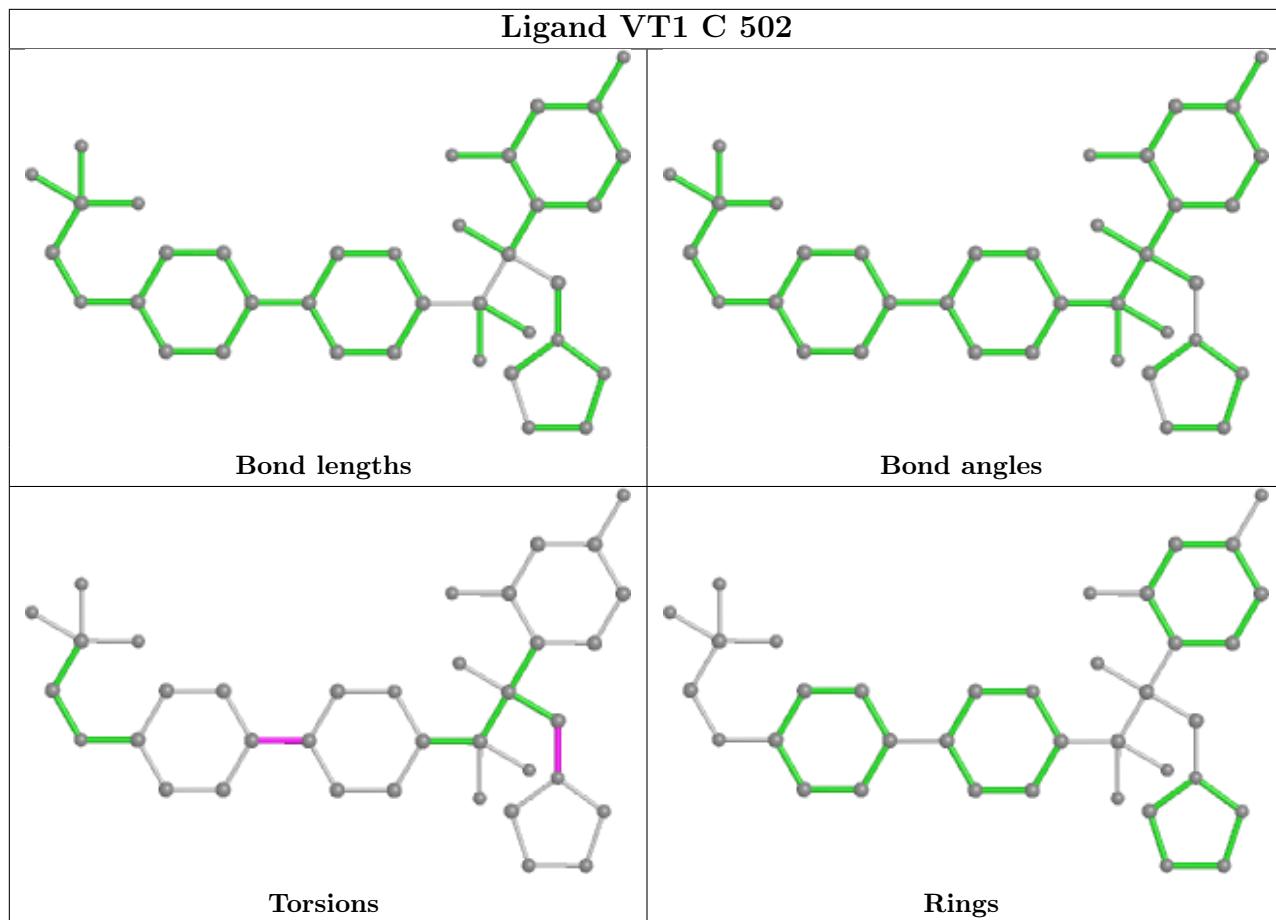
There are no ring outliers.

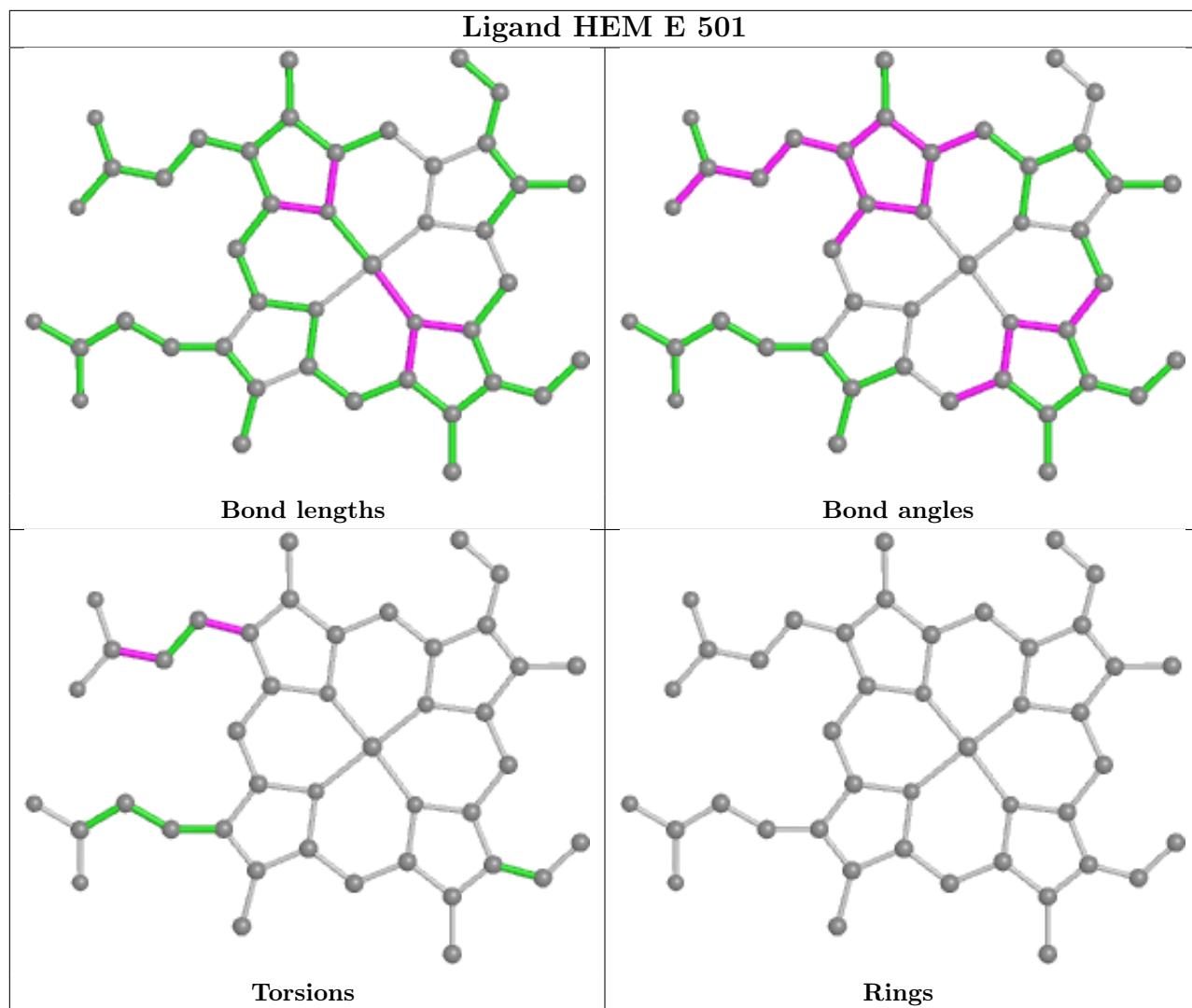
12 monomers are involved in 37 short contacts:

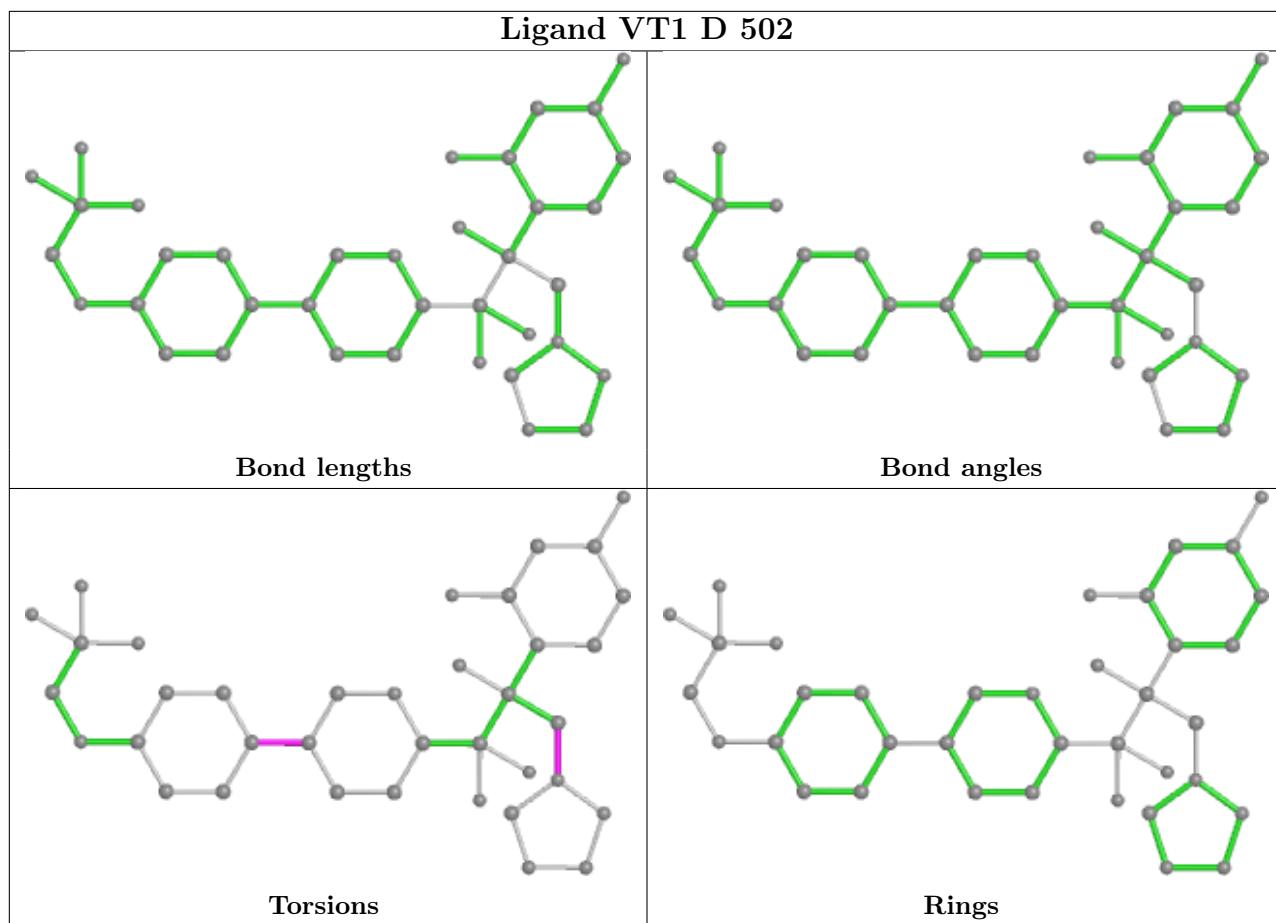
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	VT1	2	0
2	E	501	HEM	4	0
3	D	502	VT1	3	0
3	E	502	VT1	4	0
2	B	501	HEM	3	0
2	A	501	HEM	3	0
3	B	502	VT1	2	0
3	F	502	VT1	4	0
3	A	502	VT1	3	0
2	D	501	HEM	4	0
2	F	501	HEM	3	0
2	C	501	HEM	2	0

