



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:29 PM BST

PDB ID : 4G3J
Title : Sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in complex with the VNI derivative (R)-N-(1-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide [R-VNI-triazole (VNT)]
Authors : Hargrove, T.Y.; Wawrzak, Z.; Waterman, M.R.; Lepesheva, G.I.
Deposited on : 2012-07-14
Resolution : 1.83 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

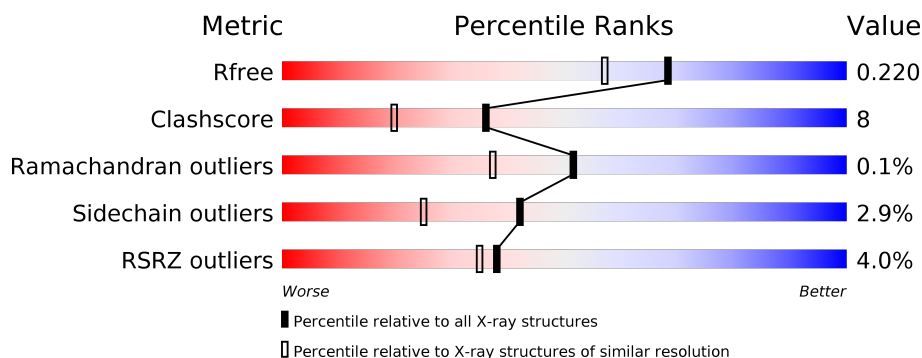
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>
1	B	448	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	C	448	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> </div>
1	D	448	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15243 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 14-alpha-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	B	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	C	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	D	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			

There are 12 discrepancies between the modelled and reference sequences:

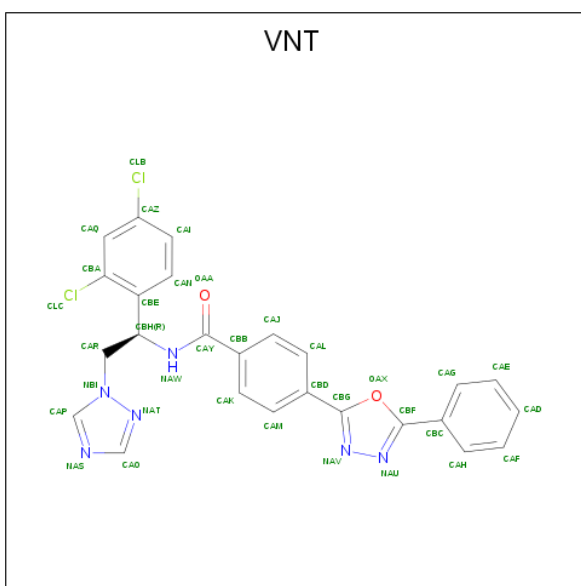
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
A	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
A	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
B	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
B	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
B	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
C	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
C	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
C	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
D	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
D	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
D	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8

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



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

- Molecule 3 is N-[(1R)-1-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (three-letter code: VNT) (formula: C₂₅H₁₈Cl₂N₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			35	25	2	6	2		
3	B	1	Total	C	Cl	N	O	0	0
			35	25	2	6	2		
3	C	1	Total	C	Cl	N	O	0	0
			35	25	2	6	2		
3	D	1	Total	C	Cl	N	O	0	0
			35	25	2	6	2		

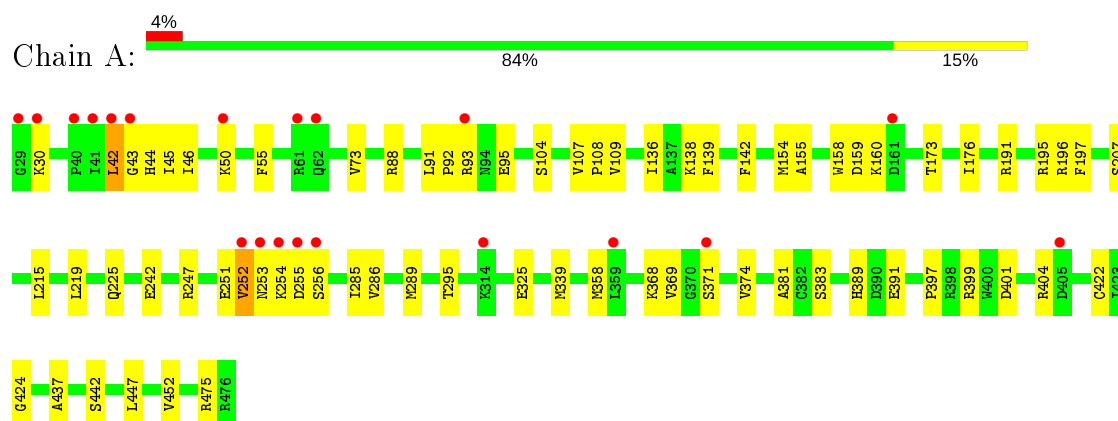
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		
4	B	226	Total	O	0	0
			226	226		
4	C	141	Total	O	0	0
			141	141		
4	D	134	Total	O	0	0
			134	134		

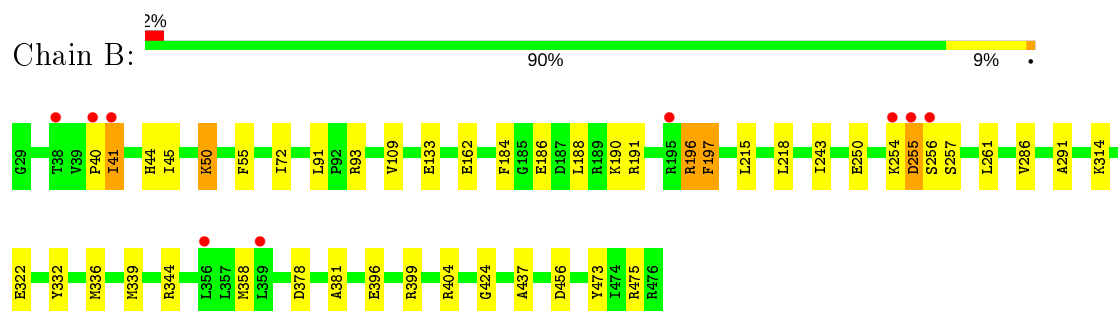
3 Residue-property plots [i](#)

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.

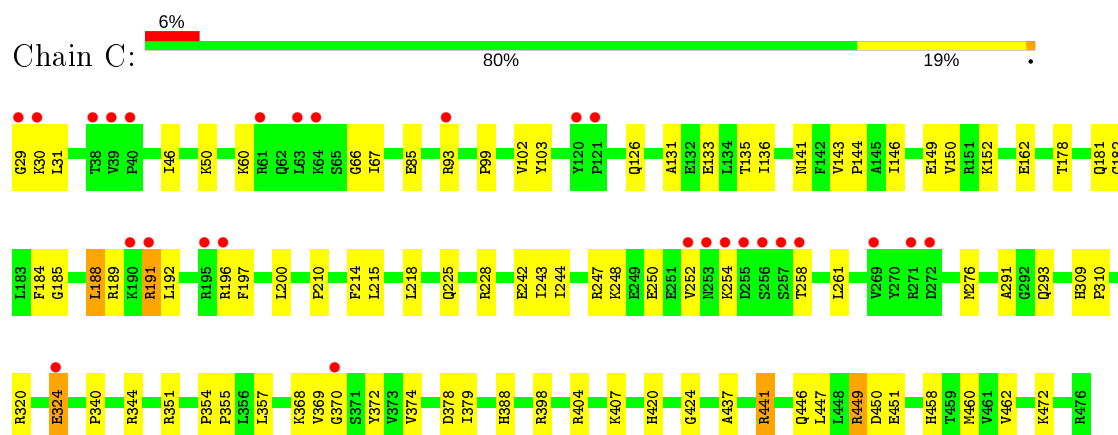
• Molecule 1: sterol 14-alpha-demethylase




• Molecule 1: sterol 14-alpha-demethylase

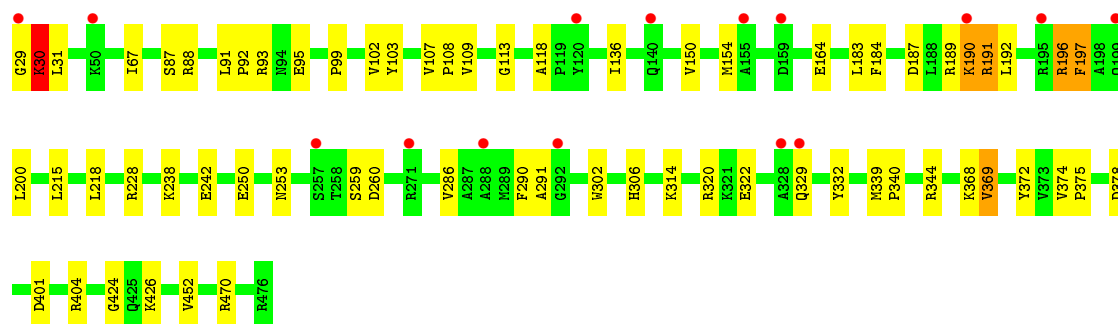


• Molecule 1: sterol 14-alpha-demethylase



● Molecule 1: sterol 14-alpha-demethylase

Chain D:  3% 85% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.01Å 79.48Å 116.35Å 74.59° 79.28° 68.48°	Depositor
Resolution (Å)	29.93 – 1.83 29.93 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.93-1.83) 97.2 (29.93-1.83)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.169 , 0.220 0.169 , 0.220	Depositor DCC
R_{free} test set	8327 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15243	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/3639	0.45	0/4922
1	B	0.33	0/3639	0.43	0/4922
1	C	0.33	0/3639	0.43	0/4922
1	D	0.32	0/3639	0.43	0/4922
All	All	0.33	0/14556	0.43	0/19688

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	378	ASP	Peptide
1	C	378	ASP	Peptide
1	D	378	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3557	0	3594	58	0
1	B	3557	0	3594	42	0
1	C	3557	0	3594	69	0
1	D	3557	0	3594	52	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	7	0
3	A	35	0	18	2	0
3	B	35	0	18	2	0
3	C	35	0	18	2	0
3	D	35	0	18	4	0
4	A	202	0	0	2	0
4	B	226	0	0	3	0
4	C	141	0	0	3	0
4	D	134	0	0	2	0
All	All	15243	0	14568	232	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 8.

