



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:12 PM EDT

PDB ID : 4G3J / pdb_00004g3j
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 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

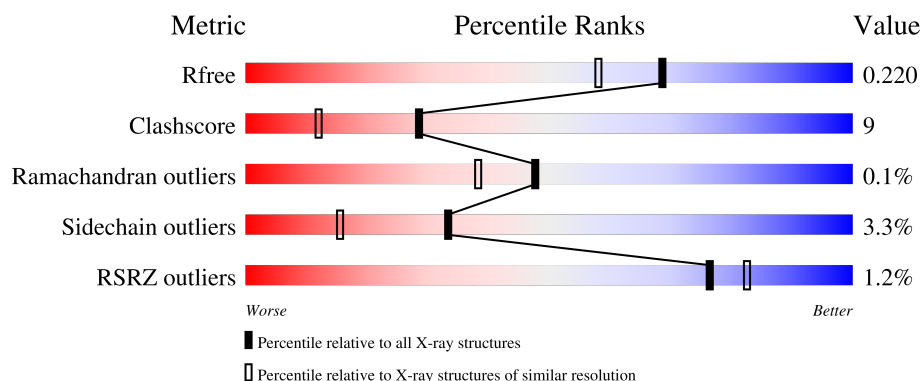
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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.

Mol	Chain	Length	Quality of chain
1	A	448	2% 84% 15% .
1	B	448	% 88% 11% .
1	C	448	% 77% 21% .
1	D	448	84% 15% .

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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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		

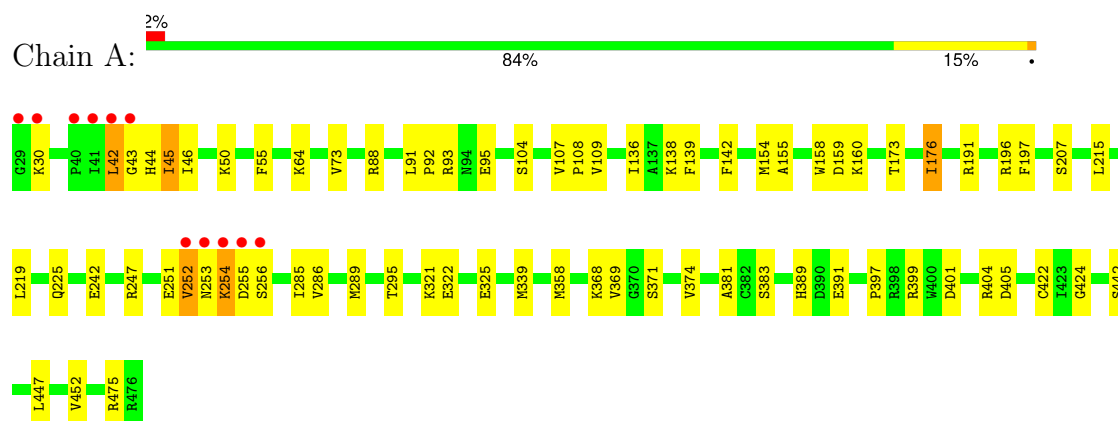
- Molecule 4 is water.

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		

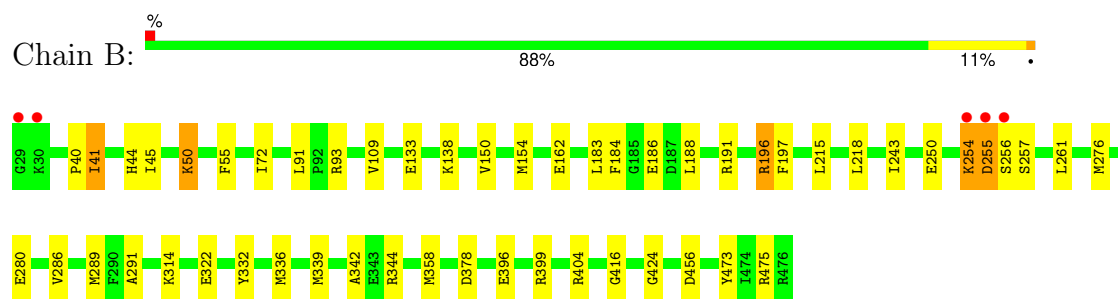
3 Residue-property plots

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.

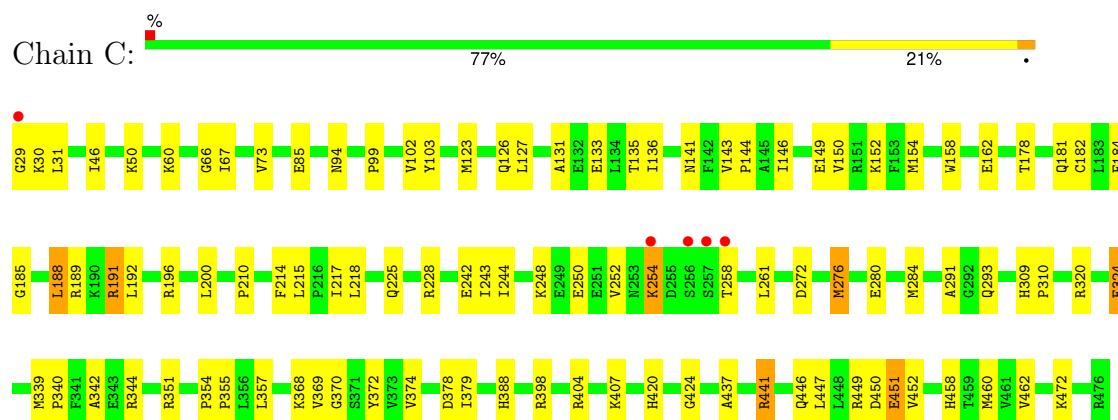
• Molecule 1: sterol 14-alpha-demethylase