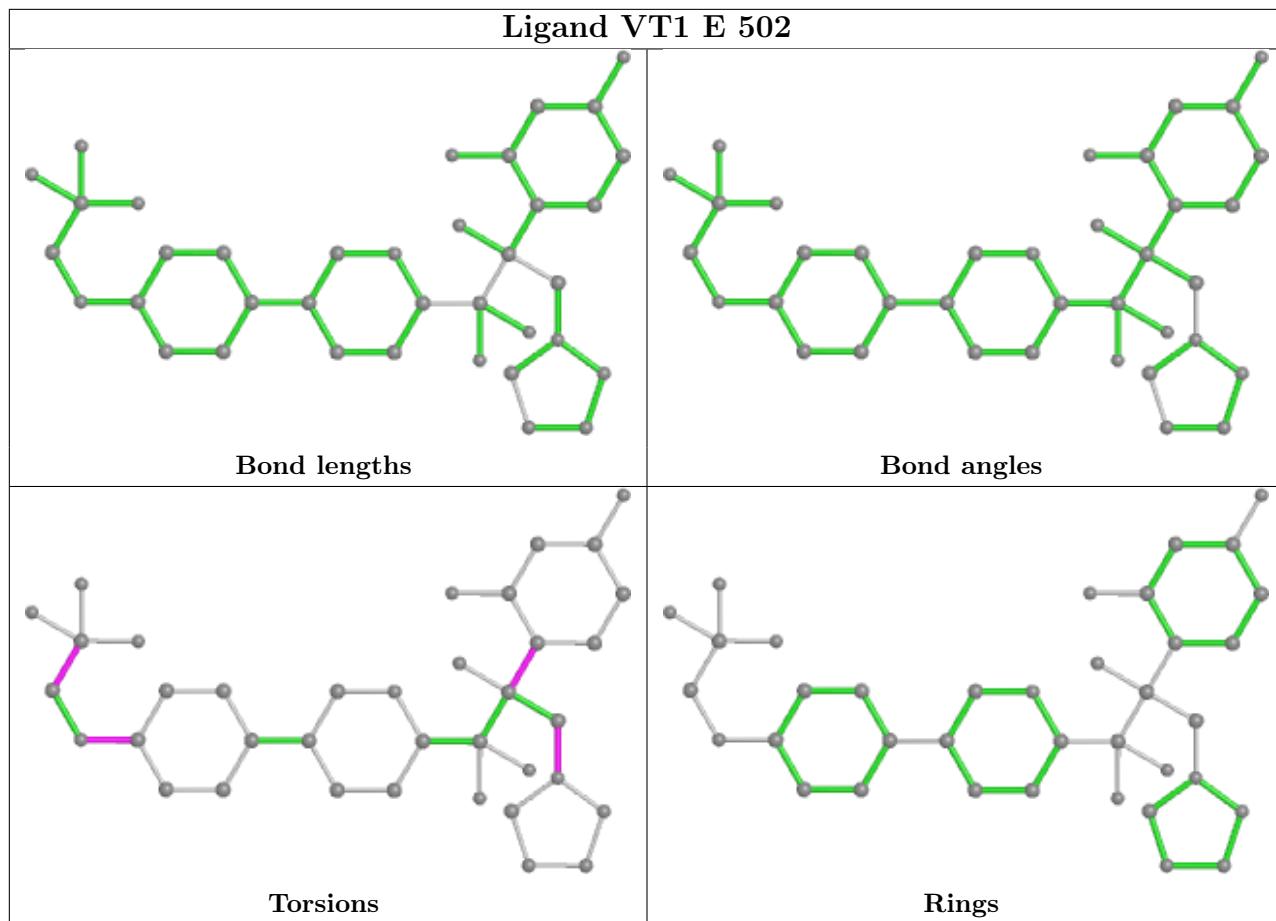
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

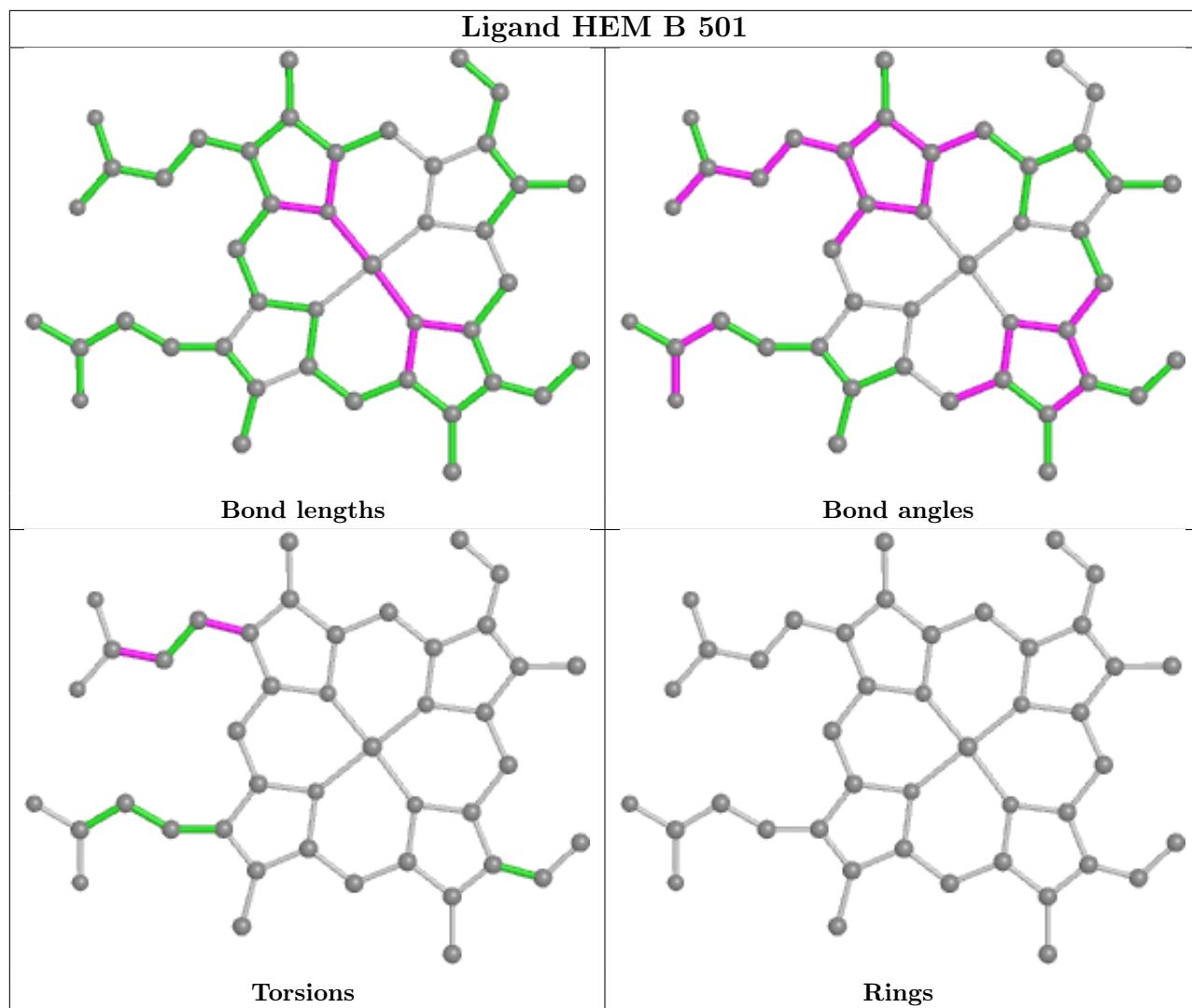
equivalents in the CSD to analyse the geometry.