All (232) 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:67:ILE:HD13	1:D:369:VAL:HG22	1.45	0.99
1:A:176:ILE:HD11	1:A:197:PHE:HD2	1.27	0.96
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.46	0.96
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.49	0.94
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.51	0.93
1:A:252:VAL:HG13	1:B:93:ARG:HH22	1.37	0.90
1:A:176:ILE:HD11	1:A:197:PHE:CD2	2.07	0.90
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.53	0.89
1:A:109:VAL:CG1	1:A:286:VAL:HG11	2.04	0.88
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.56	0.86
1:A:247:ARG:O	1:A:251:GLU:HG3	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.58	0.85
1:B:50:LYS:HB2	1:B:50:LYS:NZ	1.93	0.82
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.61	0.82
1:D:369:VAL:CG1	1:D:374:VAL:HG23	2.12	0.80
1:D:291:ALA:O	3:D:502:VNT:H7	1.82	0.79
1:D:368:LYS:HD2	1:D:372:TYR:O	1.83	0.77
1:C:188:LEU:C	1:C:188:LEU:HD12	2.04	0.77
1:D:136:ILE:HD13	1:D:426:LYS:HD2	1.65	0.77
1:D:184:PHE:O	1:D:189:ARG:NH1	2.18	0.76
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.68	0.76
1:B:332:TYR:CE2	1:B:336:MET:HG3	2.21	0.75
1:C:188:LEU:O	1:C:188:LEU:HD12	1.87	0.75
1:D:136:ILE:CD1	1:D:426:LYS:HD2	2.18	0.73
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.18	0.72
1:C:133:GLU:HG3	1:C:261:LEU:HD12	1.70	0.72
1:B:475:ARG:NH1	4:B:672:HOH:O	2.20	0.72
1:C:184:PHE:O	1:C:189:ARG:NH1	2.23	0.72
1:D:184:PHE:CE2	1:D:197:PHE:HE2	2.08	0.71
1:C:291:ALA:O	3:C:502:VNT:H7	1.91	0.71
1:A:44:HIS:HB3	1:A:55:PHE:CZ	2.26	0.71
1:C:185:GLY:HA3	1:C:258:THR:HG21	1.74	0.70
1:C:368:LYS:HE2	1:C:370:GLY:O	1.92	0.70
1:A:109:VAL:HG12	1:A:286:VAL:HG11	1.74	0.70
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.23	0.69
1:B:40:PRO:C	1:B:41:ILE:HG13	2.13	0.69
1:C:309:HIS:CG	1:C:310:PRO:HD2	2.29	0.68
1:D:369:VAL:CG1	1:D:374:VAL:CG2	2.71	0.68
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.67
1:C:248:LYS:O	1:C:252:VAL:HG23	1.95	0.67
1:A:252:VAL:HG13	1:B:93:ARG:NH2	2.08	0.67
1:C:458:HIS:CE1	4:C:716:HOH:O	2.49	0.65
1:C:250:GLU:O	1:C:254:LYS:O	2.15	0.65
1:A:207:SER:OG	1:A:225:GLN:O	2.13	0.65
1:D:99:PRO:O	1:D:102:VAL:HG22	1.97	0.64
1:C:324:GLU:O	1:C:324:GLU:HG2	1.97	0.64
1:D:369:VAL:HG11	1:D:374:VAL:HG21	1.79	0.64
1:C:188:LEU:HA	1:C:243:ILE:HD12	1.78	0.64
1:B:184:PHE:CE2	1:B:197:PHE:HE2	2.15	0.64
1:A:173:THR:O	1:A:176:ILE:HG22	1.98	0.63
1:A:252:VAL:HG22	1:B:93:ARG:NH2	2.13	0.63
2:D:501:HEM:CHC	2:D:501:HEM:HBB2	2.20	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.28	0.63
2:A:501:HEM:CHC	2:A:501:HEM:HBB2	2.25	0.63
1:C:126:GLN:HG2	1:C:276:MET:HE3	1.80	0.63
1:D:250:GLU:HA	1:D:253:ASN:OD1	1.98	0.63
1:A:109:VAL:CG1	1:A:286:VAL:CG1	2.77	0.62
1:D:87:SER:HB2	1:D:91:LEU:HD12	1.82	0.62
1:A:43:GLY:O	1:A:44:HIS:CD2	2.53	0.62
1:D:369:VAL:HG11	1:D:374:VAL:CG2	2.30	0.61
1:A:191:ARG:NH1	1:A:242:GLU:OE1	2.22	0.61
1:C:181:GLN:HA	1:C:189:ARG:NH1	2.16	0.60
1:C:191:ARG:HB2	1:C:243:ILE:HD11	1.81	0.60
1:B:50:LYS:HB2	1:B:50:LYS:HZ2	1.66	0.60
1:D:184:PHE:HE2	1:D:197:PHE:HE2	1.49	0.60
1:D:369:VAL:HG12	1:D:374:VAL:HG23	1.85	0.59
1:C:191:ARG:NH1	1:C:242:GLU:OE1	2.36	0.58
1:C:146:ILE:HG13	1:C:182:CYS:SG	2.43	0.58
1:D:31:LEU:HD22	1:D:375:PRO:HD3	1.84	0.58
1:A:424:GLY:HA3	2:A:501:HEM:C3C	2.38	0.58
1:A:88:ARG:HH21	1:A:368:LYS:HB3	1.69	0.57
2:D:501:HEM:HHC	2:D:501:HEM:CBB	2.29	0.57
1:B:291:ALA:O	3:B:502:VNT:H7	2.06	0.56
1:D:109:VAL:HG13	1:D:286:VAL:HG11	1.87	0.56
1:C:451:GLU:OE2	1:C:451:GLU:HA	2.04	0.56
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.27	0.56
1:C:225:GLN:HG3	1:C:228:ARG:HH12	1.70	0.56
1:A:399:ARG:HH11	1:A:399:ARG:HG3	1.69	0.55
1:C:188:LEU:CD1	1:C:192:LEU:HB3	2.36	0.55
1:B:188:LEU:HD13	1:B:243:ILE:HG13	1.89	0.55
1:C:126:GLN:HG2	1:C:276:MET:CE	2.36	0.55
1:A:155:ALA:O	1:A:159:ASP:HB3	2.07	0.54
1:A:138:LYS:HE3	4:A:744:HOH:O	2.06	0.54
1:D:340:PRO:O	1:D:344:ARG:HG3	2.08	0.54
1:D:290:PHE:HB3	3:D:502:VNT:CLC	2.45	0.54
1:C:215:LEU:HD23	1:C:218:LEU:CD1	2.38	0.54
1:B:250:GLU:O	1:B:254:LYS:O	2.26	0.54
1:A:93:ARG:HD3	1:A:95:GLU:HB2	1.90	0.53
1:C:340:PRO:O	1:C:344:ARG:HG3	2.09	0.53
1:C:184:PHE:HB3	1:C:188:LEU:HG	1.89	0.53
2:D:501:HEM:C1A	3:D:502:VNT:H8	2.42	0.53
1:B:339:MET:HE1	1:B:437:ALA:HB2	1.90	0.53
1:C:214:PHE:CE1	1:C:379:ILE:HD13	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:CB	1:C:243:ILE:HD11	2.39	0.53
1:D:187:ASP:O	1:D:190:LYS:HG3	2.08	0.53
1:B:50:LYS:HB2	1:B:50:LYS:HZ3	1.74	0.53
1:C:131:ALA:O	1:C:135:THR:HG23	2.08	0.53
1:C:446:GLN:OE1	1:C:472:LYS:HE3	2.08	0.53
1:C:309:HIS:CD2	1:C:310:PRO:HD2	2.43	0.53
1:C:244:ILE:O	1:C:248:LYS:HG3	2.08	0.52
1:B:424:GLY:HA3	2:B:501:HEM:C3C	2.45	0.52
1:A:252:VAL:HG11	1:B:93:ARG:HH12	1.75	0.52
1:A:46:ILE:HG22	1:A:50:LYS:HE2	1.91	0.52
1:C:188:LEU:CD1	1:C:188:LEU:C	2.74	0.52
1:C:143:VAL:HB	1:C:144:PRO:HD3	1.91	0.52
1:C:320:ARG:O	1:C:324:GLU:HB3	2.10	0.52
1:A:207:SER:O	1:A:225:GLN:HB3	2.10	0.52
1:C:437:ALA:O	1:C:441:ARG:HB2	2.10	0.51
1:B:314:LYS:NZ	4:B:674:HOH:O	2.42	0.51
1:C:181:GLN:HA	1:C:189:ARG:HH11	1.74	0.51
1:D:191:ARG:NH1	1:D:242:GLU:OE1	2.42	0.51
1:C:369:VAL:HG12	1:C:374:VAL:HG23	1.93	0.51
1:C:368:LYS:HD2	1:C:372:TYR:O	2.11	0.50
1:A:422:CYS:HB2	2:A:501:HEM:NA	2.27	0.50
1:C:215:LEU:HD23	1:C:218:LEU:HD11	1.93	0.50
1:A:253:ASN:OD1	1:A:254:LYS:N	2.45	0.49
1:A:399:ARG:HG3	1:A:399:ARG:NH1	2.25	0.49
1:B:44:HIS:HB3	1:B:55:PHE:CZ	2.48	0.49
1:C:85:GLU:OE2	1:C:370:GLY:HA2	2.13	0.48
1:D:102:VAL:HG23	1:D:103:TYR:CD2	2.48	0.48
1:D:184:PHE:HE2	1:D:197:PHE:CE2	2.30	0.48
1:D:164:GLU:HG2	1:D:470:ARG:HH21	1.79	0.48
1:D:424:GLY:HA3	2:D:501:HEM:C3C	2.49	0.48
1:C:369:VAL:CG1	1:C:374:VAL:HG23	2.43	0.48
1:D:238:LYS:HE3	1:D:242:GLU:OE2	2.13	0.48
1:A:154:MET:HG2	1:A:158:TRP:CE3	2.49	0.48
1:D:196:ARG:HG2	1:D:196:ARG:NH1	2.28	0.48
1:B:344:ARG:NH2	1:B:404:ARG:O	2.47	0.47
1:D:136:ILE:HG23	1:D:332:TYR:OH	2.14	0.47
1:A:339:MET:HE1	1:A:437:ALA:HB2	1.97	0.47
1:A:358:MET:HE3	1:A:381:ALA:HB1	1.96	0.47
1:C:451:GLU:OE2	1:C:451:GLU:CA	2.61	0.47
1:B:218:LEU:HD21	1:D:218:LEU:HD11	1.95	0.47
1:D:322:GLU:CD	1:D:339:MET:HA	2.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG22	1:B:93:ARG:CZ	2.44	0.47
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.62	0.47
1:A:191:ARG:O	1:A:196:ARG:NH2	2.48	0.46
1:A:252:VAL:CG2	1:B:93:ARG:CZ	2.93	0.46
1:A:358:MET:SD	1:A:383:SER:HB2	2.55	0.46
1:A:139:PHE:HA	1:A:142:PHE:HB2	1.98	0.46
1:B:322:GLU:CD	1:B:339:MET:HA	2.35	0.46
1:A:251:GLU:HG2	1:A:254:LYS:NZ	2.31	0.46
1:B:254:LYS:C	1:B:256:SER:N	2.69	0.46
1:B:424:GLY:HA3	2:B:501:HEM:C2C	2.51	0.46
1:C:29:GLY:O	1:C:31:LEU:N	2.42	0.46
1:C:152:LYS:HB3	1:C:152:LYS:HE2	1.72	0.46
1:C:344:ARG:NH2	1:C:404:ARG:O	2.48	0.46
1:C:67:ILE:HD13	1:C:369:VAL:HG22	1.98	0.45
1:D:192:LEU:HD12	1:D:196:ARG:HG2	1.97	0.45
1:C:424:GLY:HA3	2:C:501:HEM:C3C	2.52	0.45
1:A:73:VAL:HG11	1:A:215:LEU:HD13	1.99	0.45
1:A:254:LYS:C	1:A:256:SER:H	2.20	0.45
1:A:442:SER:O	1:A:475:ARG:HD2	2.17	0.45
1:B:399:ARG:HG3	1:B:399:ARG:HH11	1.82	0.45
1:A:252:VAL:HG11	1:B:93:ARG:NH1	2.32	0.45
1:A:389:HIS:CD2	1:A:397:PRO:HB2	2.52	0.45
1:C:149:GLU:HB2	1:C:178:THR:HG22	1.98	0.45
1:C:420:HIS:ND1	2:C:501:HEM:O2D	2.50	0.45
1:D:183:LEU:O	1:D:260:ASP:HB2	2.16	0.45
1:A:91:LEU:N	1:A:92:PRO:CD	2.80	0.44
1:C:449:ARG:HD2	4:C:630:HOH:O	2.17	0.44
2:B:501:HEM:HHC	2:B:501:HEM:CBB	2.33	0.44
1:D:91:LEU:N	1:D:92:PRO:CD	2.81	0.44
1:A:196:ARG:NH1	4:A:736:HOH:O	2.50	0.44
1:B:196:ARG:NH1	1:B:196:ARG:HG2	2.33	0.44
1:C:29:GLY:C	1:C:31:LEU:H	2.20	0.44
1:C:407:LYS:HA	1:C:407:LYS:HD3	1.81	0.44
1:C:60:LYS:HG3	1:C:66:GLY:HA2	2.00	0.44
1:A:369:VAL:HG12	1:A:374:VAL:HG23	2.00	0.43
1:B:254:LYS:O	1:B:256:SER:N	2.51	0.43
1:D:314:LYS:HB2	4:D:722:HOH:O	2.16	0.43
1:B:399:ARG:NH1	4:B:679:HOH:O	2.41	0.43
1:A:107:VAL:N	1:A:108:PRO:CD	2.81	0.43
1:A:358:MET:CE	1:A:381:ALA:HB1	2.48	0.43
1:B:254:LYS:O	1:B:255:ASP:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:HD11	1:D:426:LYS:HD2	1.96	0.43
1:B:358:MET:HE3	1:B:381:ALA:HB1	2.01	0.43
1:C:102:VAL:HG23	1:C:103:TYR:CD1	2.54	0.43
1:C:357:LEU:HD11	1:C:462:VAL:HG21	2.01	0.43
1:B:255:ASP:O	1:B:256:SER:C	2.56	0.43
1:D:302:TRP:O	1:D:306:HIS:CD2	2.71	0.43
1:D:67:ILE:CD1	1:D:369:VAL:HG22	2.32	0.43
1:C:146:ILE:O	1:C:150:VAL:HG23	2.19	0.43
1:C:293:GLN:HB3	4:C:612:HOH:O	2.17	0.43
1:A:104:SER:HB3	1:A:219:LEU:CD1	2.49	0.43
1:C:210:PRO:HG3	1:C:460:MET:SD	2.59	0.43
1:C:67:ILE:CD1	1:C:369:VAL:HG22	2.49	0.43
1:D:107:VAL:N	1:D:108:PRO:CD	2.81	0.43
1:D:136:ILE:HD11	1:D:426:LYS:CD	2.49	0.43
1:A:295:THR:HG21	3:A:502:VNT:CAO	2.48	0.43
1:C:85:GLU:HA	1:C:85:GLU:OE1	2.19	0.43
1:C:99:PRO:O	1:C:102:VAL:HG22	2.19	0.42
1:C:450:ASP:O	1:C:451:GLU:OE2	2.36	0.42
1:D:401:ASP:O	1:D:404:ARG:HG2	2.18	0.42
1:B:162:GLU:HA	1:B:473:TYR:O	2.20	0.42
1:A:176:ILE:HA	1:A:176:ILE:HD12	1.86	0.42
3:C:502:VNT:H3	3:C:502:VNT:H5	1.83	0.42
1:C:141:ASN:O	1:C:144:PRO:HD2	2.18	0.42
1:D:88:ARG:HA	1:D:88:ARG:HD2	1.80	0.42
1:A:401:ASP:O	1:A:404:ARG:HG2	2.19	0.42
1:A:42:LEU:HB3	1:A:45:ILE:HG22	2.02	0.42
1:B:456:ASP:OD1	1:B:456:ASP:C	2.58	0.42
1:D:93:ARG:HG3	1:D:95:GLU:HB2	2.02	0.42
1:A:254:LYS:O	1:A:255:ASP:HB3	2.20	0.42
1:C:146:ILE:CG1	1:C:182:CYS:SG	3.08	0.42
1:C:354:PRO:HA	1:C:355:PRO:HD3	1.88	0.41
1:B:45:ILE:HD13	1:B:72:ILE:HG23	2.01	0.41
1:D:29:GLY:O	1:D:30:LYS:HB2	2.20	0.41
1:A:285:ILE:O	1:A:289:MET:HG2	2.20	0.41
1:C:351:ARG:HD2	1:C:388:HIS:HB3	2.02	0.41
3:D:502:VNT:H5	3:D:502:VNT:H3	1.68	0.41
1:B:133:GLU:HG3	1:B:261:LEU:HD12	2.03	0.41
1:D:228:ARG:NH1	4:D:625:HOH:O	2.52	0.41
1:D:29:GLY:O	1:D:30:LYS:CB	2.68	0.41
1:B:109:VAL:HG12	1:B:286:VAL:HG11	2.03	0.41
1:D:109:VAL:CG1	1:D:286:VAL:HG11	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.85	0.41
1:A:253:ASN:ND2	1:B:91:LEU:O	2.53	0.41
1:D:87:SER:HB2	1:D:91:LEU:CD1	2.48	0.41
1:C:398:ARG:HD2	1:C:398:ARG:HA	1.87	0.41
1:D:150:VAL:HG13	1:D:154:MET:HE2	2.01	0.41
1:D:184:PHE:CE2	1:D:197:PHE:CE2	2.97	0.41
1:A:109:VAL:HG13	1:A:286:VAL:CG1	2.44	0.40
1:D:113:GLY:O	1:D:118:ALA:HB2	2.21	0.40
1:B:332:TYR:CD2	1:B:336:MET:HG3	2.57	0.40
3:B:502:VNT:H5	3:B:502:VNT:H3	1.78	0.40
1:C:424:GLY:HA3	2:C:501:HEM:C2C	2.55	0.40
3:A:502:VNT:H3	3:A:502:VNT:H5	1.85	0.40
1:B:109:VAL:CG1	1:B:286:VAL:HG11	2.51	0.40
1:A:252:VAL:CG1	1:B:93:ARG:NH2	2.81	0.40
1:A:368:LYS:HA	1:A:368:LYS:HD2	1.90	0.40
1:C:46:ILE:HG22	1:C:50:LYS:HE3	2.03	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	446/448 (100%)	436 (98%)	10 (2%)	0	100	100
1	B	446/448 (100%)	436 (98%)	10 (2%)	0	100	100
1	C	446/448 (100%)	436 (98%)	9 (2%)	1 (0%)	47	33
1	D	446/448 (100%)	438 (98%)	7 (2%)	1 (0%)	47	33
All	All	1784/1792 (100%)	1746 (98%)	36 (2%)	2 (0%)	51	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	30	LYS
1	C	30	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/390 (100%)	380 (97%)	10 (3%)	46	29
1	B	390/390 (100%)	379 (97%)	11 (3%)	43	26
1	C	390/390 (100%)	377 (97%)	13 (3%)	38	20
1	D	390/390 (100%)	378 (97%)	12 (3%)	40	23
All	All	1560/1560 (100%)	1514 (97%)	46 (3%)	42	25