• Molecule 1: sterol 14-alpha-demethylase



• Molecule 1: sterol 14-alpha-demethylase

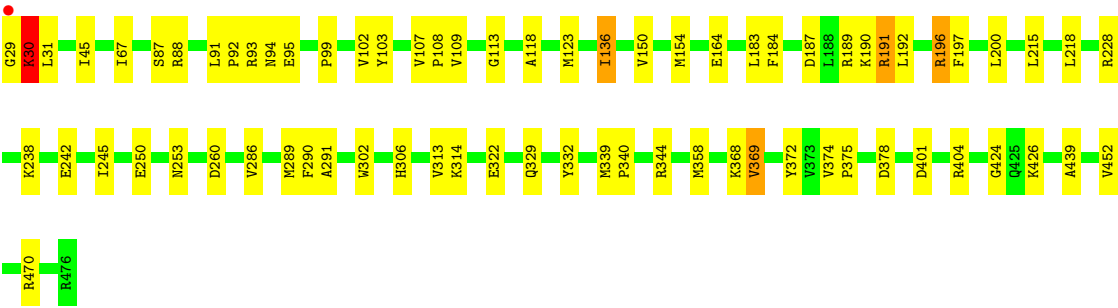


● Molecule 1: sterol 14-alpha-demethylase

Chain D:

84%

15%



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) 97.6 (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	8549 reflections (5.01%)	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)	0.38 , 52.5	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: VNT, 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	0.48	0/3639	0.69	0/4922
1	B	0.45	0/3639	0.66	0/4922
1	C	0.46	0/3639	0.70	0/4922
1	D	0.46	0/3639	0.69	0/4922
All	All	0.46	0/14556	0.68	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	61	0
1	B	3557	0	3594	49	0
1	C	3557	0	3594	77	0
1	D	3557	0	3594	59	0
2	A	43	0	30	6	0
2	B	43	0	30	7	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	3	0
4	B	226	0	0	4	0
4	C	141	0	0	3	0
4	D	134	0	0	3	0
All	All	15243	0	14568	257	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 9.

All (257) 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:HBB2	2:A:501:HEM:HHC	1.53	0.89
1:A:109:VAL:CG1	1:A:286:VAL:HG11	2.04	0.88
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	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:HBC2	2:B:501:HEM:HMC2	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:C:188:LEU:HD12	1:C:188:LEU:C	2.04	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: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:HD12	1:C:188:LEU:O	1.87	0.74
1:D:136:ILE:CD1	1:D:426:LYS:HD2	2.18	0.73
1:B:40:PRO:C	1:B:41:ILE:HG13	2.13	0.72
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
1:D:150:VAL:HG13	1:D:154:MET:HE3	1.73	0.69
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.23	0.69
1:D:150:VAL:CG1	1:D:154:MET:HE3	2.23	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:HG2	1:C:324:GLU:O	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

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:NH2	2.13	0.63
2:D:501:HEM:HBB2	2:D:501:HEM:CHC	2.20	0.63
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.28	0.63
2:A:501:HEM:HBB2	2:A:501:HEM:CHC	2.25	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:154:MET:HE1	1:D:439:ALA:HA	1.81	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:126:GLN:HG2	1:C:276:MET:HE3	1.83	0.60
1:C:191:ARG:HB2	1:C:243:ILE:HD11	1.81	0.60
1:C:188:LEU:C	1:C:188:LEU:CD1	2.74	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:B:183:LEU:HD12	1:B:289:MET:HE1	1.84	0.58
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:C:451:GLU:OE2	1:C:451:GLU:HA	2.04	0.56
1:D:109:VAL:HG13	1:D:286:VAL:HG11	1.87	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:HG3	1:A:399:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:214:PHE:CE1	1:C:379:ILE:HD13	2.44	0.53
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:D:154:MET:HE1	1:D:439:ALA:CA	2.38	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:46:ILE:HG22	1:A:50:LYS:HE2	1.91	0.52
1:A:252:VAL:HG11	1:B:93:ARG:HH12	1.75	0.52
1:D:322:GLU:CD	1:D:339:MET:HA	2.34	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:B:276:MET:HE2	1:B:280:GLU:HB3	1.91	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:C:181:GLN:HA	1:C:189:ARG:HH11	1.74	0.51
1:B:314:LYS:NZ	4:B:674:HOH:O	2.42	0.51
1:D:191:ARG:NH1	1:D:242:GLU:OE1	2.42	0.51
1:B:322:GLU:CD	1:B:339:MET:HA	2.35	0.51
1:C:339:MET:HE2	1:C:342:ALA:CB	2.41	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:B:150:VAL:CG1	1:B:154:MET:HE3	2.41	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:254:LYS:C	1:A:256:SER:H	2.20	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:29:GLY:C	1:C:31:LEU:H	2.20	0.49
1:B:254:LYS:C	1:B:256:SER:N	2.69	0.49
1:A:154:MET:HE2	1:A:158:TRP:CZ3	2.48	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LYS:O	1:B:255:ASP:C	2.56	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:C:154:MET:HE2	1:C:158:TRP:CZ3	2.49	0.48
1:D:196:ARG:NH1	1:D:196:ARG:HG2	2.28	0.48
1:B:344:ARG:NH2	1:B:404:ARG:O	2.47	0.47
1:A:251:GLU:HG2	1:A:254:LYS:HZ2	1.79	0.47
1:D:136:ILE:HG23	1:D:332:TYR:OH	2.14	0.47
1:B:255:ASP:O	1:B:256:SER:C	2.56	0.47
1:D:183:LEU:HD12	1:D:289:MET:HE1	1.97	0.47
1:B:218:LEU:HD21	1:D:218:LEU:HD11	1.95	0.47
1:C:451:GLU:OE2	1:C:451:GLU:CA	2.61	0.47
1:A:252:VAL:HG22	1:B:93:ARG:CZ	2.44	0.47
1:D:94:ASN:ND2	1:D:123:MET:HE1	2.30	0.47
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.62	0.47
1:B:456:ASP:OD1	1:B:456:ASP:C	2.58	0.47
1:C:94:ASN:HD21	1:C:123:MET:HE1	1.80	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:A:251:GLU:HG2	1:A:254:LYS:NZ	2.31	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:HE2	1:C:152:LYS:HB3	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: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:127:LEU:HD23	1:C:284:MET:HE1	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:407:LYS:HD3	1:C:407:LYS:HA	1.81	0.44
1:B:254:LYS:C	1:B:256:SER:H	2.24	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:D:136:ILE:HD11	1:D:426:LYS:HD2	1.96	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:D:67:ILE:CD1	1:D:369:VAL:HG22	2.32	0.43
1:D:302:TRP:O	1:D:306:HIS:CD2	2.71	0.43
1:C:146:ILE:O	1:C:150:VAL:HG23	2.19	0.43
1:C:272:ASP:C	1:C:272:ASP:OD1	2.60	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:67:ILE:CD1	1:C:369:VAL:HG22	2.49	0.43
1:C:210:PRO:HG3	1:C:460:MET:SD	2.59	0.43
1:D:358:MET:HE3	1:D:358:MET:HB3	1.87	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:A:322:GLU:CD	1:A:339:MET:HA	2.43	0.43
1:C:85:GLU:OE1	1:C:85:GLU:HA	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:HD12	1:A:176:ILE:HA	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:HD2	1:D:88:ARG:HA	1.80	0.42
1:A:321:LYS:NZ	4:A:793:HOH:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:C	1:A:256:SER:N	2.76	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:C:29:GLY:C	1:C:31:LEU:N	2.78	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:B:138:LYS:NZ	4:B:766:HOH:O	2.52	0.42
1:C:146:ILE:CG1	1:C:182:CYS:SG	3.08	0.42
1:B:332:TYR:CD1	1:B:332:TYR:C	2.98	0.41
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:29:GLY:O	1:D:30:LYS:CB	2.68	0.41
1:D:228:ARG:NH1	4:D:625:HOH:O	2.52	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
1:B:339:MET:HE2	1:B:342:ALA:CB	2.51	0.41
1:B:416:GLY:N	2:B:501:HEM:HMA3	2.35	0.41
1:C:276:MET:HE2	1:C:280:GLU:HB3	2.02	0.41
1:A:253:ASN:ND2	1:B:91:LEU:O	2.53	0.41
1:B:358:MET:HE3	1:B:358:MET:HB3	1.90	0.41
1:C:339:MET:HE2	1:C:342:ALA:HB3	2.03	0.41
1:D:87:SER:HB2	1:D:91:LEU:CD1	2.48	0.41
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.85	0.41
1:C:398:ARG:HA	1:C:398:ARG:HD2	1.87	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:H3	3:B:502:VNT:H5	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:D:30:LYS:NZ	4:D:724:HOH:O	2.54	0.40
1:A:368:LYS:HD2	1:A:368:LYS:HA	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%)	43	34
1	D	446/448 (100%)	438 (98%)	7 (2%)	1 (0%)	43	34
All	All	1784/1792 (100%)	1746 (98%)	36 (2%)	2 (0%)	48	38