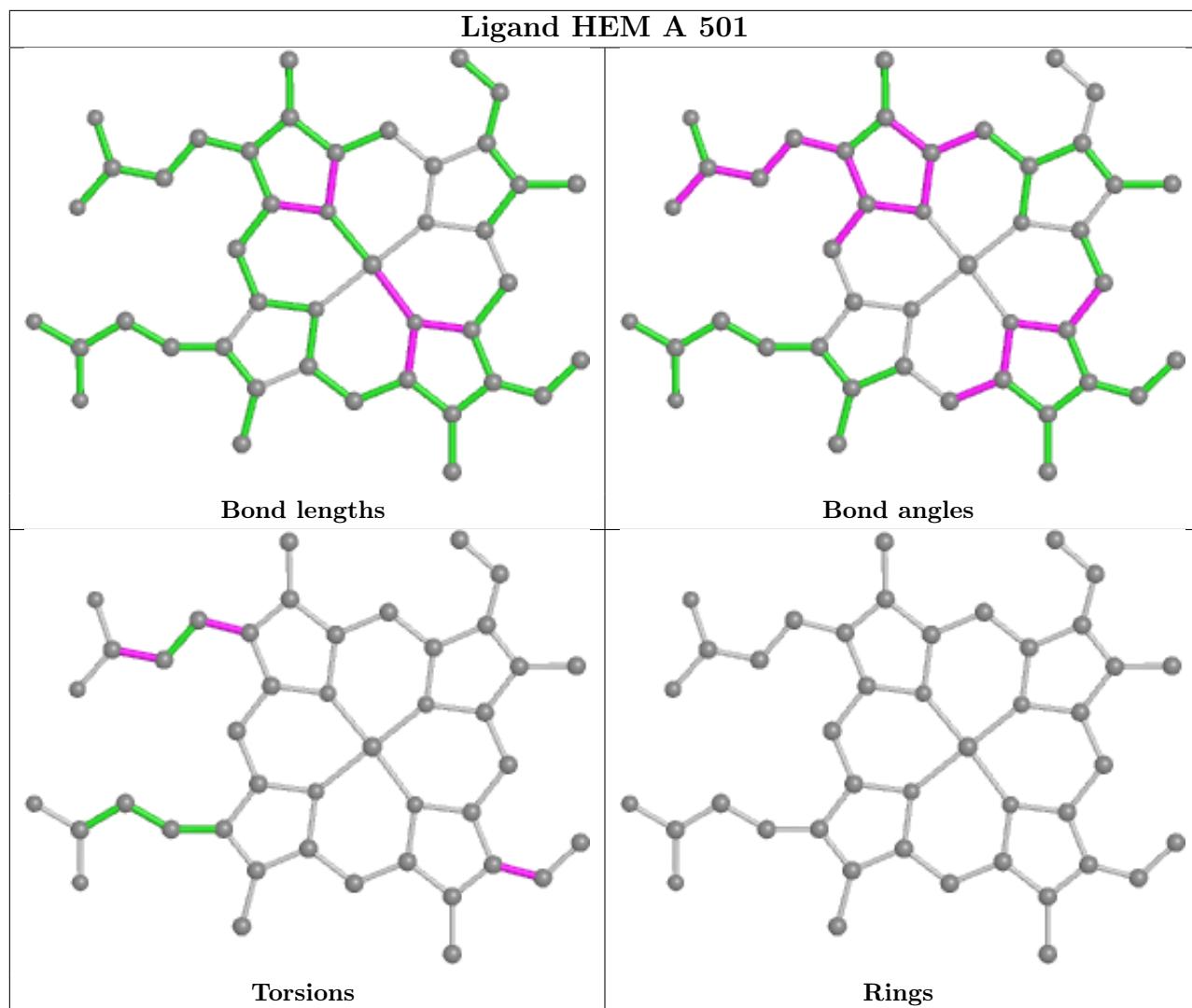


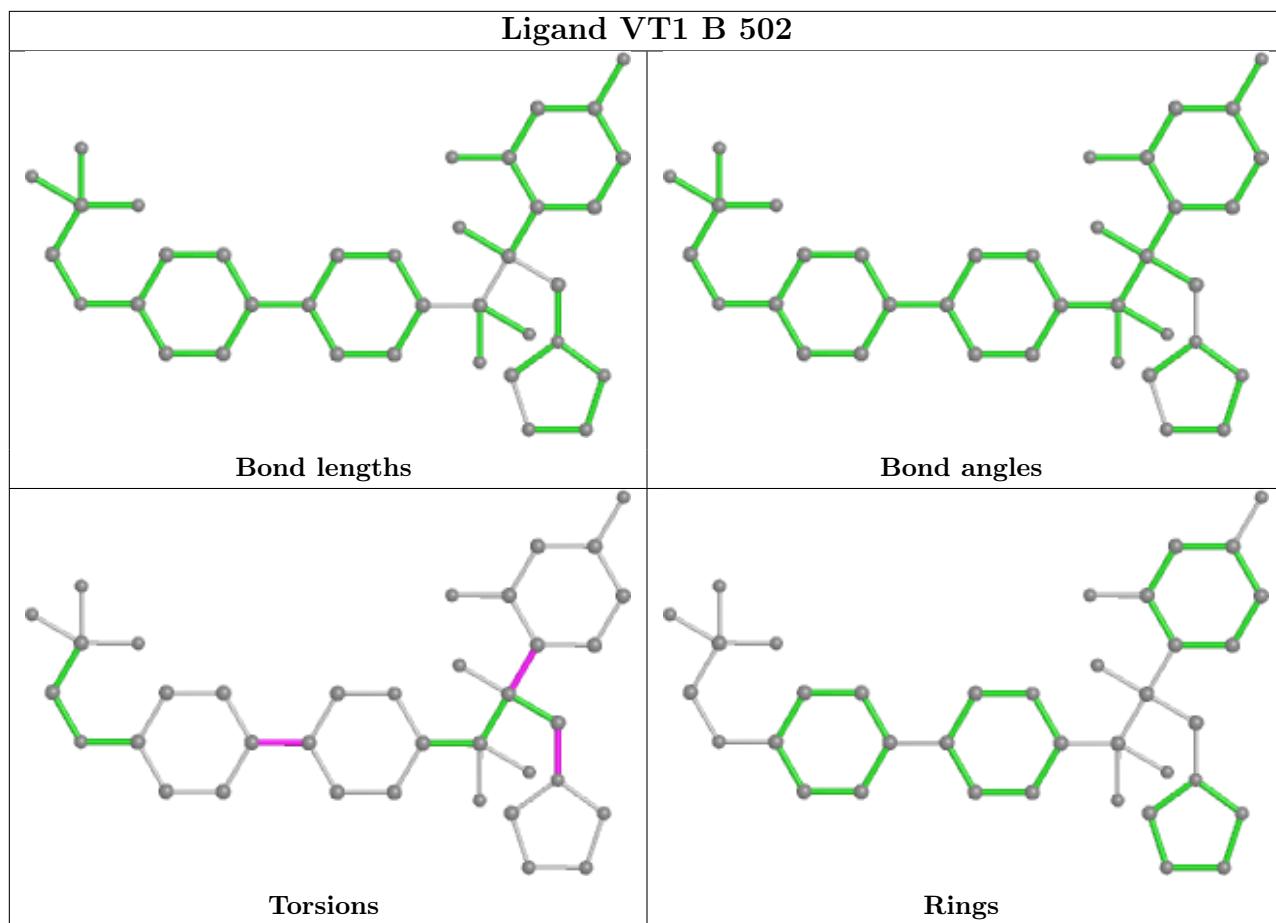


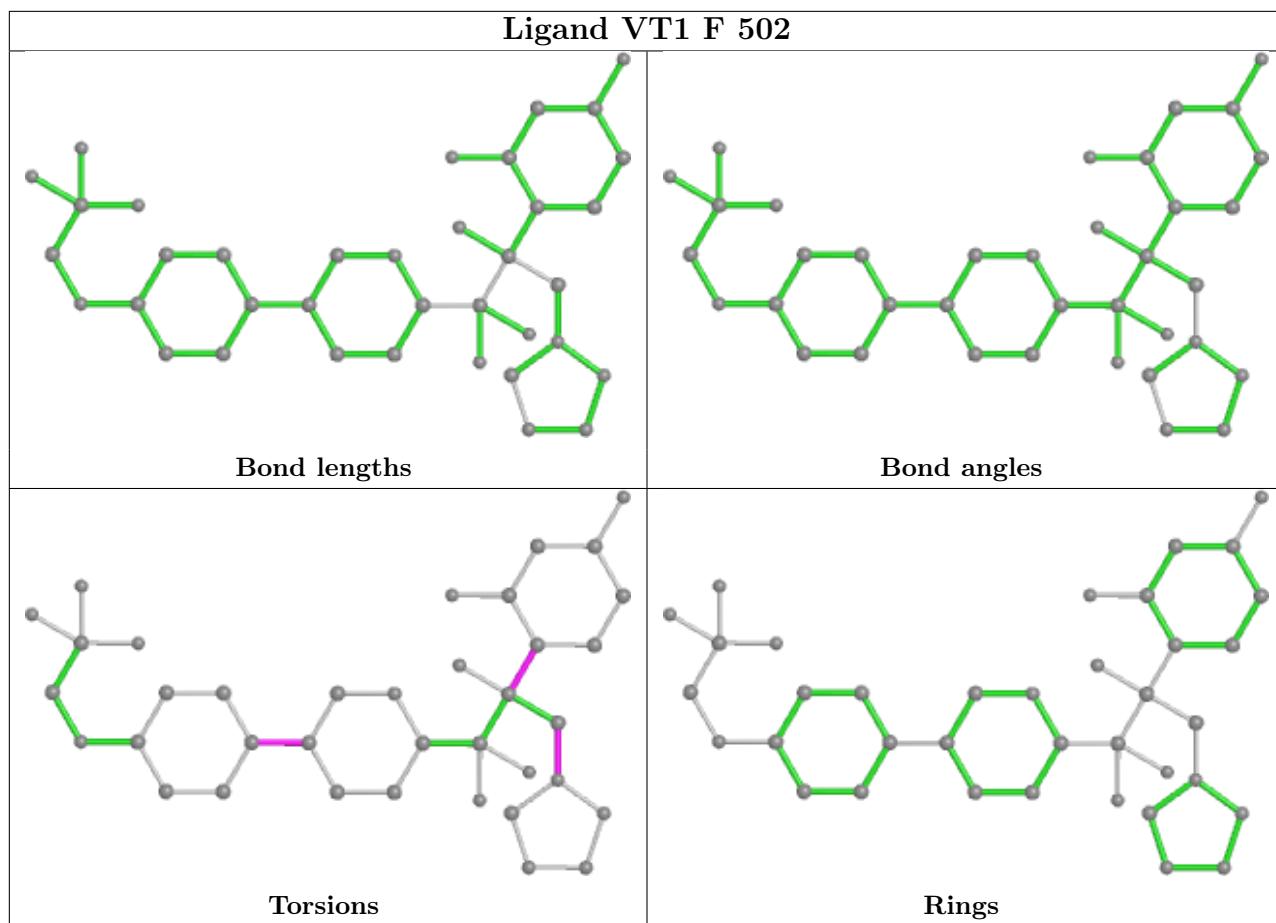


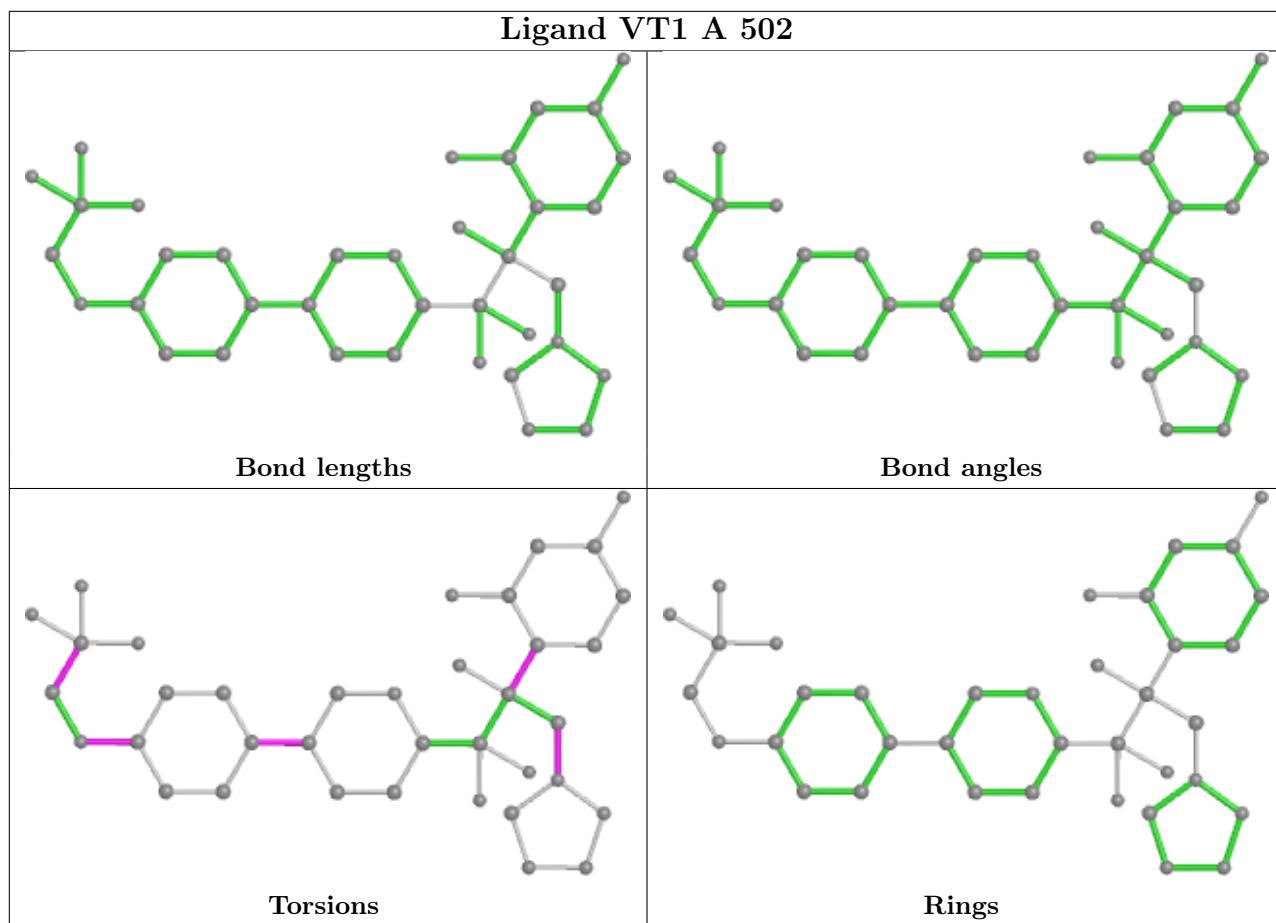


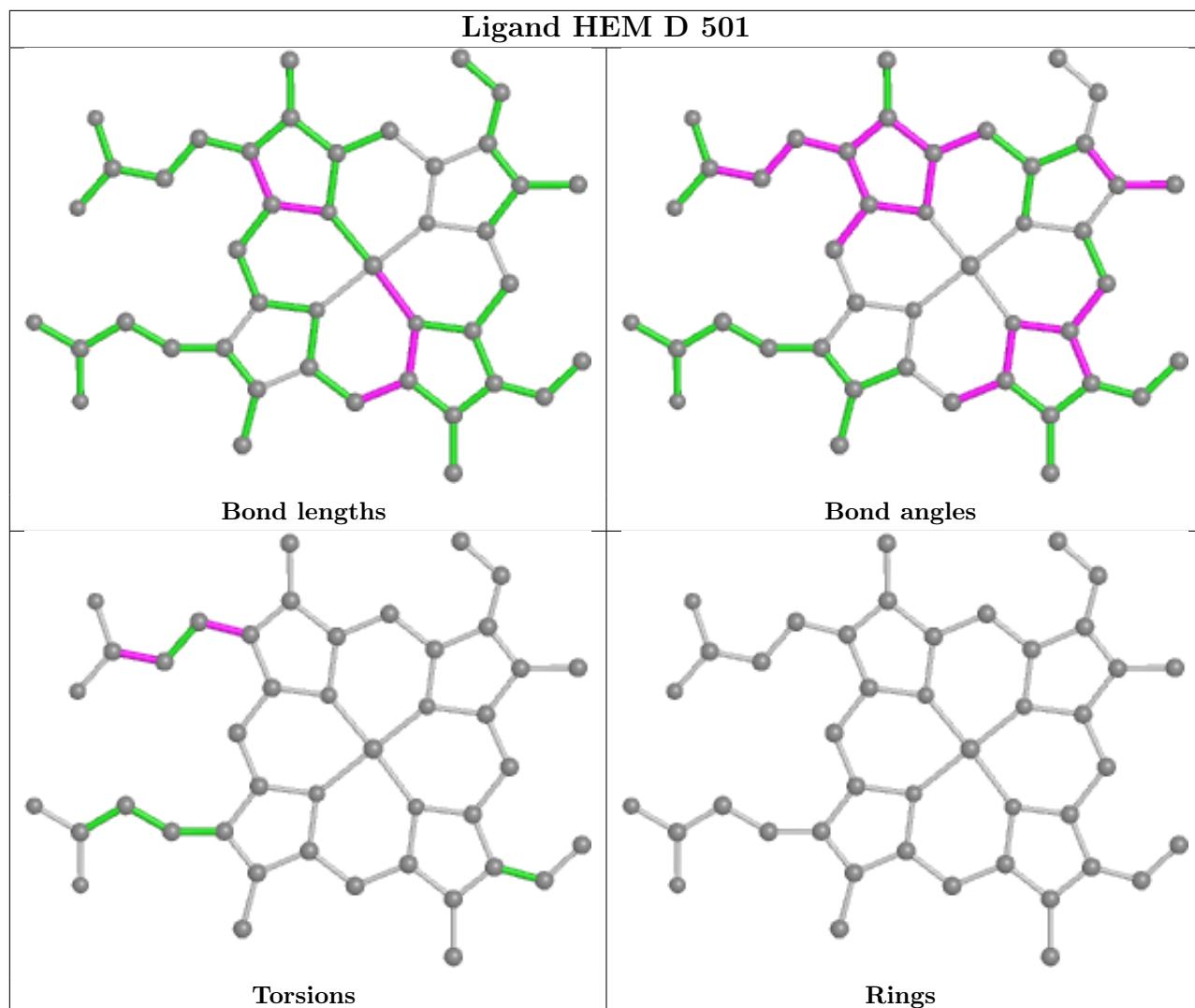


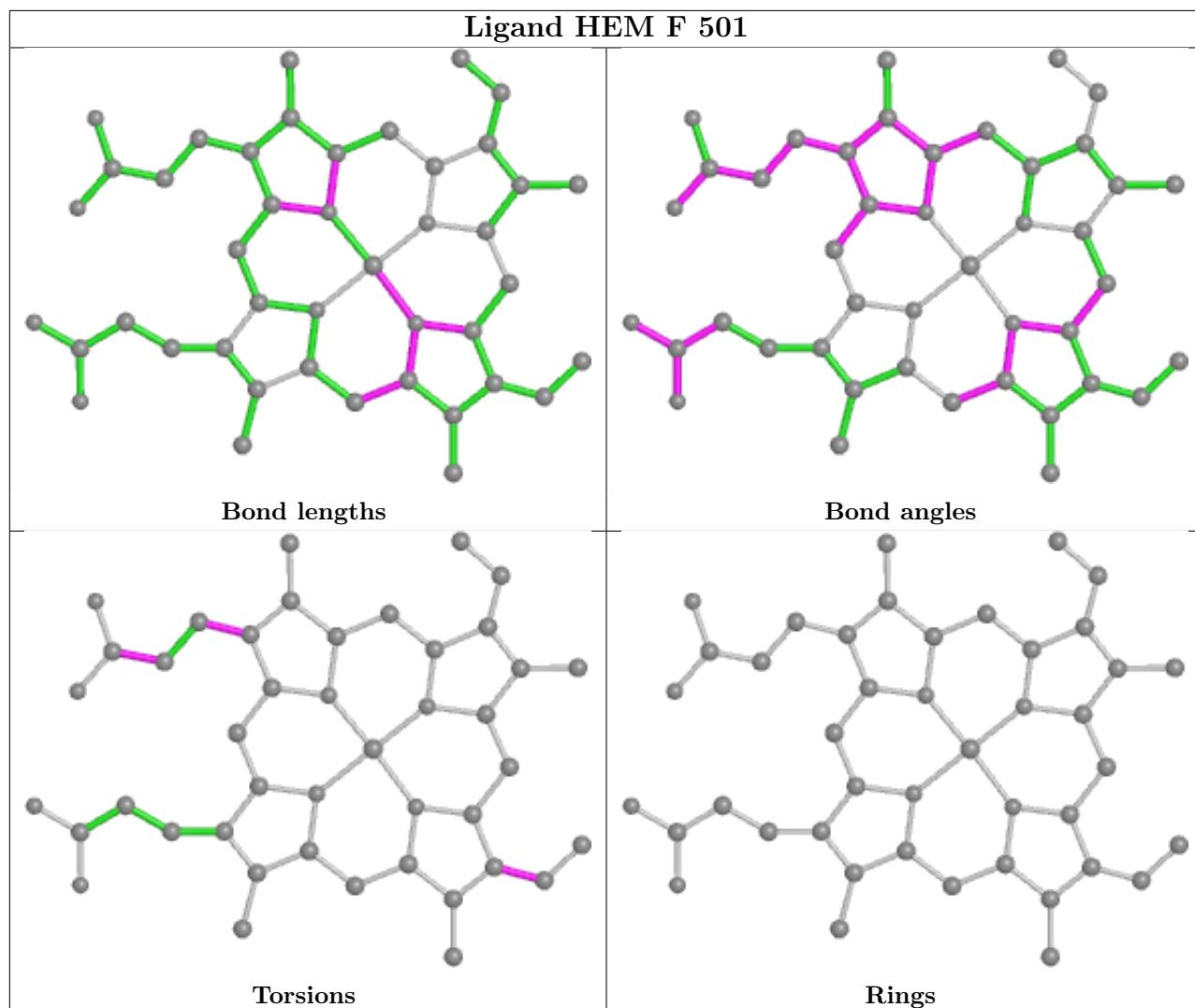


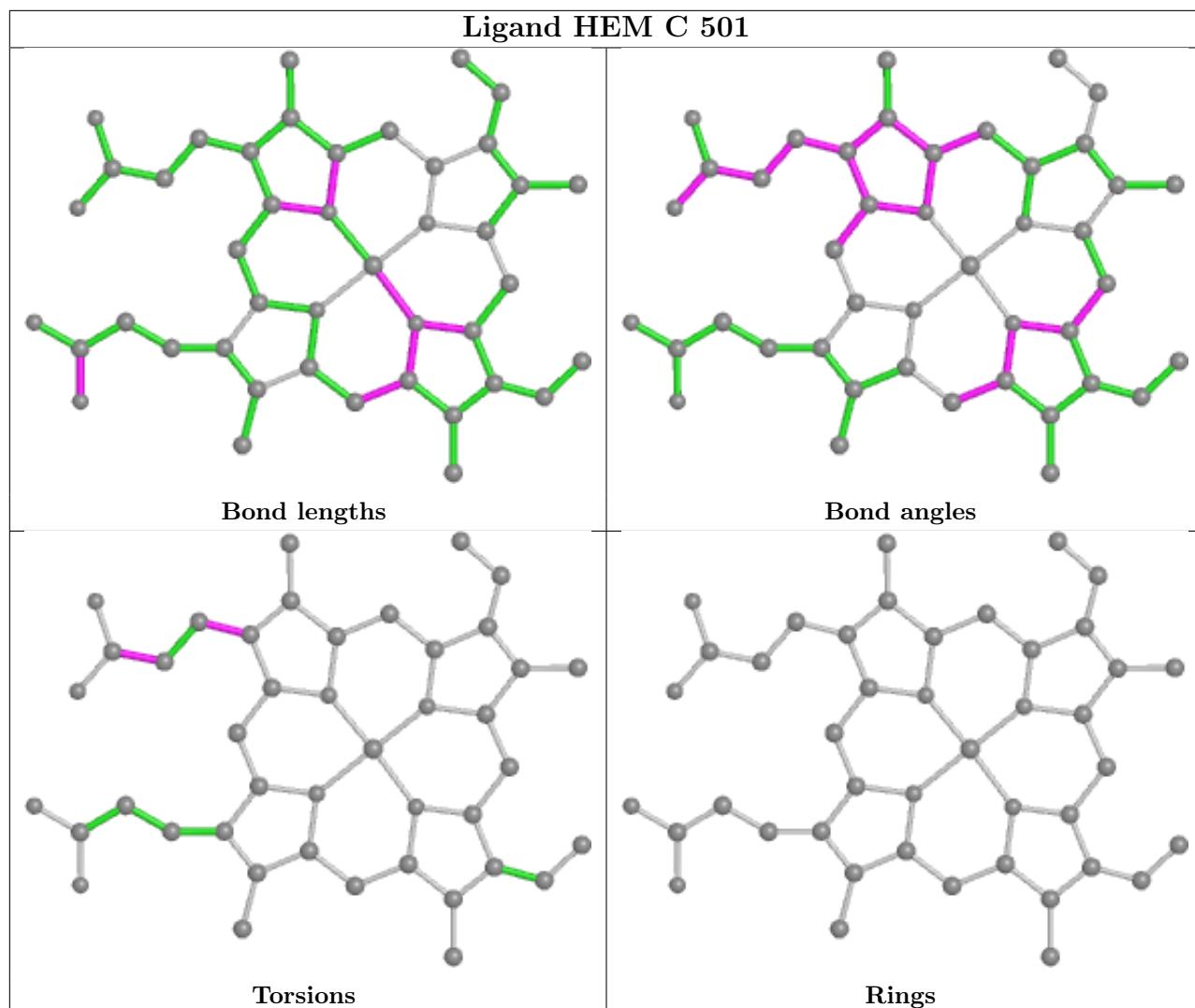












5.7 Other polymers [\(i\)](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	413/460 (89%)	0.07	14 (3%) 45 52	11, 33, 67, 119	0
1	B	413/460 (89%)	0.05	12 (2%) 51 58	15, 35, 68, 135	0
1	C	413/460 (89%)	0.32	28 (6%) 17 22	16, 43, 85, 126	0
1	D	413/460 (89%)	0.41	25 (6%) 21 27	18, 47, 83, 138	0
1	E	413/460 (89%)	0.44	25 (6%) 21 27	18, 48, 86, 127	0
1	F	413/460 (89%)	0.49	30 (7%) 15 20	16, 53, 88, 134	0
All	All	2478/2760 (89%)	0.30	134 (5%) 25 32	11, 43, 83, 138	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	GLY	13.6
1	B	75	TYR	8.4
1	F	274	GLY	7.9
1	D	276	GLU	7.5
1	F	276	GLU	6.9
1	D	74	LYS	6.8
1	E	274	GLY	6.8
1	C	274	GLY	6.4
1	A	274	GLY	6.4
1	B	274	GLY	6.4
1	C	469	THR	6.3
1	F	75	TYR	6.3
1	E	276	GLU	6.3
1	E	75	TYR	6.2
1	A	75	TYR	5.9
1	A	469	THR	5.8