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	136	ILE
1	A	160	LYS
1	A	195	ARG
1	A	252	VAL
1	A	325	GLU
1	A	371	SER
1	A	391	GLU
1	A	447	LEU
1	A	452	VAL
1	B	41	ILE
1	B	50	LYS
1	B	186	GLU
1	B	190	LYS
1	B	191	ARG
1	B	196	ARG
1	B	197	PHE
1	B	215	LEU
1	B	255	ASP
1	B	257	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	396	GLU
1	C	93	ARG
1	C	136	ILE
1	C	162	GLU
1	C	188	LEU
1	C	191	ARG
1	C	196	ARG
1	C	197	PHE
1	C	200	LEU
1	C	247	ARG
1	C	324	GLU
1	C	441	ARG
1	C	447	LEU
1	C	449	ARG
1	D	30	LYS
1	D	190	LYS
1	D	191	ARG
1	D	196	ARG
1	D	197	PHE
1	D	200	LEU
1	D	215	LEU
1	D	259	SER
1	D	320	ARG
1	D	329	GLN
1	D	369	VAL
1	D	452	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	VNT	D	502	2	30,39,39	3.37	6 (20%)	44,54,54	1.55	6 (13%)
2	HEM	C	501	1,3	27,50,50	0.80	1 (3%)	17,82,82	1.31	1 (5%)
2	HEM	A	501	1,3	27,50,50	0.81	1 (3%)	17,82,82	1.17	2 (11%)
3	VNT	B	502	2	30,39,39	3.57	5 (16%)	44,54,54	1.42	5 (11%)
2	HEM	D	501	1,3	27,50,50	0.83	2 (7%)	17,82,82	1.42	3 (17%)
2	HEM	B	501	1,3	27,50,50	0.88	1 (3%)	17,82,82	1.35	4 (23%)
3	VNT	A	502	2	30,39,39	3.92	5 (16%)	44,54,54	1.38	4 (9%)
3	VNT	C	502	2	30,39,39	2.97	5 (16%)	44,54,54	1.13	3 (6%)