All (2) Ramachandran outliers are listed below:

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

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	390/390 (100%)	376 (96%)	14 (4%)	31	13
1	B	390/390 (100%)	380 (97%)	10 (3%)	40	23
1	C	390/390 (100%)	375 (96%)	15 (4%)	29	12
1	D	390/390 (100%)	378 (97%)	12 (3%)	35	18
All	All	1560/1560 (100%)	1509 (97%)	51 (3%)	33	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	45	ILE
1	A	64	LYS
1	A	136	ILE
1	A	160	LYS
1	A	176	ILE
1	A	252	VAL
1	A	254	LYS
1	A	325	GLU
1	A	371	SER
1	A	391	GLU
1	A	405	ASP
1	A	447	LEU
1	A	452	VAL
1	B	41	ILE
1	B	50	LYS
1	B	186	GLU
1	B	191	ARG
1	B	196	ARG
1	B	215	LEU
1	B	254	LYS
1	B	255	ASP
1	B	257	SER
1	B	396	GLU
1	C	73	VAL
1	C	136	ILE
1	C	162	GLU
1	C	188	LEU
1	C	191	ARG
1	C	196	ARG
1	C	200	LEU
1	C	217	ILE
1	C	254	LYS
1	C	276	MET
1	C	324	GLU
1	C	441	ARG
1	C	447	LEU
1	C	451	GLU
1	C	452	VAL
1	D	30	LYS
1	D	45	ILE
1	D	136	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	191	ARG
1	D	196	ARG
1	D	200	LEU
1	D	215	LEU
1	D	245	ILE
1	D	313	VAL
1	D	329	GLN
1	D	369	VAL
1	D	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	B	47	GLN
1	B	148	HIS
1	B	181	GLN
1	B	315	HIS
1	C	47	GLN
1	C	148	HIS
1	C	181	GLN
1	C	333	ASN
1	D	47	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](#)

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	39,39,39	3.64	12 (30%)	53,54,54	1.48	11 (20%)
3	VNT	A	502	2	39,39,39	3.87	11 (28%)	53,54,54	1.57	11 (20%)
2	HEM	A	501	3,1	50,50,50	1.36	5 (10%)	67,82,82	1.34	9 (13%)
2	HEM	C	501	3,1	50,50,50	1.47	8 (16%)	67,82,82	1.36	7 (10%)
2	HEM	D	501	3,1	50,50,50	1.38	5 (10%)	67,82,82	1.41	12 (17%)
2	HEM	B	501	3,1	50,50,50	1.43	8 (16%)	67,82,82	1.33	7 (10%)
3	VNT	C	502	2	39,39,39	3.23	11 (28%)	53,54,54	1.37	9 (16%)
3	VNT	B	502	2	39,39,39	4.59	11 (28%)	53,54,54	1.57	10 (18%)

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	-	10/24/24/24	0/5/5/5
3	VNT	A	502	2	-	3/24/24/24	0/5/5/5
2	HEM	A	501	3,1	-	1/14/54/54	-
2	HEM	C	501	3,1	-	2/14/54/54	-
2	HEM	D	501	3,1	-	1/14/54/54	-
2	HEM	B	501	3,1	-	2/14/54/54	-
3	VNT	C	502	2	-	2/24/24/24	0/5/5/5
3	VNT	B	502	2	-	6/24/24/24	0/5/5/5