1	C	277	GLN	5.7
1	B	276	GLU	5.7
1	D	75	TYR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	469	THR	5.4
1	E	330	ILE	5.3
1	F	254	ALA	5.3
1	F	469	THR	5.2
1	E	469	THR	5.1
1	A	276	GLU	4.9
1	D	469	THR	4.6
1	D	275	GLU	4.4
1	E	333	GLU	4.1
1	C	275	GLU	4.1
1	A	74	LYS	4.0
1	C	276	GLU	3.9
1	A	273	ARG	3.7
1	F	74	LYS	3.7
1	D	484	THR	3.6
1	C	170	LYS	3.6
1	E	275	GLU	3.6
1	C	462	GLU	3.6
1	F	378	ASP	3.5
1	C	75	TYR	3.5
1	D	278	ALA	3.5
1	D	171	SER	3.5
1	B	275	GLU	3.4
1	A	170	LYS	3.4
1	E	169	ASP	3.4
1	D	419	ALA	3.4
1	E	444	ILE	3.4
1	B	277	GLN	3.2
1	F	166	ALA	3.2
1	E	417	LYS	3.2
1	A	334	PHE	3.1
1	E	468	TYR	3.1
1	D	314	ASN	3.1
1	D	169	ASP	3.0
1	F	419	ALA	3.0
1	B	170	LYS	3.0
1	F	484	THR	3.0
1	F	251	GLU	2.9
1	A	275	GLU	2.9
1	C	314	ASN	2.9
1	E	448	TRP	2.9
1	C	484	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	335	GLY	2.9
1	C	74	LYS	2.9
1	C	417	LYS	2.9
1	C	171	SER	2.8
1	C	273	ARG	2.8
1	F	171	SER	2.8
1	C	482	ARG	2.8
1	F	471	MET	2.8
1	D	462	GLU	2.8
1	D	277	GLN	2.8
1	C	413	VAL	2.7
1	A	468	TYR	2.7
1	A	336	ASP	2.7
1	C	336	ASP	2.7
1	C	325	GLU	2.7
1	B	76	GLY	2.7
1	F	275	GLU	2.7