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	VNT	D	502	2	-	4/18/24/24	0/5/5/5
2	HEM	C	501	1,3	-	0/6/54/54	-
2	HEM	A	501	1,3	-	0/6/54/54	-
3	VNT	B	502	2	-	3/18/24/24	0/5/5/5
2	HEM	D	501	1,3	-	0/6/54/54	-
2	HEM	B	501	1,3	-	0/6/54/54	-
3	VNT	A	502	2	-	1/18/24/24	0/5/5/5
3	VNT	C	502	2	-	2/18/24/24	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	VNT	NAT-NBI	-16.39	1.12	1.35
3	B	502	VNT	NAU-NAV	-12.78	1.12	1.37
3	D	502	VNT	NAT-NBI	-10.88	1.20	1.35
3	B	502	VNT	NAT-NBI	-10.58	1.20	1.35
3	D	502	VNT	NAU-NAV	-10.40	1.17	1.37
3	A	502	VNT	NAU-NAV	-10.31	1.17	1.37
3	C	502	VNT	NAT-NBI	-9.55	1.22	1.35
3	C	502	VNT	NAU-NAV	-9.23	1.19	1.37
3	D	502	VNT	CBE-CBH	-7.80	1.40	1.52
3	B	502	VNT	CBE-CBH	-7.58	1.40	1.52
3	C	502	VNT	CBE-CBH	-6.76	1.41	1.52
3	A	502	VNT	CBE-CBH	-6.63	1.41	1.52
3	B	502	VNT	CBB-CAY	-5.46	1.38	1.50
3	D	502	VNT	CBB-CAY	-5.26	1.39	1.50
3	A	502	VNT	CBB-CAY	-4.86	1.40	1.50
3	C	502	VNT	CBB-CAY	-4.64	1.40	1.50
3	C	502	VNT	CBA-CLC	-3.86	1.64	1.73
3	A	502	VNT	CBA-CLC	-3.41	1.65	1.73
3	D	502	VNT	CAZ-CLB	-3.33	1.67	1.74
3	B	502	VNT	CBA-CLC	-3.14	1.66	1.73
3	D	502	VNT	CBA-CLC	-3.11	1.66	1.73
2	B	501	HEM	C4D-C3D	2.75	1.48	1.42
2	C	501	HEM	C4D-C3D	2.52	1.48	1.42
2	D	501	HEM	C4D-C3D	2.48	1.48	1.42
2	A	501	HEM	C4D-C3D	2.47	1.48	1.42
2	D	501	HEM	C1A-NA	2.18	1.40	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	VNT	NAS-CAP-NBI	-5.41	105.69	112.24
3	A	502	VNT	CAR-CBH-NAW	-4.87	101.96	110.45
3	B	502	VNT	NAS-CAP-NBI	-4.63	106.64	112.24
3	A	502	VNT	NAS-CAP-NBI	-4.50	106.80	112.24
3	D	502	VNT	CAP-NAS-CAO	4.15	107.01	102.34
3	C	502	VNT	NAS-CAP-NBI	-3.71	107.76	112.24
3	B	502	VNT	CAR-CBH-NAW	-3.70	103.99	110.45
3	B	502	VNT	CAP-NAS-CAO	3.61	106.41	102.34
3	D	502	VNT	CAR-CBH-NAW	-3.41	104.50	110.45
3	C	502	VNT	CAP-NAS-CAO	3.05	105.78	102.34
2	C	501	HEM	CBA-CAA-C2A	-2.68	107.54	112.49
3	B	502	VNT	CAN-CBE-CBA	2.65	119.45	116.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C1D-C2D-C3D	-2.55	105.22	107.00
2	D	501	HEM	C1D-C2D-C3D	-2.50	105.25	107.00
3	B	502	VNT	CBH-NAW-CAY	-2.36	119.30	122.34
3	A	502	VNT	CBA-CAQ-CAZ	2.33	121.32	118.71
3	D	502	VNT	CAN-CBE-CBA	2.33	119.13	116.81
2	D	501	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
3	C	502	VNT	CAR-CBH-NAW	-2.25	106.52	110.45
2	B	501	HEM	CAD-CBD-CGD	-2.18	109.01	112.67
2	A	501	HEM	C1D-C2D-C3D	-2.16	105.49	107.00
2	B	501	HEM	CMC-C2C-C3C	2.08	128.56	124.68
2	D	501	HEM	CMC-C2C-C3C	2.05	128.51	124.68
3	D	502	VNT	CAQ-CBA-CBE	-2.04	119.97	122.41
2	B	501	HEM	CBA-CAA-C2A	-2.04	108.73	112.49
3	D	502	VNT	CAQ-CAZ-CLB	2.01	121.66	119.15
3	A	502	VNT	CBE-CBH-NAW	2.01	115.50	111.47
2	A	501	HEM	CMC-C2C-C3C	2.00	128.43	124.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	VNT	CAM-CBD-CBG-NAV
3	D	502	VNT	CAL-CBD-CBG-NAV
3	D	502	VNT	CBA-CBE-CBH-CAR
3	C	502	VNT	CBA-CBE-CBH-CAR
3	D	502	VNT	CAN-CBE-CBH-CAR
3	B	502	VNT	CAN-CBE-CBH-CAR
3	C	502	VNT	CAN-CBE-CBH-CAR
3	B	502	VNT	CAM-CBD-CBG-NAV
3	B	502	VNT	CBE-CBH-NAW-CAY
3	A	502	VNT	CBE-CBH-NAW-CAY

There are no ring outliers.

8 monomers are involved in 34 short contacts:

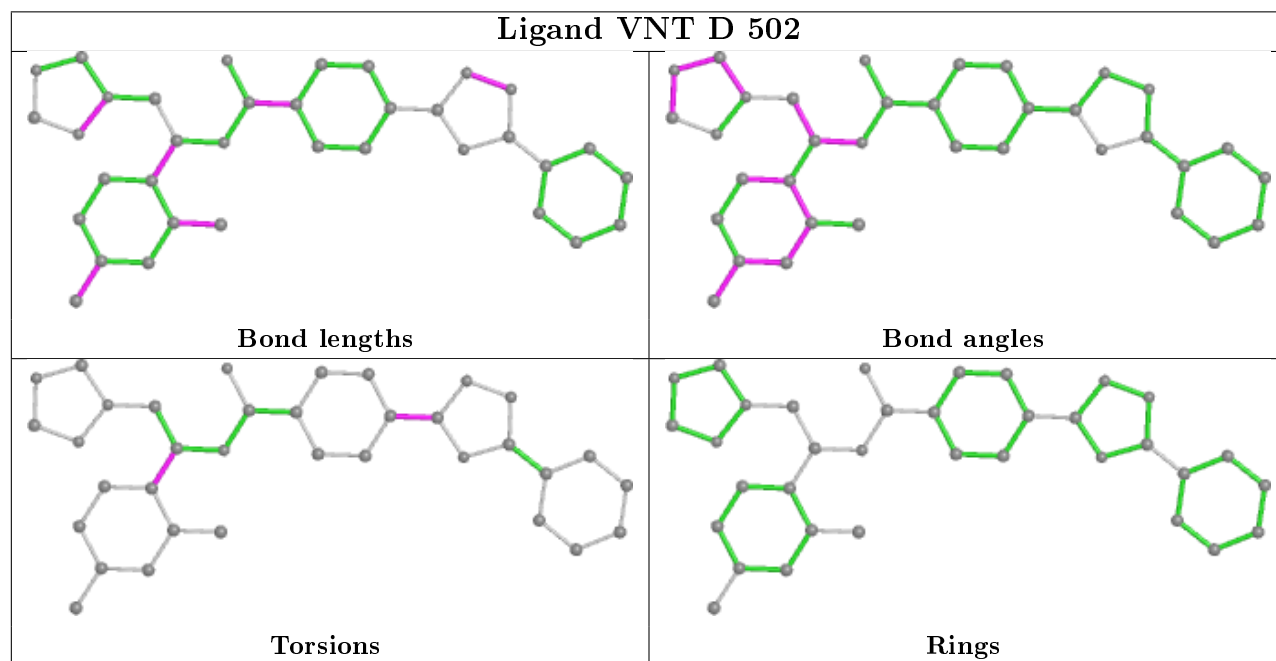
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	VNT	4	0
2	C	501	HEM	6	0
2	A	501	HEM	6	0
3	B	502	VNT	2	0
2	D	501	HEM	7	0