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	VNT	OAX-CBF	-14.04	1.14	1.37
3	B	502	VNT	NAU-NAV	-12.70	1.12	1.39
3	A	502	VNT	NBI-NAT	-12.48	1.12	1.36
3	B	502	VNT	OAX-CBG	-12.32	1.17	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	VNT	NAU-NAV	-10.51	1.17	1.39
3	A	502	VNT	NAU-NAV	-10.43	1.17	1.39
3	C	502	VNT	NAU-NAV	-9.44	1.19	1.39
3	D	502	VNT	NBI-NAT	-8.40	1.20	1.36
3	A	502	VNT	OAX-CBF	-8.35	1.23	1.37
3	D	502	VNT	OAX-CBF	-8.33	1.23	1.37
3	B	502	VNT	NBI-NAT	-8.17	1.20	1.36
3	D	502	VNT	CBE-CBH	-8.13	1.40	1.52
3	B	502	VNT	CBD-CBG	-8.00	1.31	1.47
3	B	502	VNT	CBE-CBH	-7.90	1.40	1.52
3	A	502	VNT	OAX-CBG	-7.76	1.24	1.37
3	B	502	VNT	CBC-CBF	-7.52	1.32	1.47
3	C	502	VNT	NBI-NAT	-7.41	1.22	1.36
3	D	502	VNT	CBD-CBG	-7.21	1.32	1.47
3	C	502	VNT	CBE-CBH	-7.05	1.41	1.52
3	A	502	VNT	CBE-CBH	-6.91	1.41	1.52
3	D	502	VNT	CBC-CBF	-6.79	1.33	1.47
3	A	502	VNT	CBD-CBG	-6.76	1.33	1.47
3	C	502	VNT	CBC-CBF	-6.71	1.33	1.47
3	A	502	VNT	CBC-CBF	-6.67	1.33	1.47
3	C	502	VNT	CBD-CBG	-6.45	1.34	1.47
3	C	502	VNT	OAX-CBG	-6.10	1.27	1.37
3	D	502	VNT	OAX-CBG	-6.09	1.27	1.37
2	C	501	HEM	FE-NB	5.67	2.12	1.94
3	C	502	VNT	OAX-CBF	-5.64	1.28	1.37
3	B	502	VNT	CBB-CAY	-5.19	1.38	1.50
2	D	501	HEM	FE-NB	5.06	2.10	1.94
3	D	502	VNT	CBB-CAY	-5.00	1.39	1.50
2	A	501	HEM	FE-NB	4.95	2.10	1.94
2	B	501	HEM	FE-NB	4.92	2.10	1.94
3	A	502	VNT	CBB-CAY	-4.62	1.40	1.50
3	C	502	VNT	CBB-CAY	-4.41	1.40	1.50
3	C	502	VNT	CBA-CLC	-3.86	1.64	1.73
2	D	501	HEM	FE-NC	3.51	2.06	1.95
2	B	501	HEM	FE-NC	3.47	2.06	1.95
3	A	502	VNT	CBA-CLC	-3.41	1.65	1.73
2	A	501	HEM	FE-NC	3.18	2.05	1.95
3	B	502	VNT	CBA-CLC	-3.14	1.66	1.73
3	D	502	VNT	CBA-CLC	-3.10	1.66	1.73
3	D	502	VNT	CAZ-CLB	-3.06	1.67	1.74
3	D	502	VNT	CBF-NAU	3.00	1.33	1.29
3	B	502	VNT	CBF-NAU	2.91	1.33	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	VNT	CBG-NAV	2.91	1.33	1.29
2	D	501	HEM	C1B-NB	-2.90	1.35	1.40
2	B	501	HEM	C1B-NB	-2.89	1.35	1.40
2	A	501	HEM	C1B-NB	-2.81	1.35	1.40
2	C	501	HEM	C1B-NB	-2.78	1.35	1.40
3	C	502	VNT	CBF-NAU	2.72	1.33	1.29
2	B	501	HEM	C3C-C2C	2.70	1.42	1.37
2	C	501	HEM	FE-NC	2.68	2.04	1.95
2	C	501	HEM	C3B-C4B	2.65	1.50	1.44
3	B	502	VNT	CBG-NAV	2.52	1.33	1.29
2	C	501	HEM	C4D-ND	-2.49	1.35	1.40
3	A	502	VNT	CBF-NAU	2.49	1.33	1.29
3	D	502	VNT	CBG-NAV	2.48	1.33	1.29
2	A	501	HEM	C4D-ND	-2.47	1.36	1.40
2	D	501	HEM	C3C-C2C	2.40	1.42	1.37
2	A	501	HEM	C3B-C4B	2.37	1.49	1.44
2	B	501	HEM	C3B-C4B	2.35	1.49	1.44
2	B	501	HEM	C4D-ND	-2.30	1.36	1.40
2	C	501	HEM	C3C-C2C	2.27	1.41	1.37
3	A	502	VNT	CBG-NAV	2.21	1.32	1.29
2	B	501	HEM	C4D-C3D	2.21	1.48	1.45
2	C	501	HEM	C1D-C2D	2.20	1.49	1.44
2	B	501	HEM	C1D-C2D	2.19	1.49	1.44
2	D	501	HEM	C4D-ND	-2.02	1.36	1.40
2	C	501	HEM	C1D-ND	-2.01	1.34	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	VNT	CAR-NBI-CAP	-4.67	119.03	129.48
3	B	502	VNT	CAR-NBI-NAT	3.90	129.76	121.26
3	A	502	VNT	CAO-NAT-NBI	3.66	111.05	102.60
2	D	501	HEM	CHC-C4B-NB	3.60	128.29	124.42
2	C	501	HEM	CHD-C4C-NC	3.47	128.23	124.45
3	A	502	VNT	CAR-CBH-NAW	-3.43	101.96	110.71
3	D	502	VNT	OAX-CBF-CBC	3.32	124.51	118.73
3	C	502	VNT	OAX-CBG-CBD	3.19	124.29	118.73