1	D	170	LYS	2.7
1	F	468	TYR	2.7
1	F	258	VAL	2.6
1	F	273	ARG	2.6
1	D	471	MET	2.6
1	D	418	GLN	2.6
1	D	251	GLU	2.6
1	F	462	GLU	2.6
1	C	317	LYS	2.6
1	A	471	MET	2.6
1	D	417	LYS	2.6
1	E	334	PHE	2.5
1	F	328	GLU	2.5
1	E	471	MET	2.5
1	B	468	TYR	2.5
1	C	378	ASP	2.5
1	E	414	GLU	2.4
1	E	314	ASN	2.4
1	D	166	ALA	2.4
1	F	132	ALA	2.4
1	D	321	PRO	2.4
1	E	484	THR	2.4
1	F	485	ARG	2.4
1	E	277	GLN	2.4
1	C	337	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	482	ARG	2.3
1	E	171	SER	2.3
1	B	331	ARG	2.3
1	E	413	VAL	2.3
1	F	336	ASP	2.3
1	C	169	ASP	2.3
1	D	328	GLU	2.2
1	C	328	GLU	2.2
1	A	462	GLU	2.2
1	A	378	ASP	2.2
1	F	277	GLN	2.2
1	D	399	GLU	2.2
1	C	302	THR	2.1
1	F	106	ALA	2.1
1	B	169	ASP	2.1
1	F	454	ASN	2.1
1	C	306	THR	2.1
1	C	406	GLN	2.1
1	E	406	GLN	2.1
1	F	272	TYR	2.1
1	F	465	LYS	2.1
1	B	273	ARG	2.1
1	D	173	THR	2.1
1	F	313	ALA	2.1
1	E	345	LYS	2.0
1	C	468	TYR	2.0
1	C	330	ILE	2.0
1	F	414	GLU	2.0
1	E	74	LYS	2.0
1	E	278	ALA	2.0
1	F	377	LYS	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

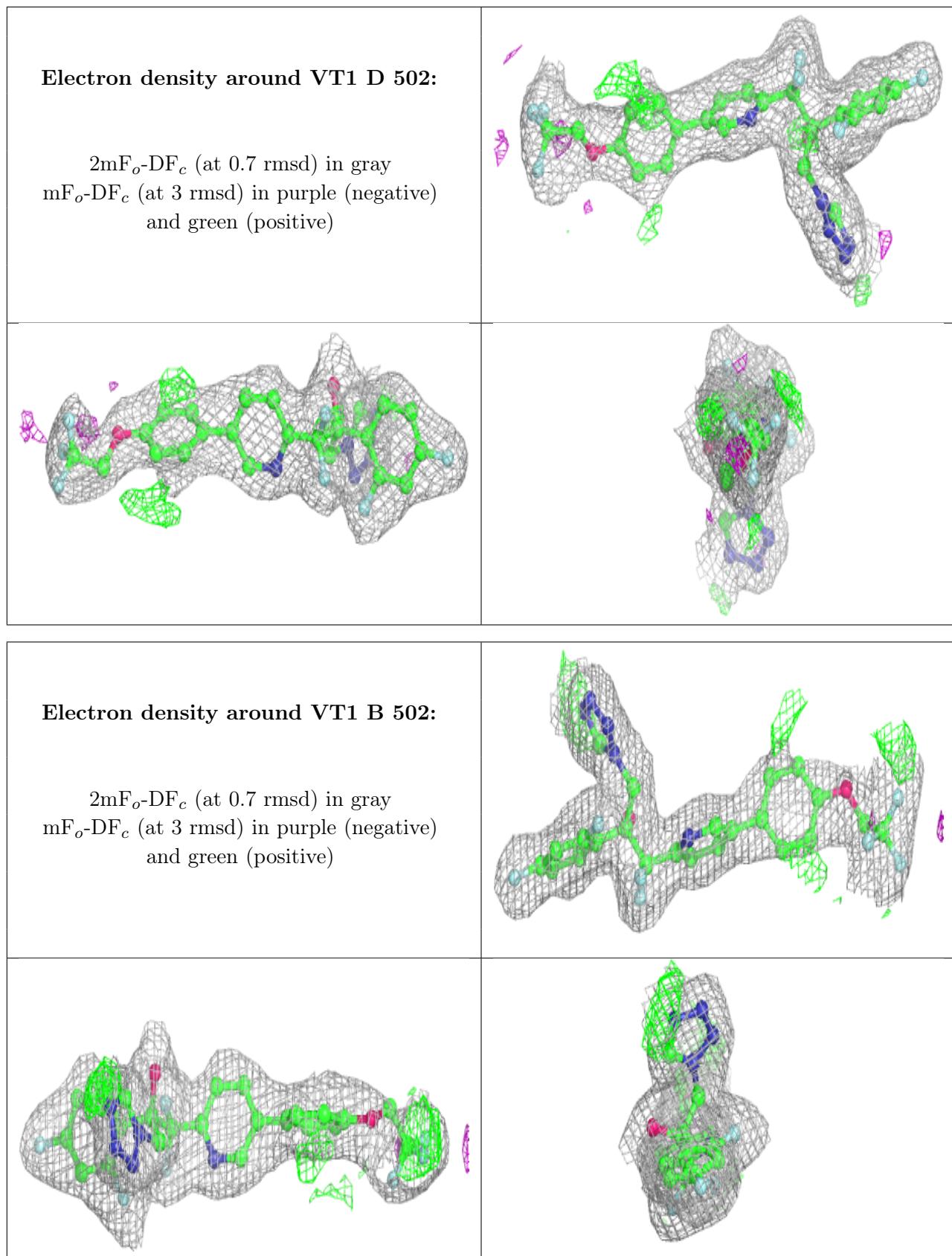
There are no monosaccharides in this entry.