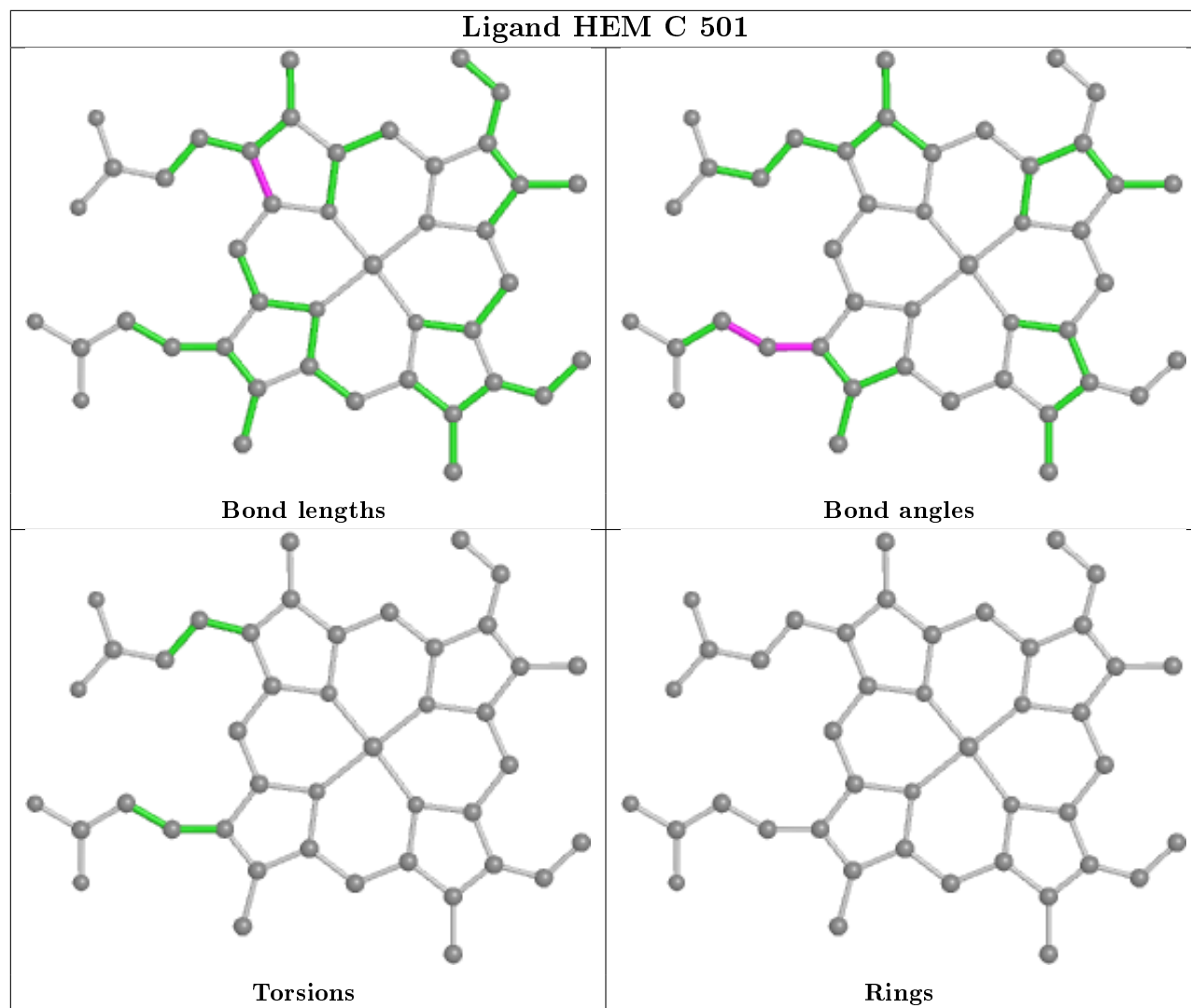
Continued on next page...

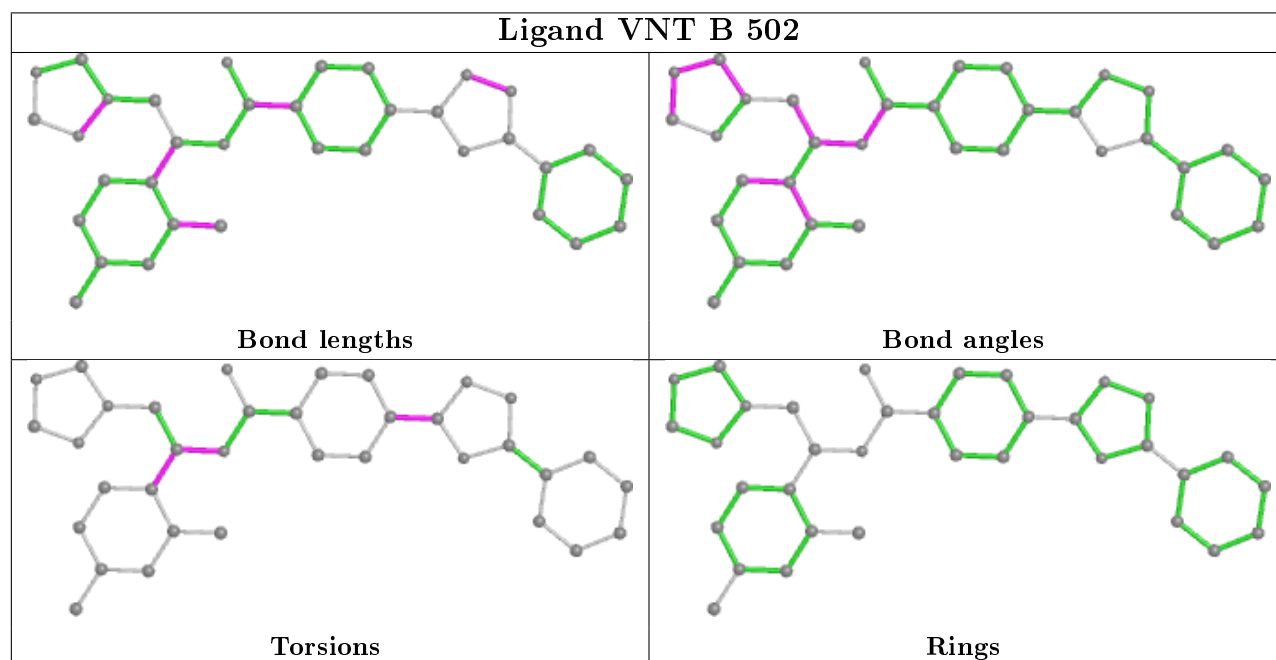
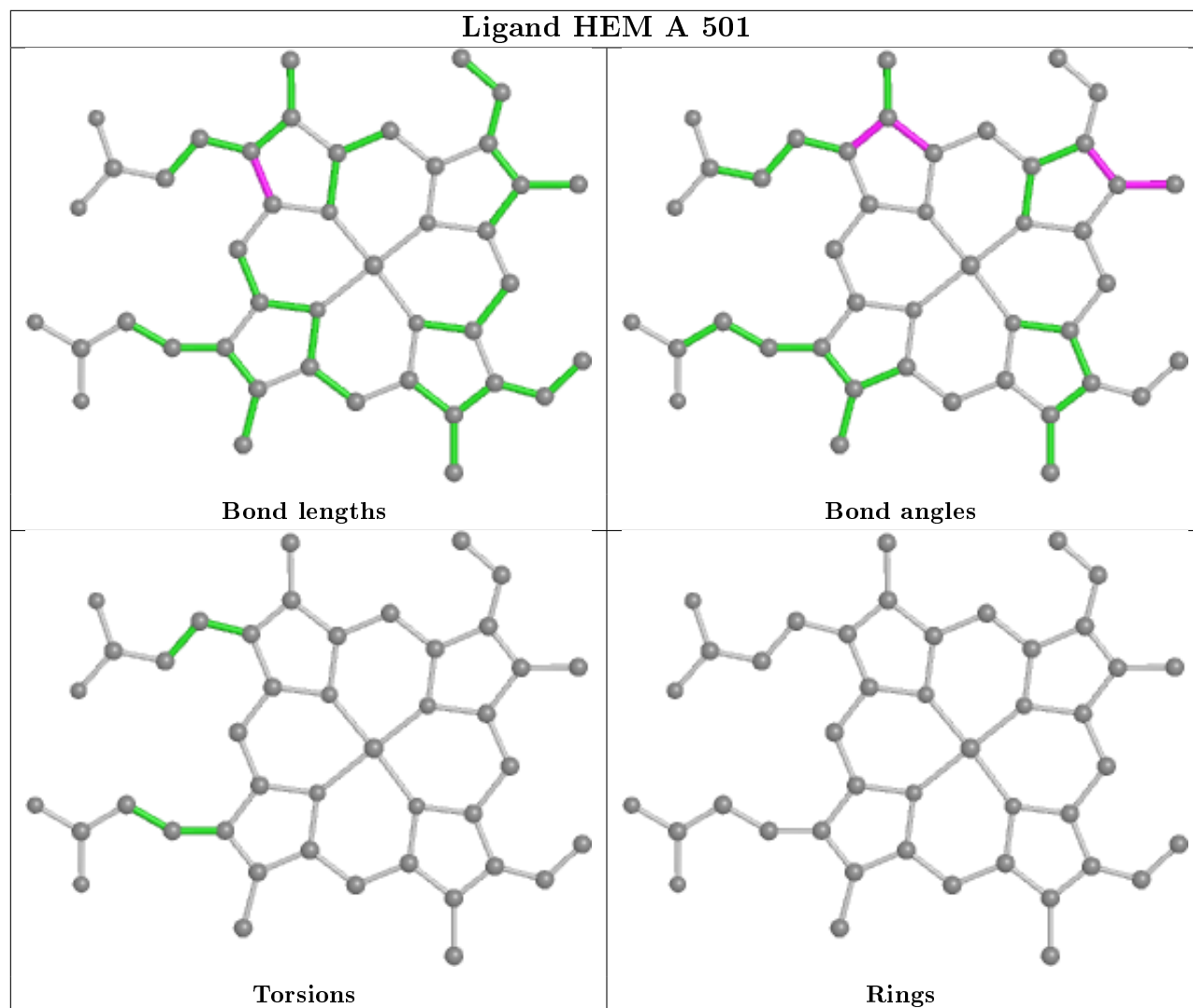
Continued from previous page...