2	A	501	HEM	CHC-C4B-NB	3.19	127.86	124.42
2	B	501	HEM	CHC-C4B-NB	3.14	127.80	124.42
3	A	502	VNT	OAX-CBF-CBC	3.07	124.07	118.73
3	C	502	VNT	OAX-CBF-CBC	3.03	124.00	118.73
3	C	502	VNT	CAO-NAT-NBI	3.01	109.57	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	VNT	CAO-NAT-NBI	3.01	109.56	102.60
3	A	502	VNT	OAX-CBG-NAV	-2.99	109.64	112.34
3	A	502	VNT	OAX-CBG-CBD	2.99	123.95	118.73
3	D	502	VNT	NAT-CAO-NAS	-2.96	106.44	114.90
3	A	502	VNT	NAT-CAO-NAS	-2.94	106.50	114.90
3	A	502	VNT	OAX-CBF-NAU	-2.85	109.77	112.34
3	A	502	VNT	CBF-OAX-CBG	2.79	105.33	102.64
3	B	502	VNT	CBF-OAX-CBG	2.79	105.33	102.64
3	B	502	VNT	NAT-CAO-NAS	-2.78	106.97	114.90
3	C	502	VNT	NAT-CAO-NAS	-2.70	107.20	114.90
2	C	501	HEM	CHA-C4D-C3D	-2.69	120.26	125.23
3	B	502	VNT	CAO-NAT-NBI	2.68	108.80	102.60
3	C	502	VNT	CAR-NBI-CAP	-2.65	123.55	129.48
3	B	502	VNT	CAR-CBH-NAW	-2.63	103.99	110.71
3	D	502	VNT	CBC-CBF-NAU	-2.63	124.28	128.36
2	D	501	HEM	CHD-C4C-NC	2.63	127.31	124.45
3	B	502	VNT	CAN-CBE-CBA	2.62	119.45	116.82
2	B	501	HEM	CHD-C4C-NC	2.58	127.27	124.45
3	A	502	VNT	CAR-NBI-CAP	-2.56	123.75	129.48
3	B	502	VNT	CBH-NAW-CAY	-2.55	119.30	122.34
2	D	501	HEM	CHD-C1D-C2D	-2.54	121.02	125.03
3	C	502	VNT	CAR-NBI-NAT	2.52	126.75	121.26
3	D	502	VNT	OAX-CBG-CBD	2.51	123.09	118.73
2	C	501	HEM	C3D-C4D-ND	2.50	112.91	110.17
3	B	502	VNT	OAX-CBF-CBC	2.48	123.04	118.73
2	D	501	HEM	CMD-C2D-C1D	2.47	128.89	125.03
2	D	501	HEM	C1B-NB-C4B	2.43	108.09	105.21
3	D	502	VNT	CAR-CBH-NAW	-2.43	104.50	110.71
2	D	501	HEM	CHA-C4D-ND	2.35	127.28	124.37
3	A	502	VNT	CBA-CAQ-CAZ	2.31	121.32	118.72
3	D	502	VNT	CAQ-CBA-CBE	-2.30	119.97	122.46
3	D	502	VNT	CAN-CBE-CBA	2.30	119.13	116.82
2	D	501	HEM	CAD-C3D-C4D	2.30	128.70	124.70
3	D	502	VNT	NBI-CAP-NAS	-2.28	105.69	110.42
2	B	501	HEM	C1B-NB-C4B	2.27	107.90	105.21
2	B	501	HEM	CHD-C1D-C2D	-2.25	121.47	125.03
3	C	502	VNT	CBD-CBG-NAV	-2.22	124.92	128.36
2	A	501	HEM	CHD-C1D-C2D	-2.21	121.54	125.03
2	A	501	HEM	C1B-NB-C4B	2.21	107.82	105.21
2	C	501	HEM	C1A-CHA-C4D	-2.19	121.11	126.25
2	A	501	HEM	CHD-C4C-NC	2.18	126.83	124.45
2	D	501	HEM	O2D-CGD-CBD	2.18	120.89	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	VNT	CBH-NAW-CAY	-2.16	119.77	122.34
2	A	501	HEM	C1A-CHA-C4D	-2.15	121.20	126.25
3	C	502	VNT	CBC-CBF-NAU	-2.13	125.05	128.36
2	D	501	HEM	CHA-C4D-C3D	-2.13	121.31	125.23
2	C	501	HEM	O2D-CGD-CBD	2.12	120.71	114.00
3	D	502	VNT	CBH-NAW-CAY	-2.11	119.83	122.34
2	C	501	HEM	CHC-C4B-NB	2.11	126.69	124.42
2	D	501	HEM	C1A-CHA-C4D	-2.10	121.30	126.25
2	A	501	HEM	CHB-C1B-NB	2.10	126.97	124.37
2	D	501	HEM	CHD-C1D-ND	2.09	126.68	124.42
2	B	501	HEM	C2D-C1D-ND	2.09	112.32	109.90
2	A	501	HEM	CHD-C1D-ND	2.09	126.67	124.42
2	A	501	HEM	O2D-CGD-CBD	2.07	120.53	114.00
3	A	502	VNT	CBE-CBH-NAW	2.06	115.50	111.44
2	D	501	HEM	C2D-C1D-ND	2.04	112.26	109.90
3	D	502	VNT	CAL-CBD-CBG	-2.04	117.48	120.56
2	B	501	HEM	C3D-C4D-ND	2.02	112.39	110.17
2	B	501	HEM	CHB-C1B-NB	2.02	126.86	124.37
2	A	501	HEM	CHB-C1B-C2B	-2.01	121.23	126.95
2	C	501	HEM	C2B-C1B-NB	2.01	112.15	109.84
3	B	502	VNT	CBC-CBF-NAU	-2.00	125.25	128.36