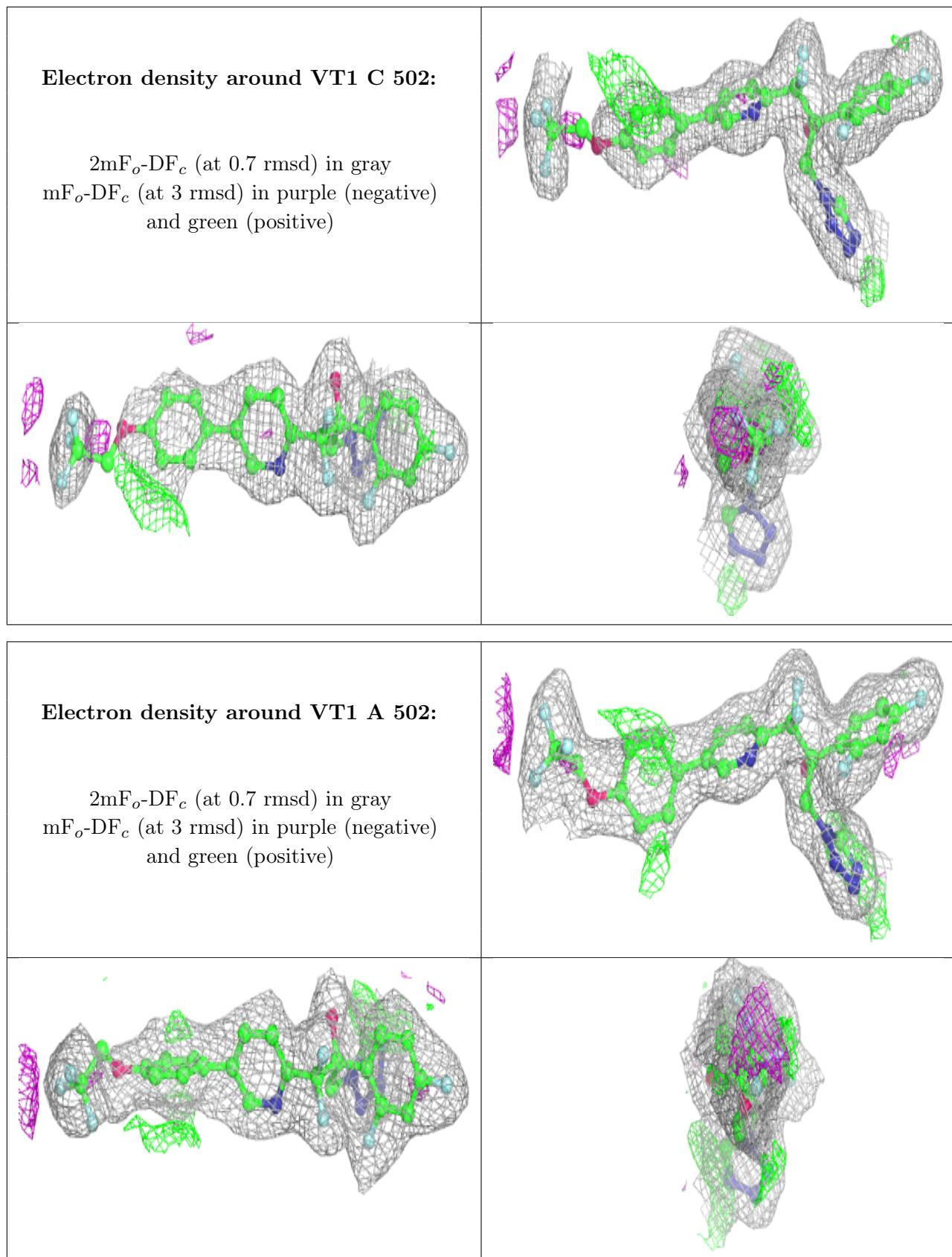
6.4 Ligands [\(i\)](#)

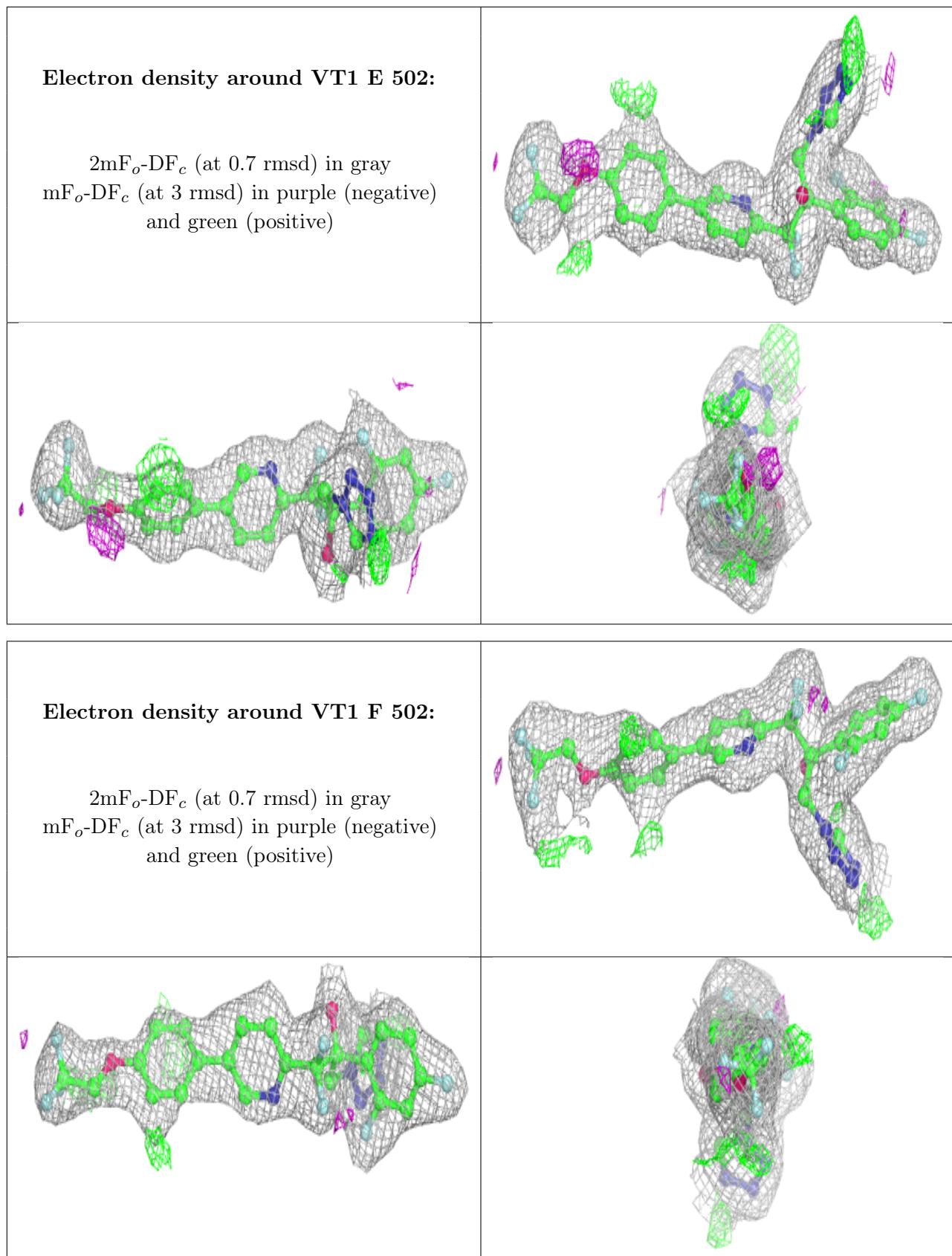
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