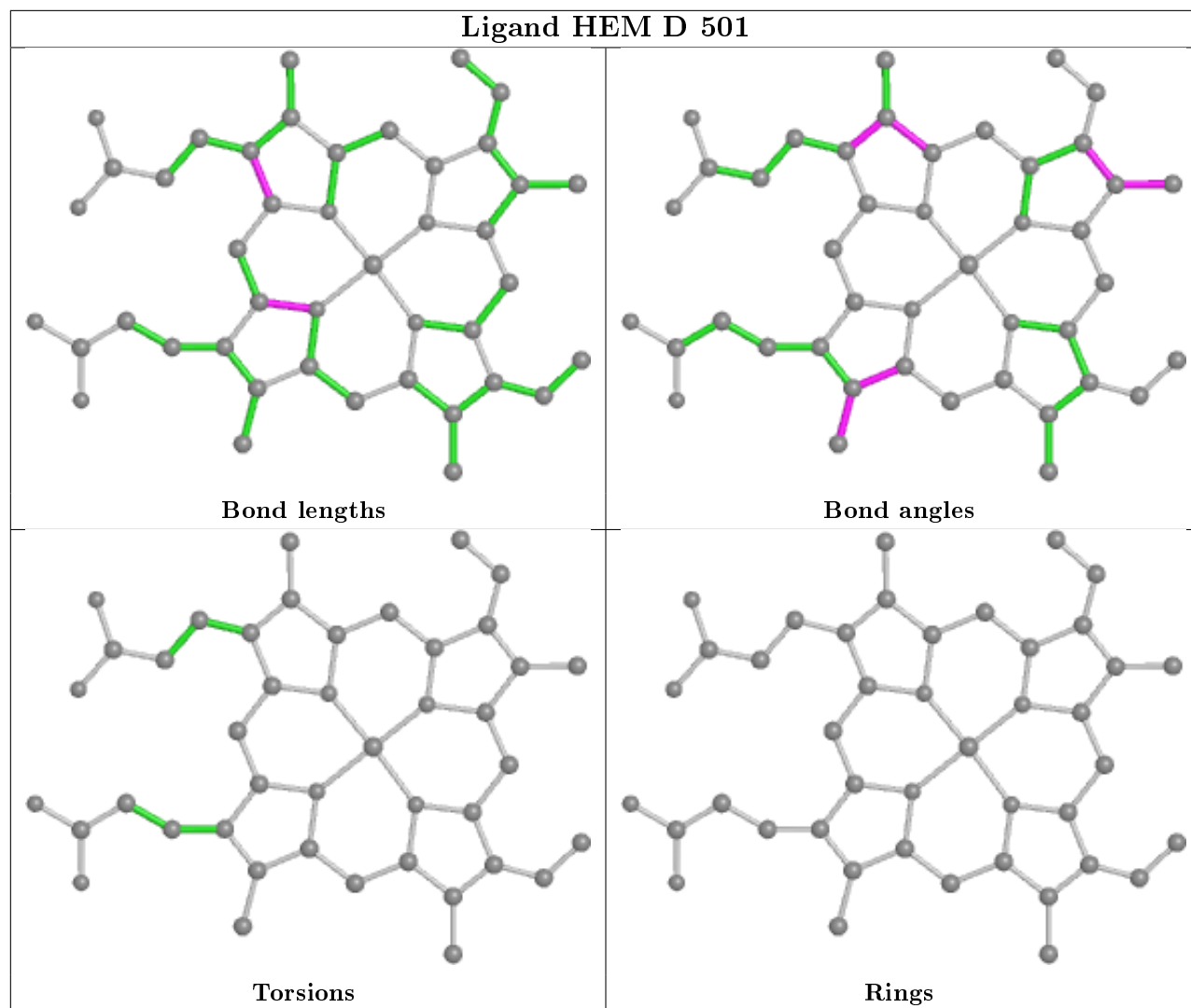
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	6	0
3	A	502	VNT	2	0
3	C	502	VNT	2	0

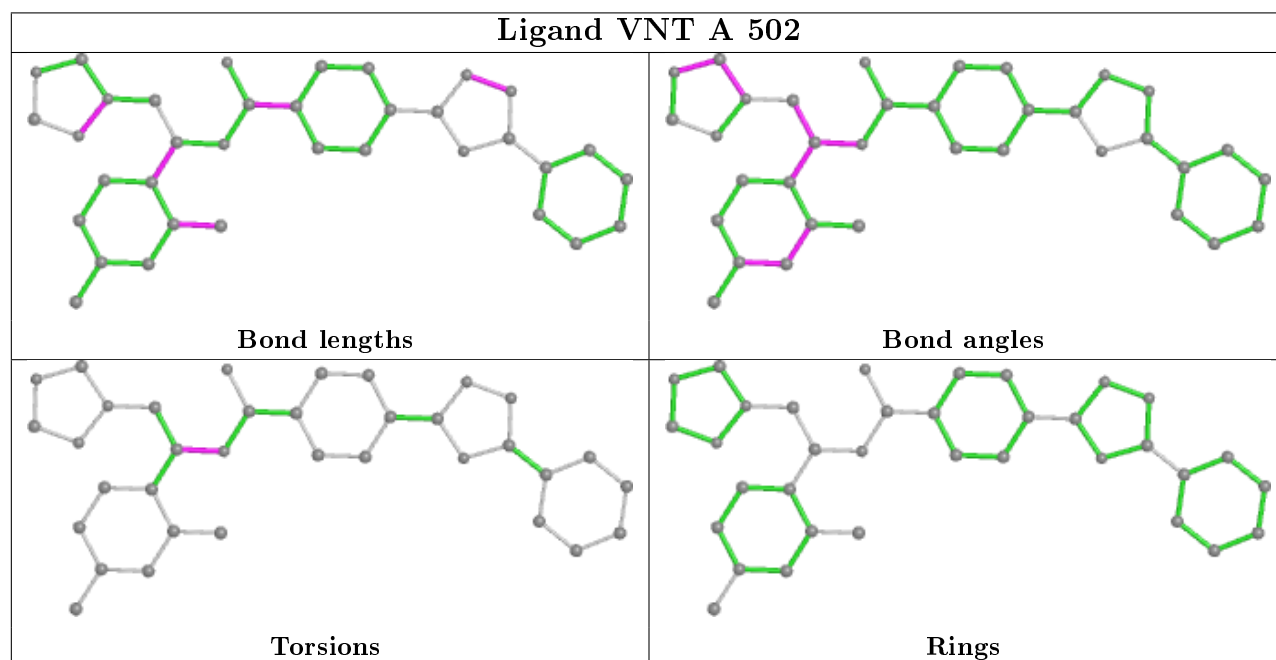
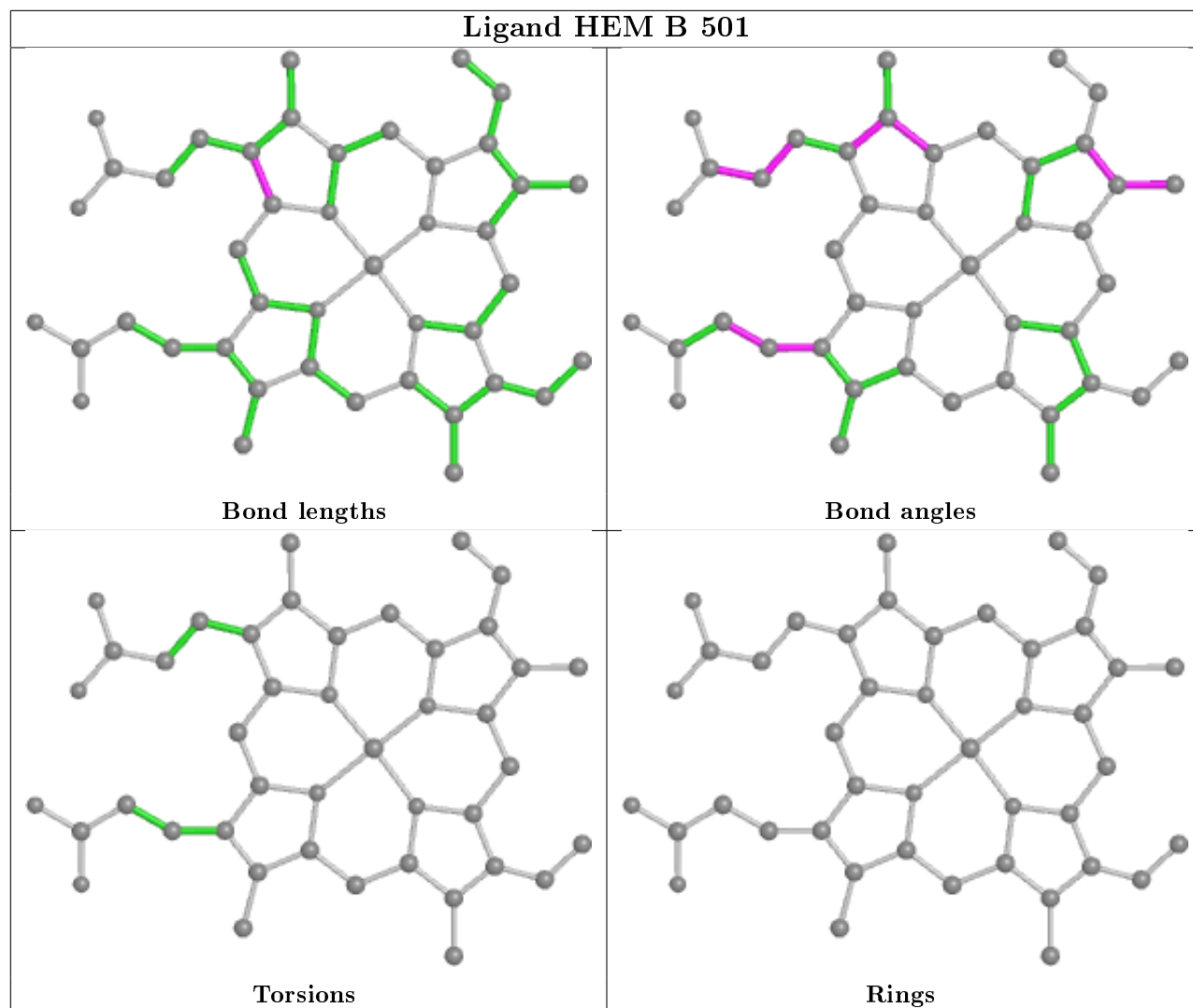
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