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	VNT	CAM-CBD-CBG-OAX
3	D	502	VNT	CAL-CBD-CBG-OAX
3	D	502	VNT	CAM-CBD-CBG-NAV
3	D	502	VNT	CAL-CBD-CBG-NAV
3	B	502	VNT	CAM-CBD-CBG-OAX
3	B	502	VNT	CAL-CBD-CBG-OAX
3	D	502	VNT	CAH-CBC-CBF-OAX
3	D	502	VNT	CAG-CBC-CBF-OAX
3	B	502	VNT	CAM-CBD-CBG-NAV
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
3	A	502	VNT	CAM-CBD-CBG-OAX
3	D	502	VNT	CBA-CBE-CBH-CAR
3	D	502	VNT	CAG-CBC-CBF-NAU
3	B	502	VNT	CAL-CBD-CBG-NAV

Continued on next page...

Continued from previous page...

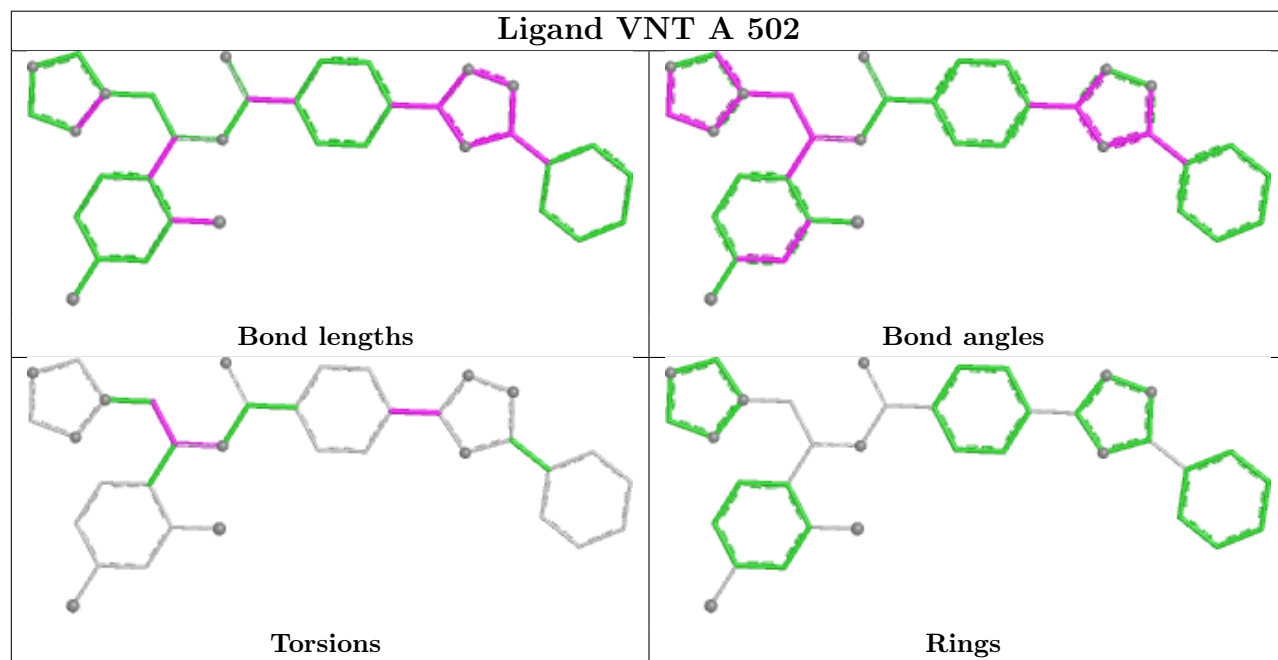
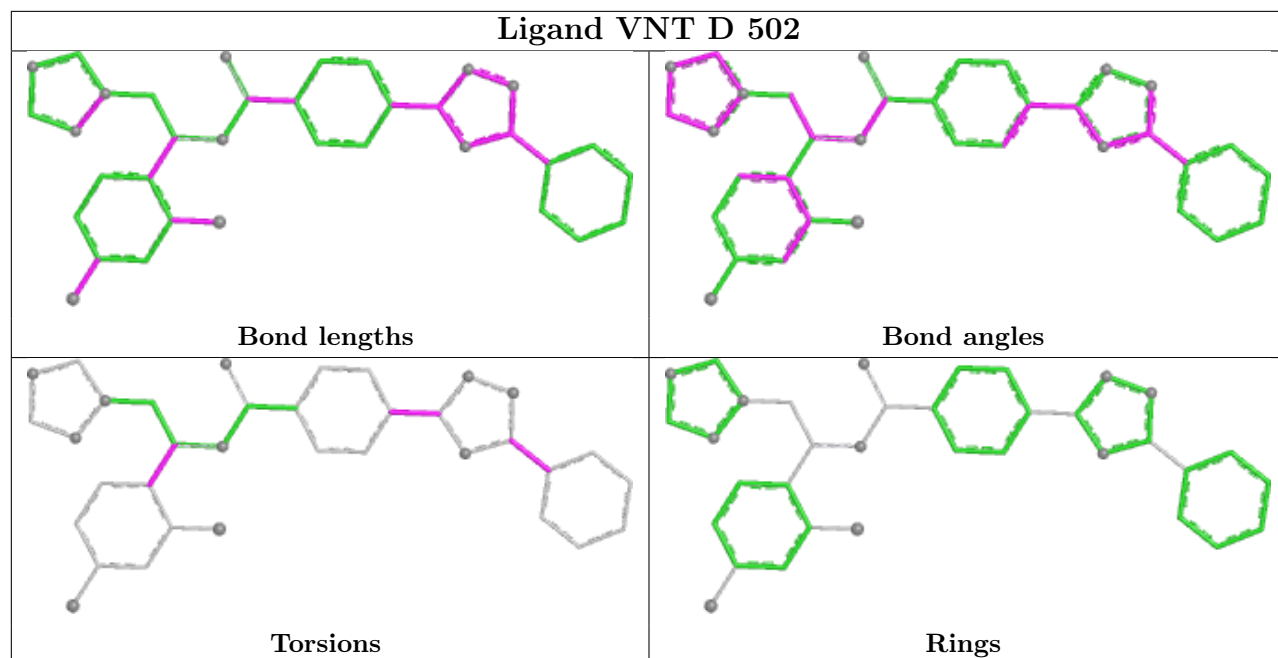
Mol	Chain	Res	Type	Atoms
3	D	502	VNT	CAH-CBC-CBF-NAU
2	C	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O1D
3	A	502	VNT	CBE-CBH-NAW-CAY
3	B	502	VNT	CBE-CBH-NAW-CAY
3	B	502	VNT	CAN-CBE-CBH-CAR
3	C	502	VNT	CAN-CBE-CBH-CAR
3	D	502	VNT	CAN-CBE-CBH-CAR
3	C	502	VNT	CBA-CBE-CBH-CAR
2	B	501	HEM	CAD-CBD-CGD-O2D
3	A	502	VNT	NBI-CAR-CBH-CBE