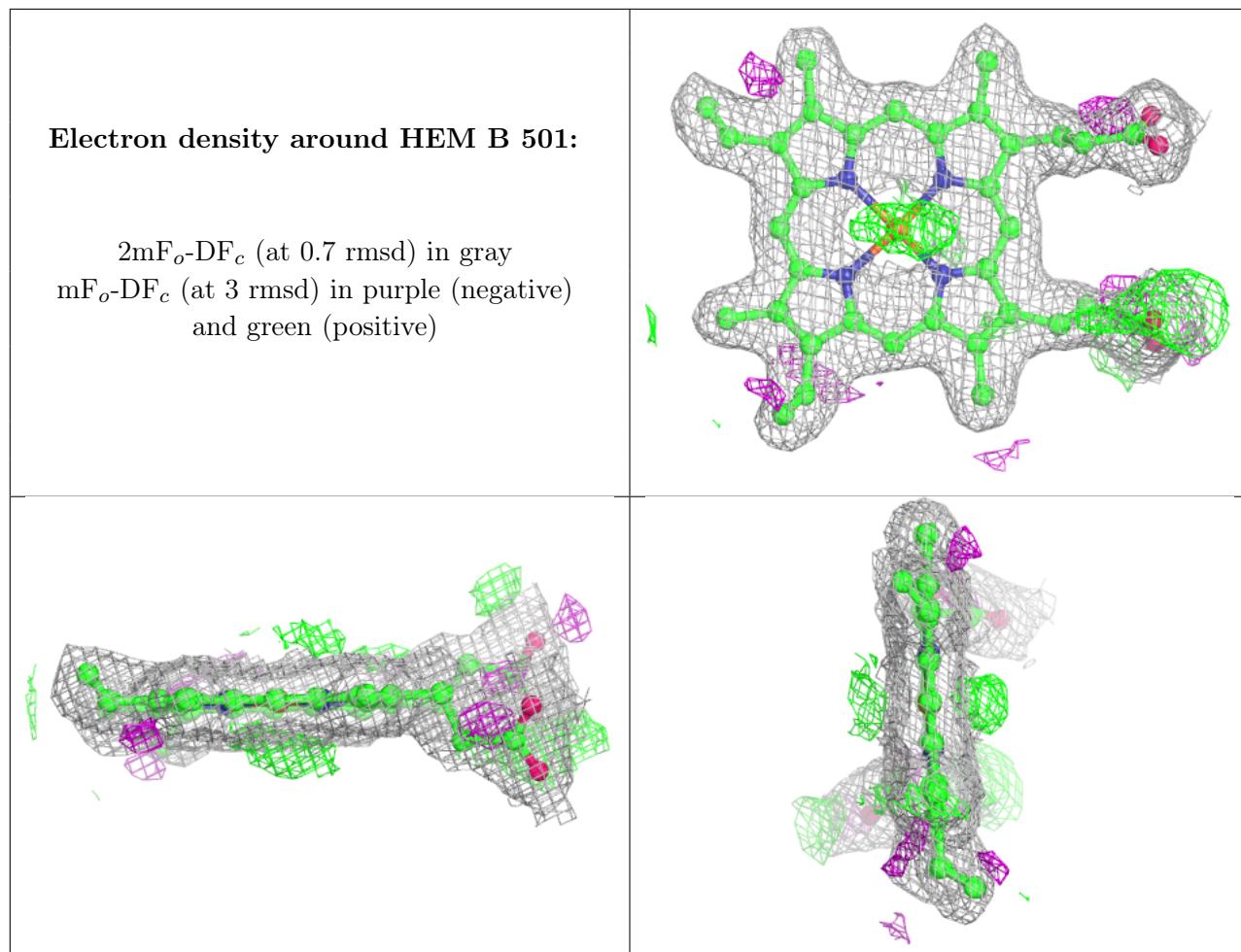
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VT1	D	502	37/37	0.93	0.19	20,30,91,92	0
3	VT1	B	502	37/37	0.94	0.18	12,27,87,96	0
3	VT1	C	502	37/37	0.94	0.19	15,25,100,111	0
3	VT1	A	502	37/37	0.94	0.18	9,23,87,91	0
3	VT1	E	502	37/37	0.94	0.16	12,29,76,82	0
3	VT1	F	502	37/37	0.94	0.19	20,37,103,108	0
2	HEM	B	501	43/43	0.97	0.15	14,15,21,26	0
2	HEM	C	501	43/43	0.97	0.17	17,20,26,28	0
2	HEM	E	501	43/43	0.97	0.16	12,21,26,34	0
2	HEM	F	501	43/43	0.97	0.17	17,21,34,39	0
2	HEM	A	501	43/43	0.97	0.15	8,10,15,17	0
2	HEM	D	501	43/43	0.98	0.16	16,19,28,31	0

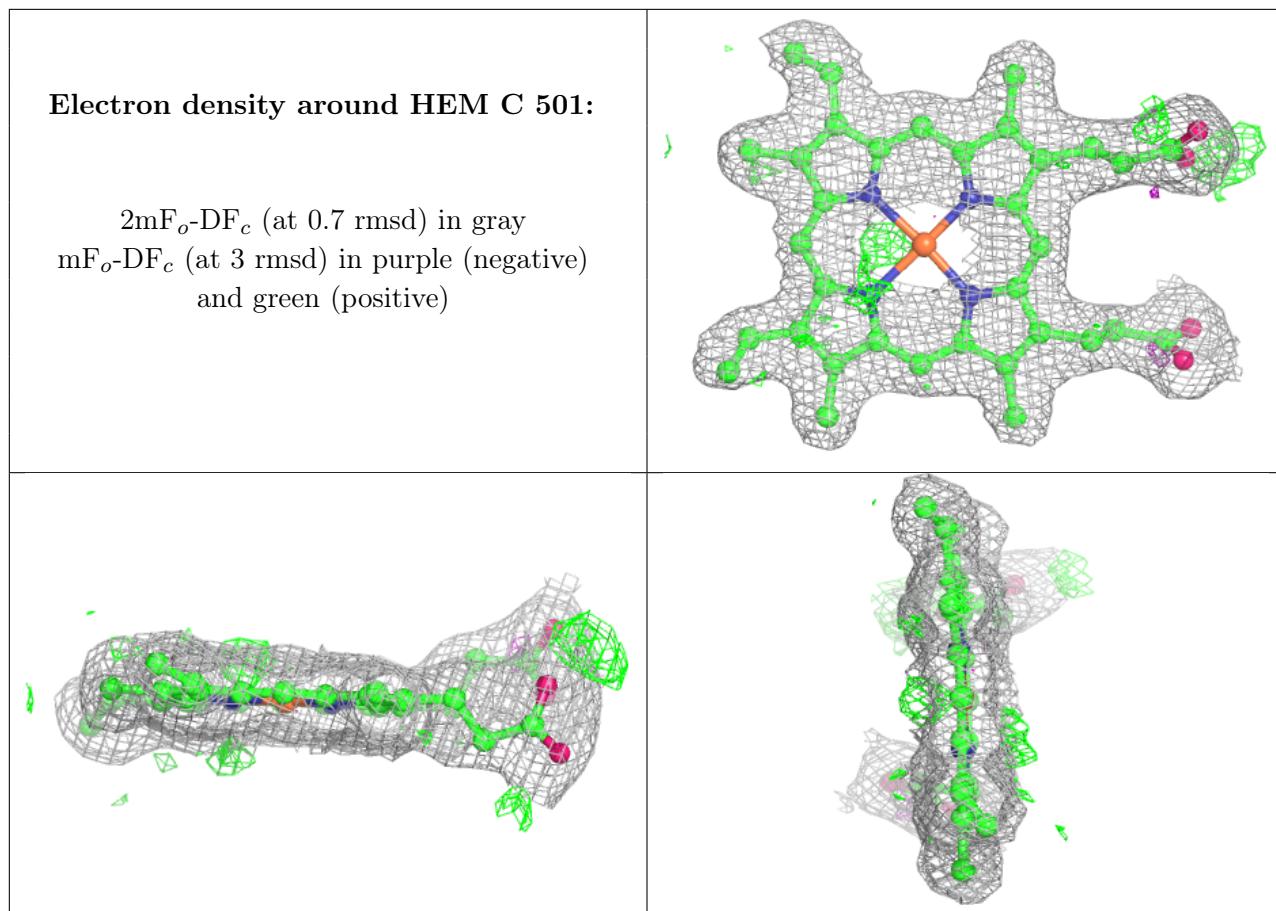
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