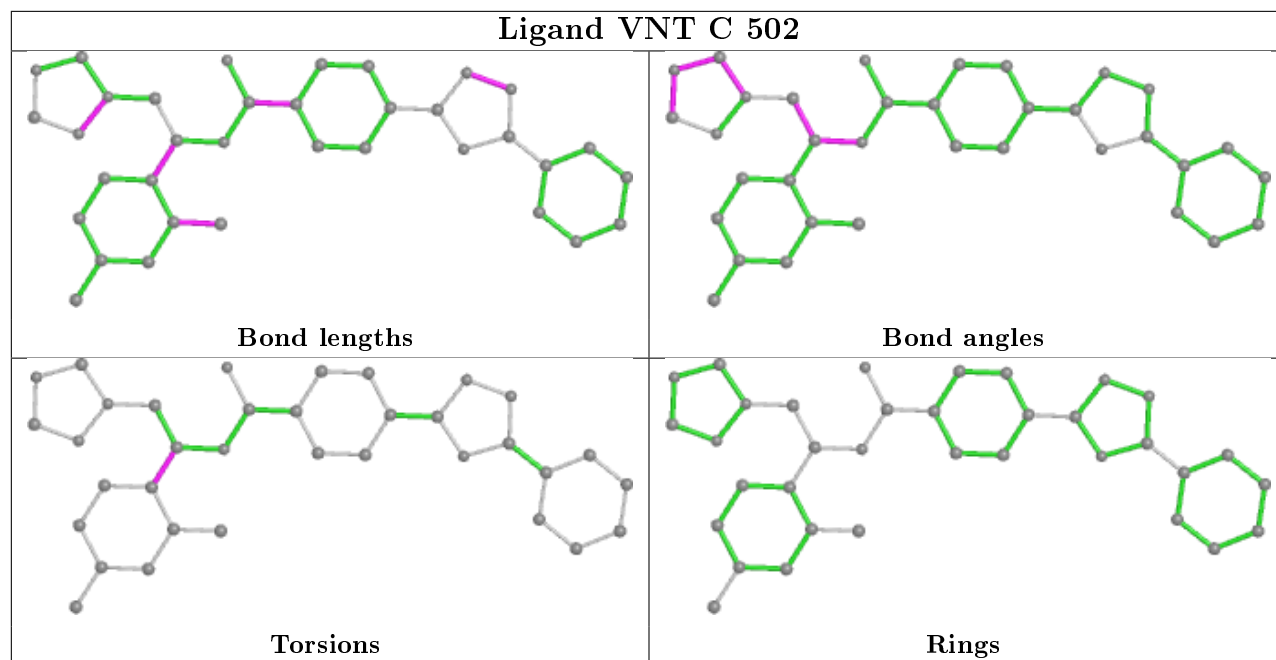












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/448 (100%)	0.10	20 (4%) 33 30	18, 31, 54, 119	0
1	B	448/448 (100%)	-0.12	9 (2%) 65 64	18, 30, 48, 107	0
1	C	448/448 (100%)	0.12	27 (6%) 21 19	23, 38, 62, 104	0
1	D	448/448 (100%)	0.07	15 (3%) 46 43	21, 36, 57, 76	0
All	All	1792/1792 (100%)	0.04	71 (3%) 38 35	18, 34, 57, 119	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	12.6
1	A	255	ASP	12.2
1	A	252	VAL	10.9
1	A	254	LYS	8.9
1	A	29	GLY	8.4
1	C	256	SER	7.9
1	C	29	GLY	7.0
1	B	255	ASP	6.7
1	A	41	ILE	6.7
1	A	43	GLY	5.4
1	D	29	GLY	5.4
1	C	257	SER	5.1
1	B	256	SER	5.1
1	A	256	SER	4.8
1	C	254	LYS	4.1
1	D	195	ARG	3.8
1	C	121	PRO	3.5
1	C	195	ARG	3.4
1	B	254	LYS	3.4
1	C	64	LYS	3.3
1	C	255	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	30	LYS	3.2
1	C	191	ARG	3.1
1	D	190	LYS	3.1
1	B	41	ILE	3.1
1	C	271	ARG	3.0
1	D	120	TYR	3.0
1	C	30	LYS	2.9
1	C	61	ARG	2.9
1	D	257	SER	2.9
1	C	38	THR	2.8
1	B	359	LEU	2.7
1	B	195	ARG	2.7
1	D	159	ASP	2.7
1	D	329	GLN	2.6
1	C	258	THR	2.6
1	D	50	LYS	2.6
1	D	199	GLN	2.6
1	A	42	LEU	2.5
1	A	40	PRO	2.5
1	D	155	ALA	2.5
1	C	196	ARG	2.5
1	C	63	LEU	2.4
1	C	120	TYR	2.4
1	C	40	PRO	2.4
1	A	61	ARG	2.3
1	C	269	VAL	2.3
1	D	292	GLY	2.3
1	C	190	LYS	2.3
1	A	50	LYS	2.3
1	C	93	ARG	2.2
1	C	324	GLU	2.2
1	B	40	PRO	2.2
1	A	371	SER	2.2
1	B	356	LEU	2.2
1	C	252	VAL	2.2
1	A	161	ASP	2.2
1	A	314	LYS	2.2
1	D	328	ALA	2.2
1	A	62	GLN	2.2
1	C	39	VAL	2.2
1	A	93	ARG	2.1
1	A	359	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	38	THR	2.1
1	C	370	GLY	2.1
1	A	405	ASP	2.1
1	D	288	ALA	2.1
1	C	253	ASN	2.1
1	D	140	GLN	2.1
1	C	272	ASP	2.0
1	D	271	ARG	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](#)

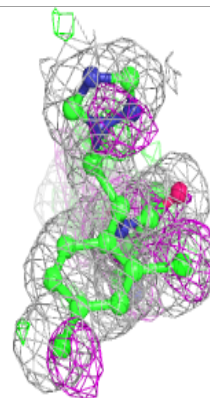
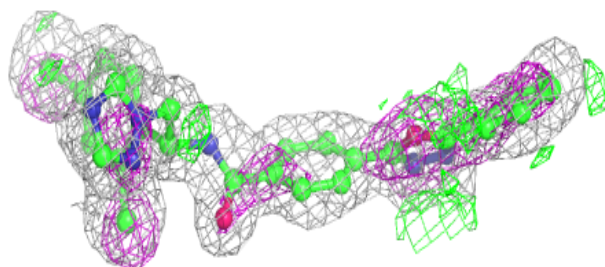
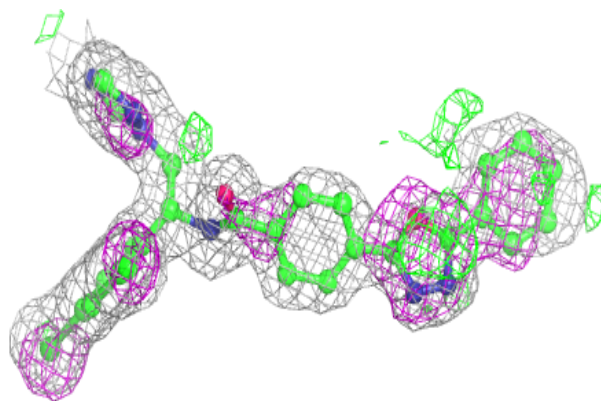
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VNT	D	502	35/35	0.86	0.13	21,23,26,27	0
3	VNT	B	502	35/35	0.90	0.11	20,22,25,26	0
3	VNT	C	502	35/35	0.91	0.11	21,22,24,27	0
3	VNT	A	502	35/35	0.92	0.11	19,22,25,25	0
2	HEM	D	501	43/43	0.98	0.15	18,23,32,42	0
2	HEM	B	501	43/43	0.98	0.15	16,20,26,37	0
2	HEM	A	501	43/43	0.98	0.12	17,20,28,33	0
2	HEM	C	501	43/43	0.98	0.14	23,28,41,50	0

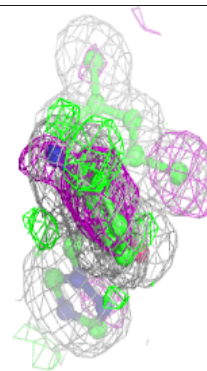
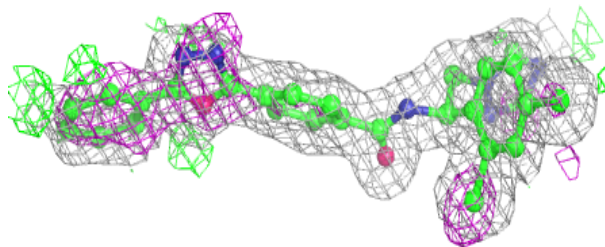
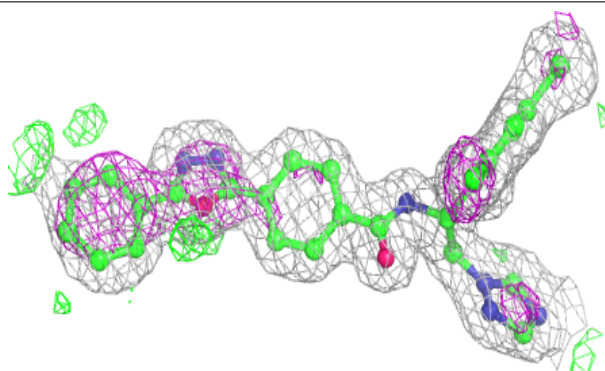
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VNT D 502:

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

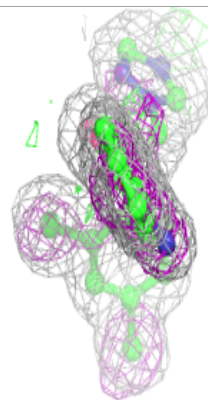
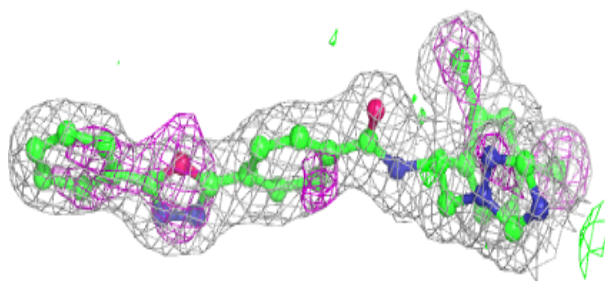
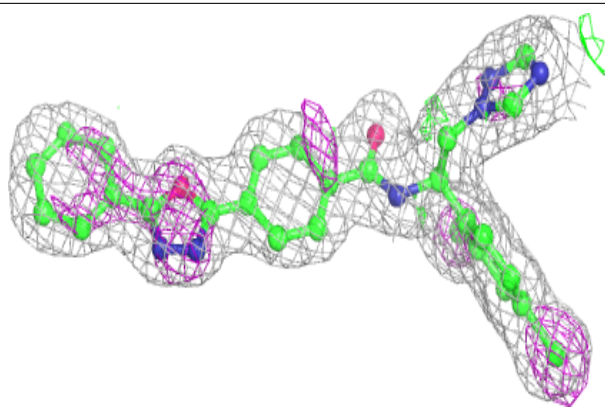
**Electron density around VNT B 502:**