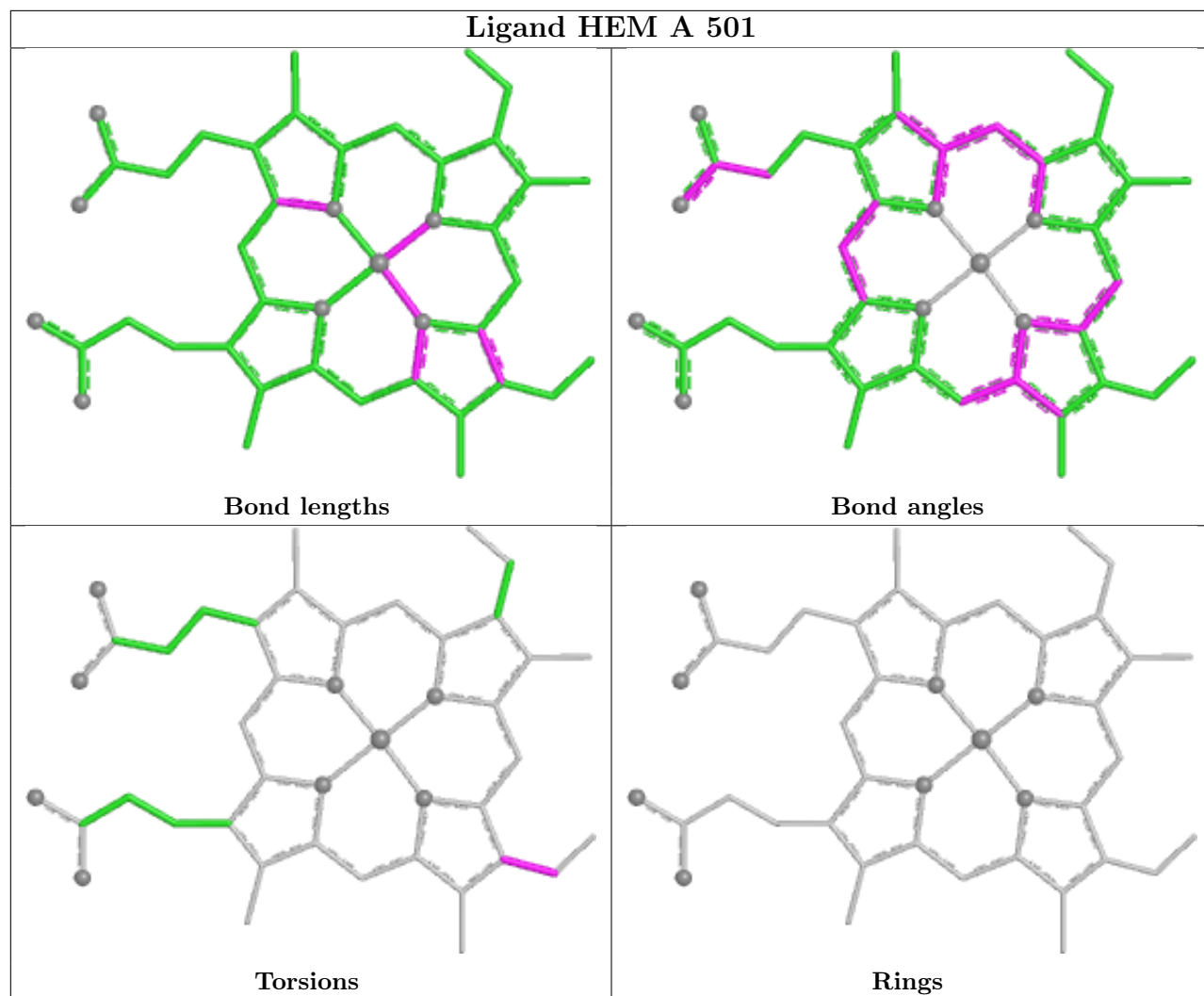
There are no ring outliers.