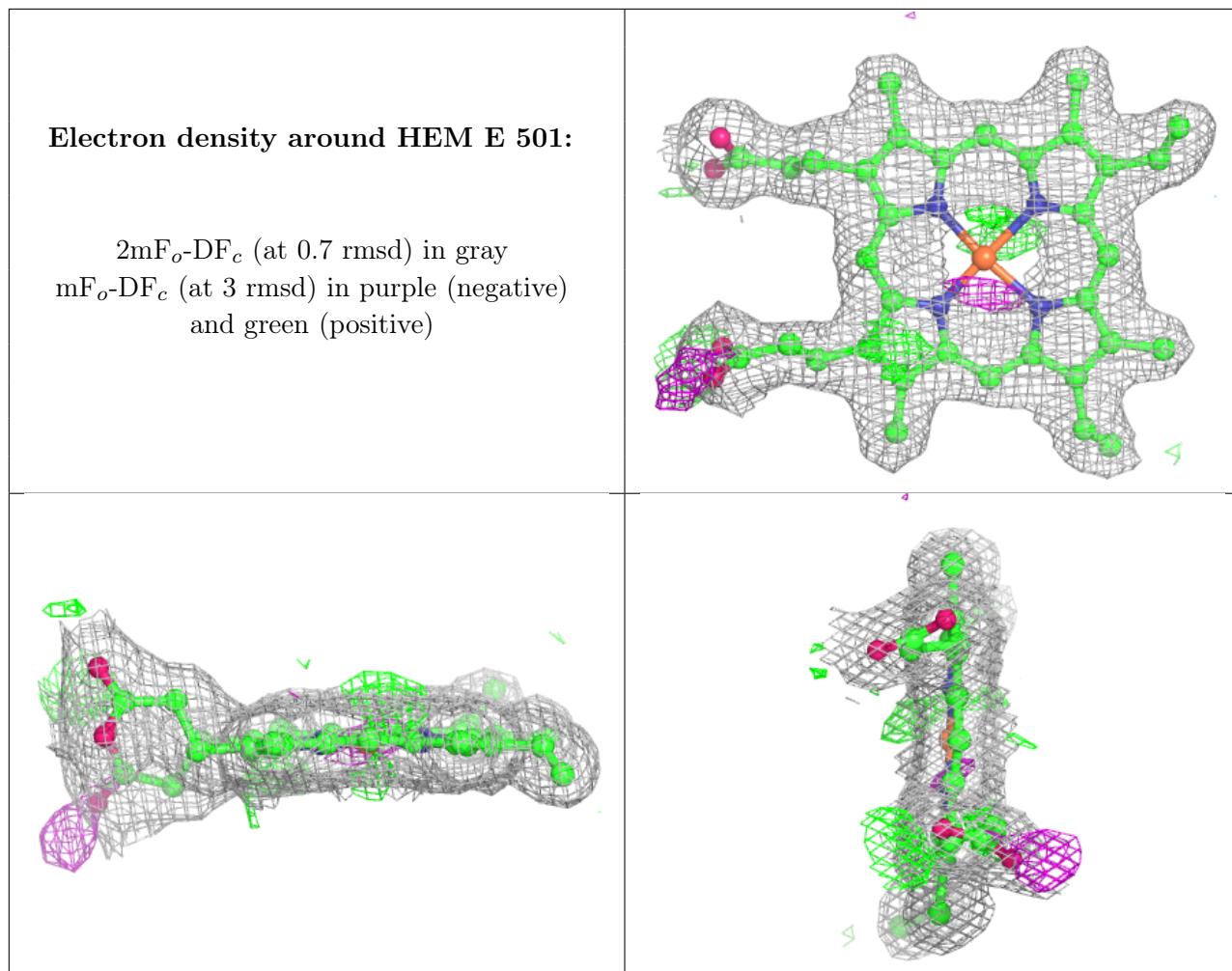


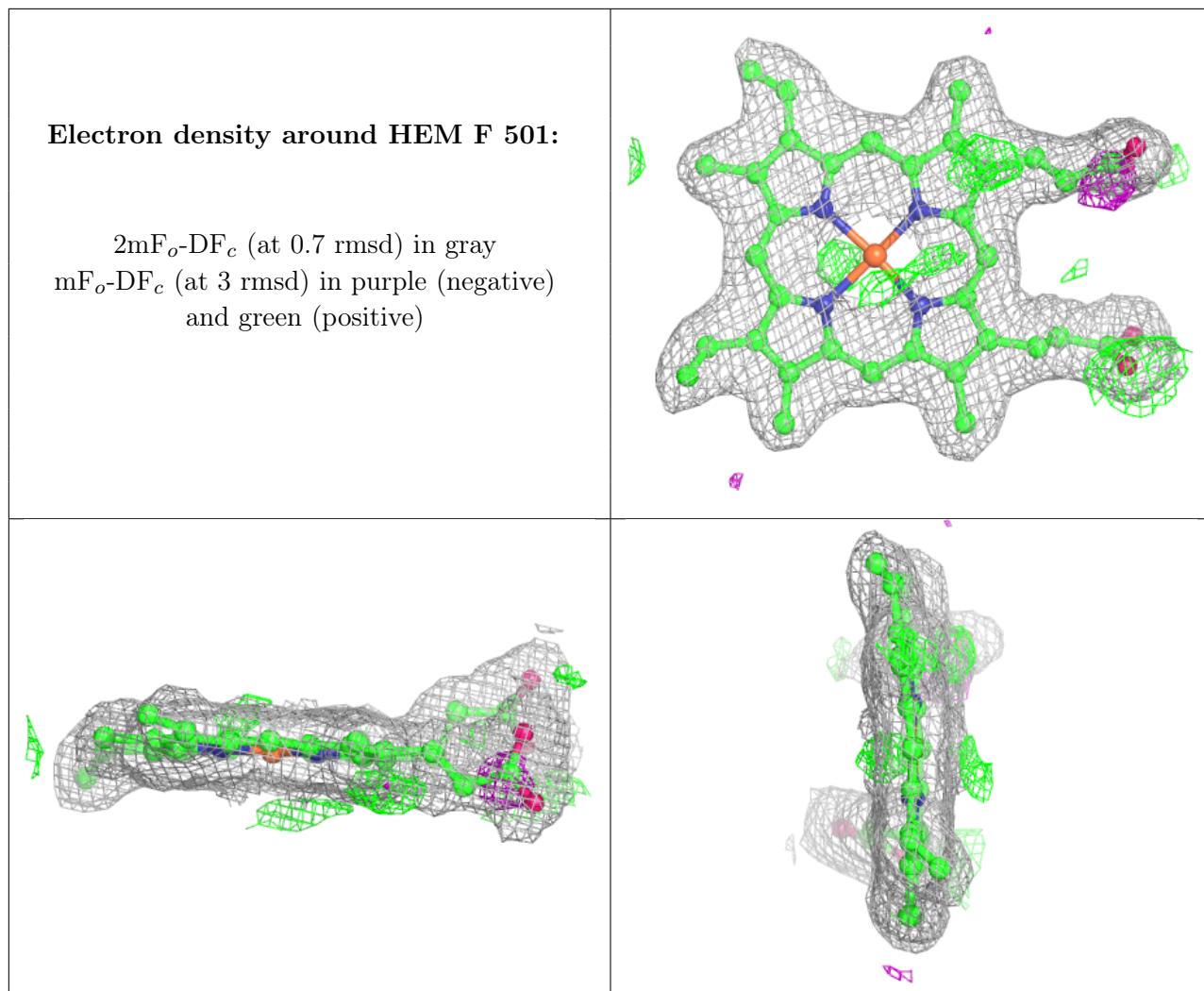


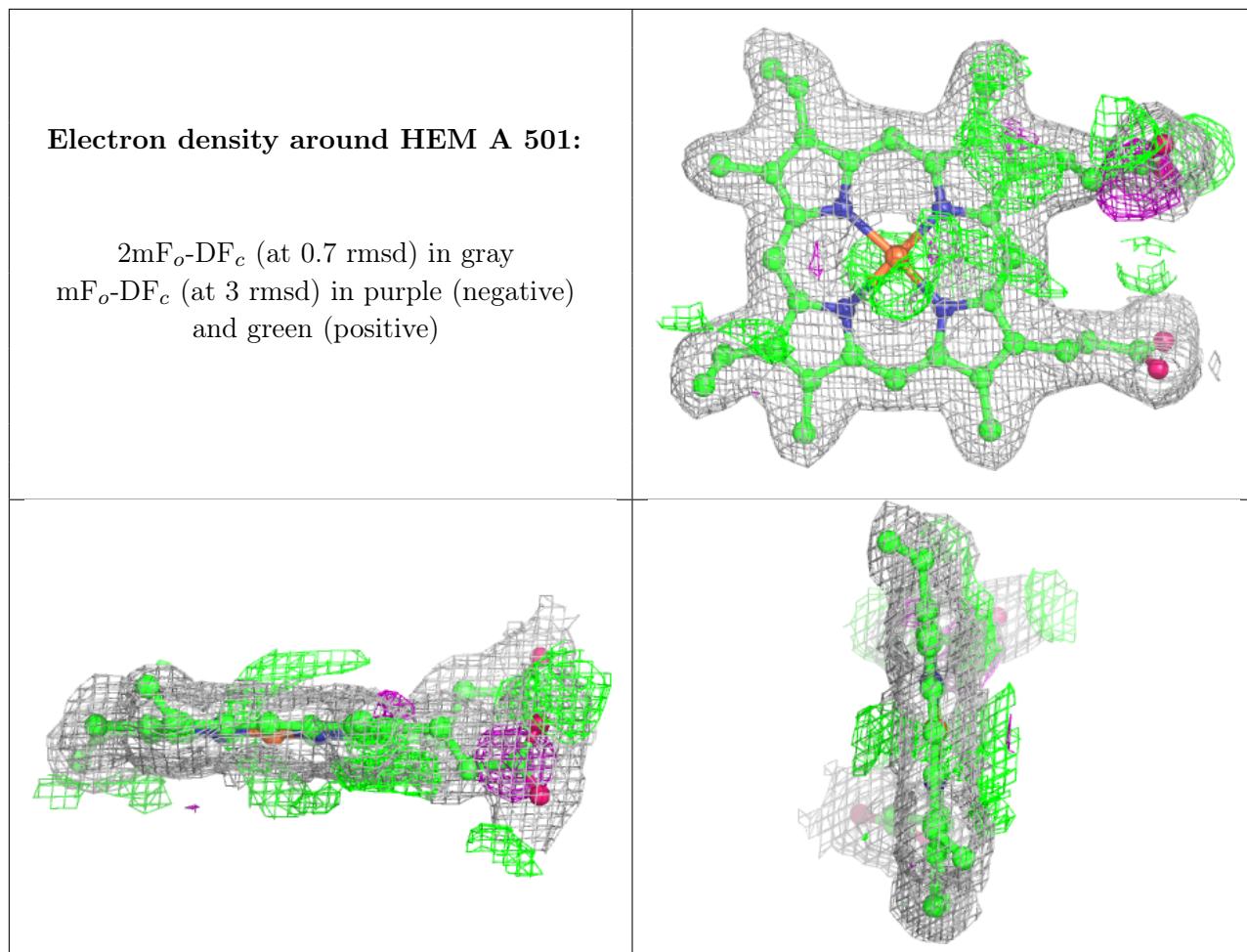


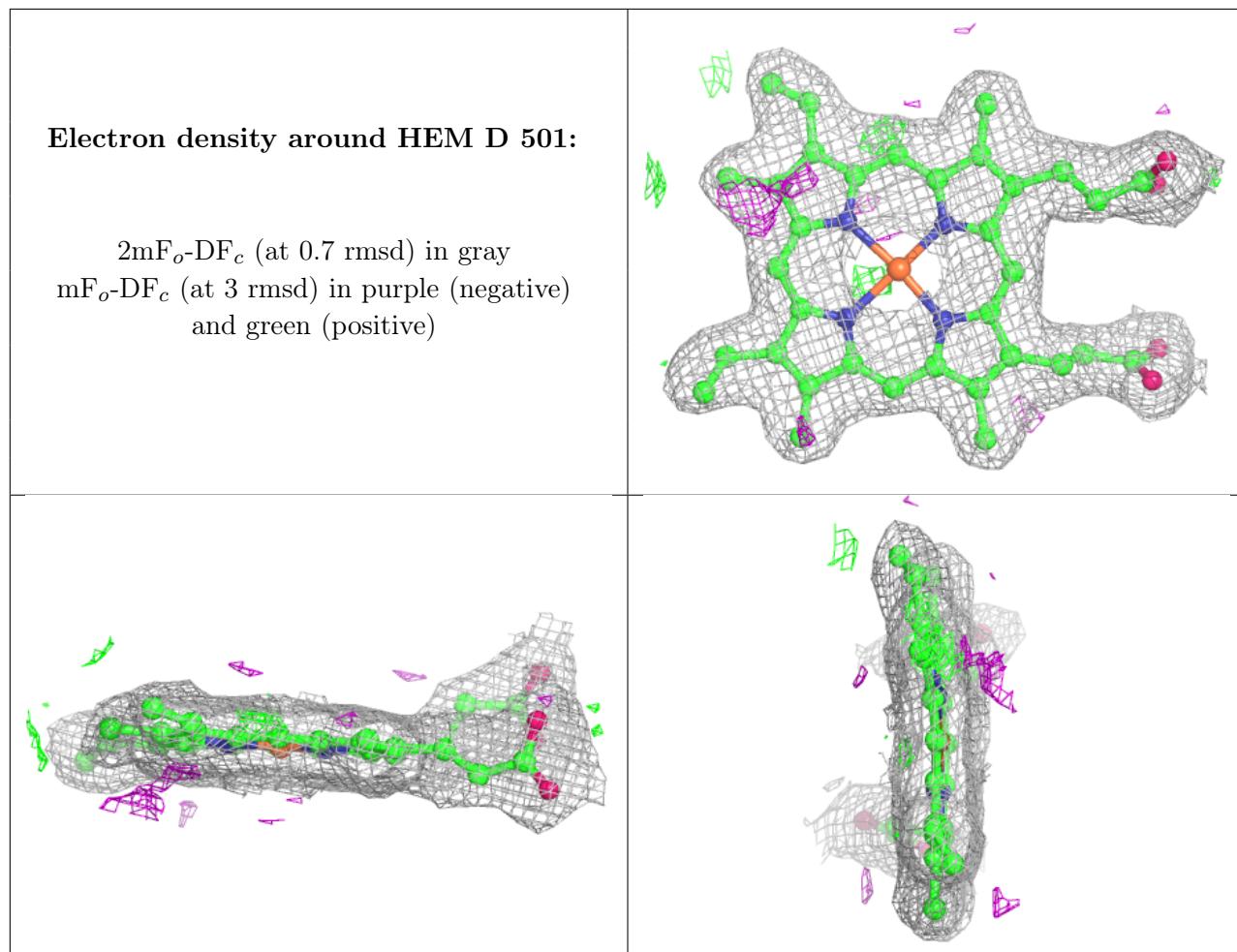












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.