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

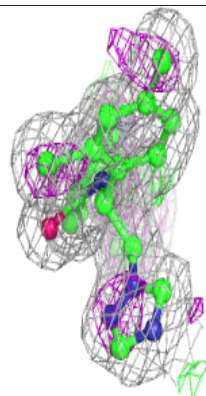
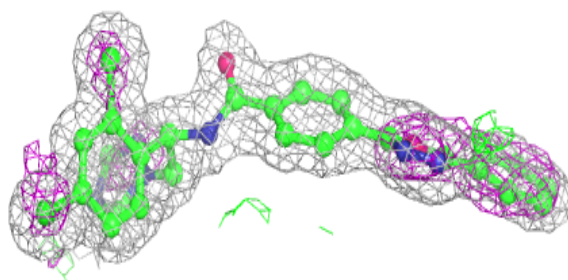
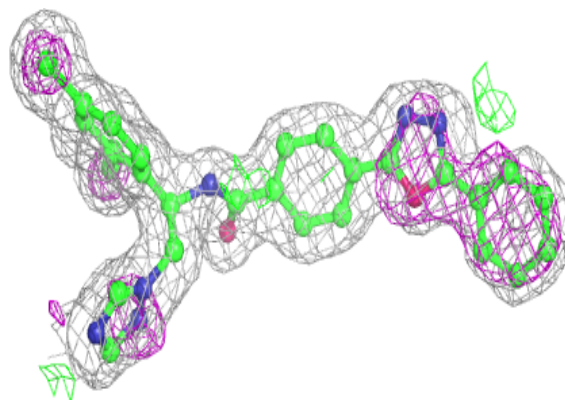


Electron density around VNT C 502:

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

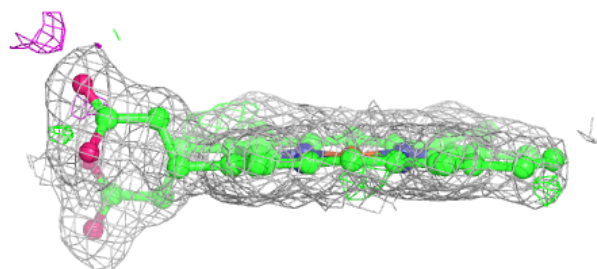
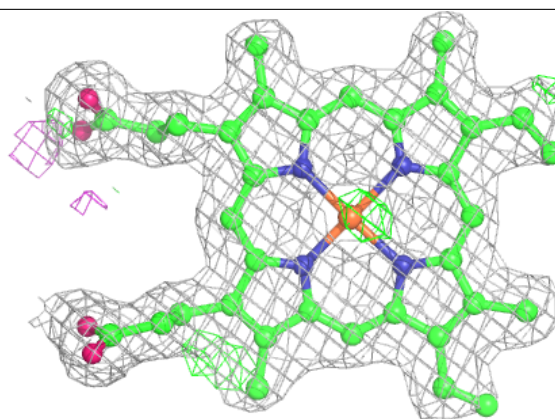
**Electron density around VNT A 502:**

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



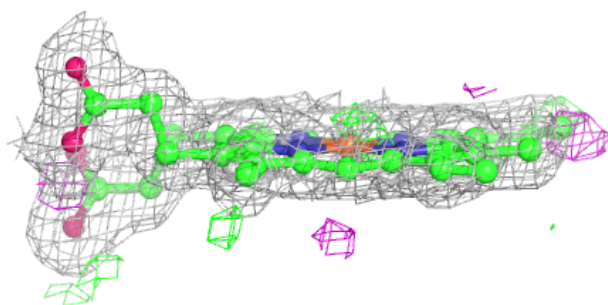
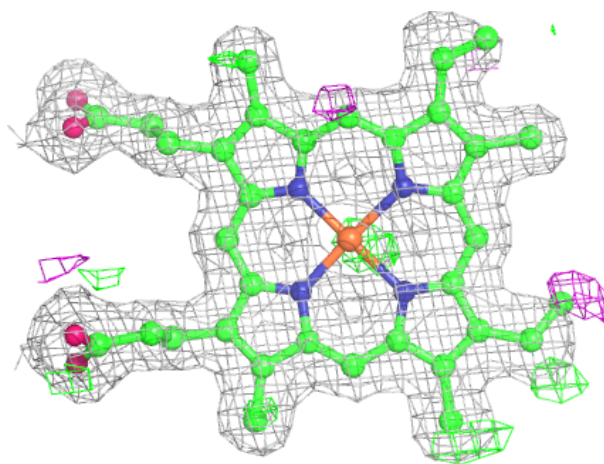
Electron density around HEM D 501:

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



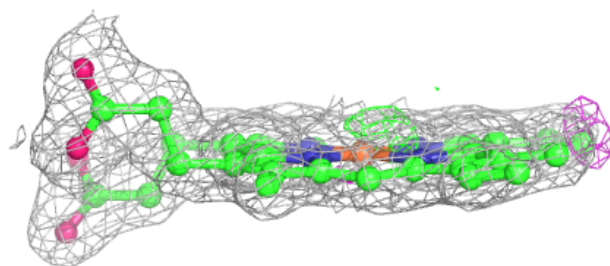
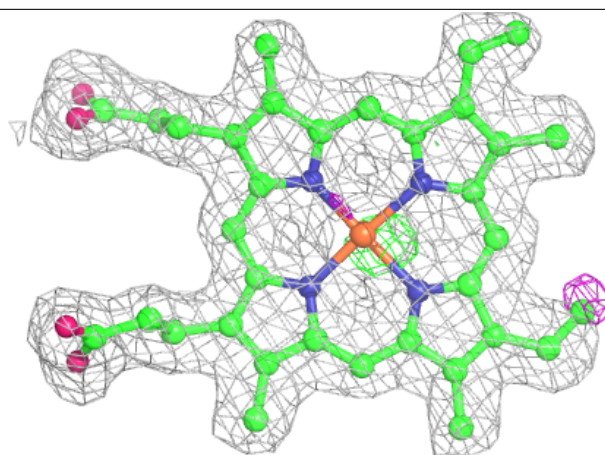
Electron density around HEM B 501:

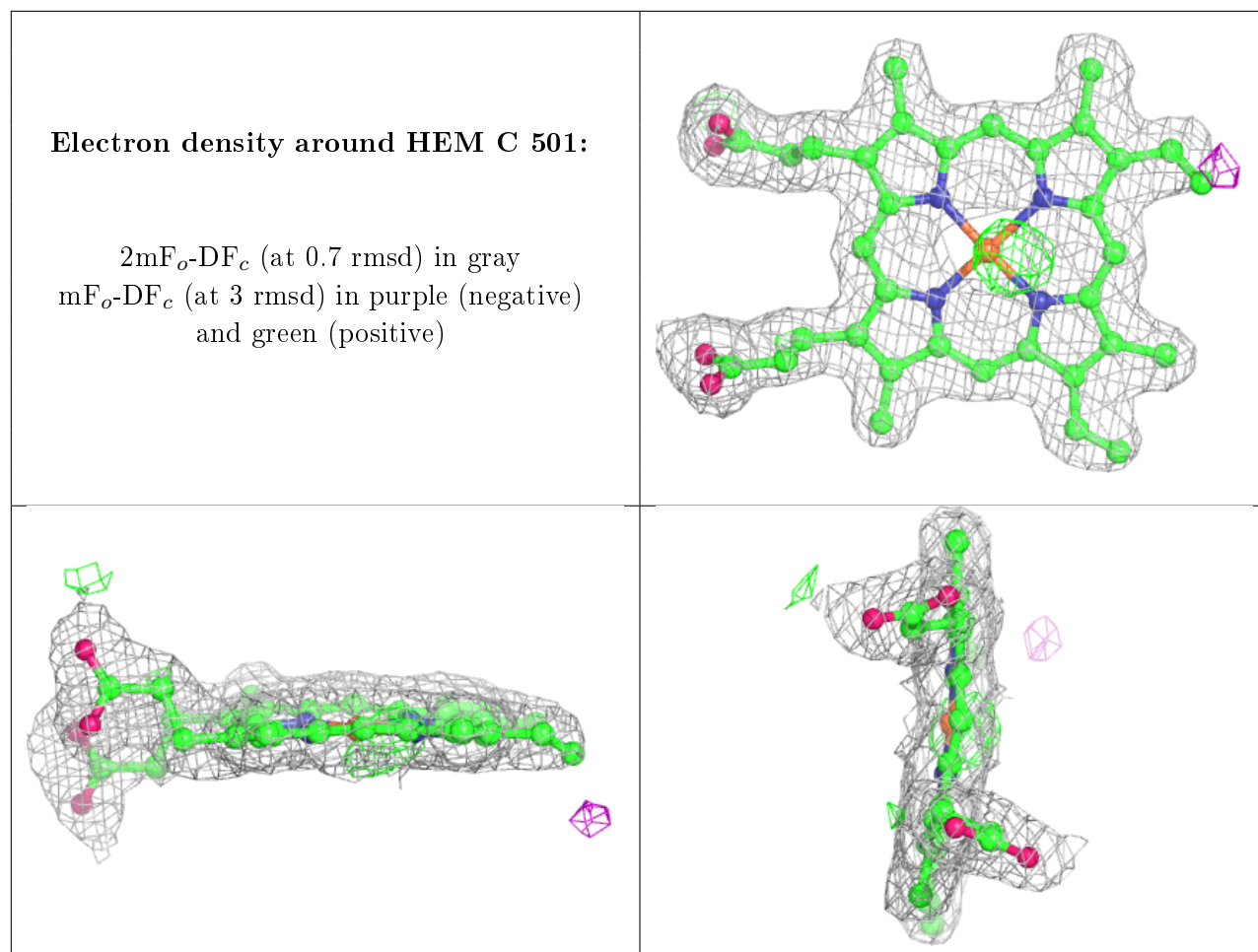
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 501:

$2mF_o-DF_c$ (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.