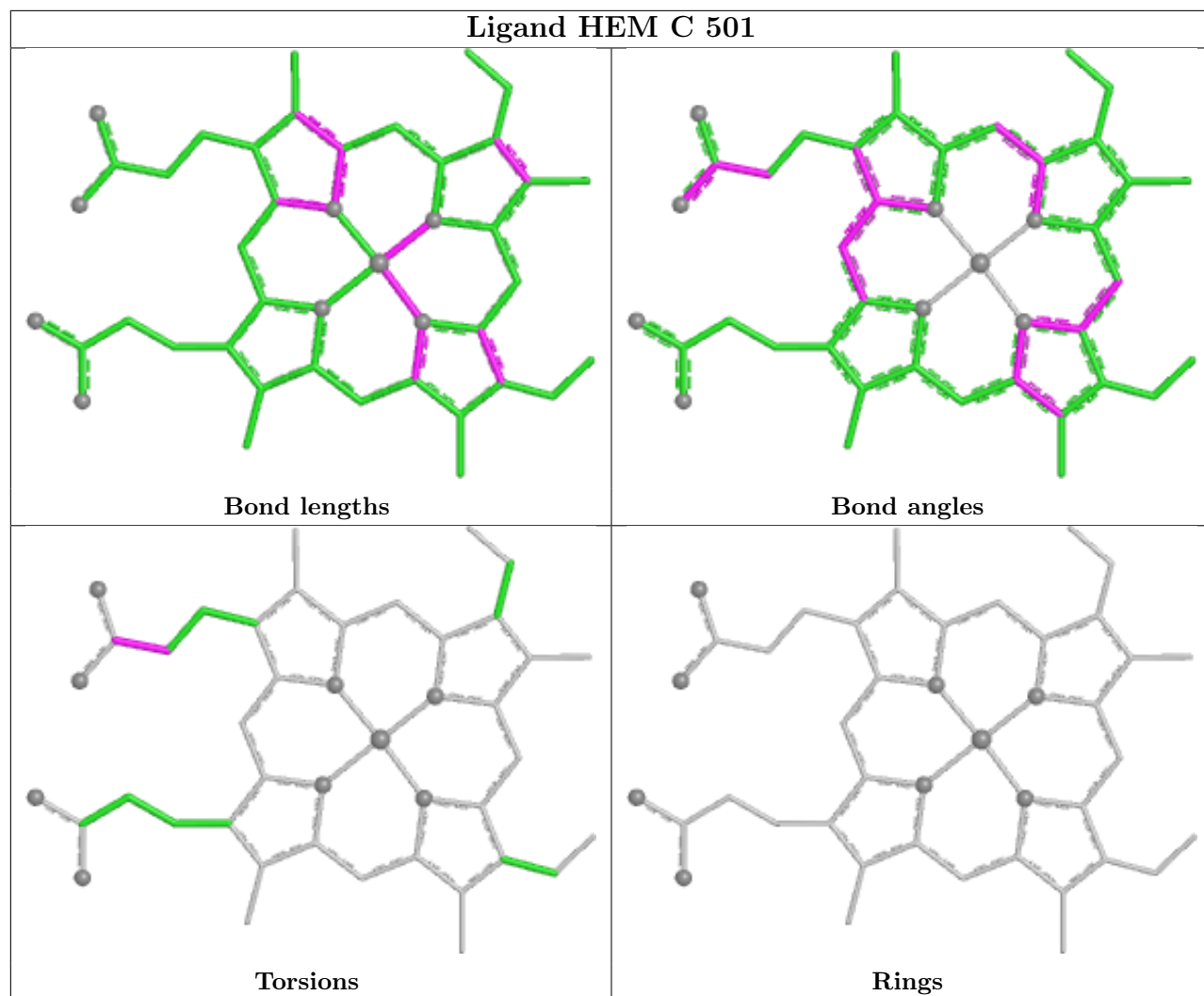
8 monomers are involved in 35 short contacts:

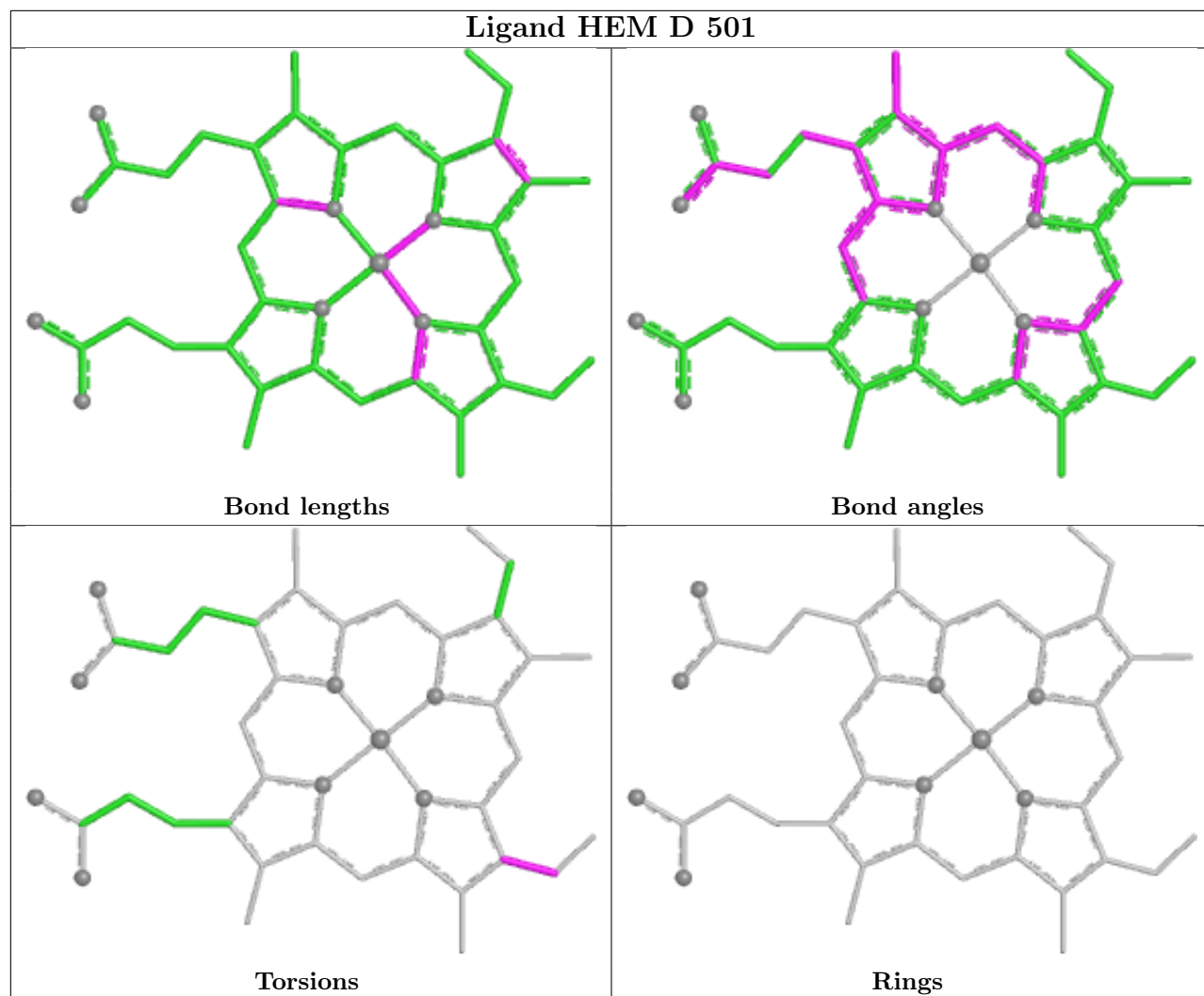
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	VNT	4	0
3	A	502	VNT	2	0
2	A	501	HEM	6	0
2	C	501	HEM	6	0
2	D	501	HEM	7	0
2	B	501	HEM	7	0
3	C	502	VNT	2	0
3	B	502	VNT	2	0

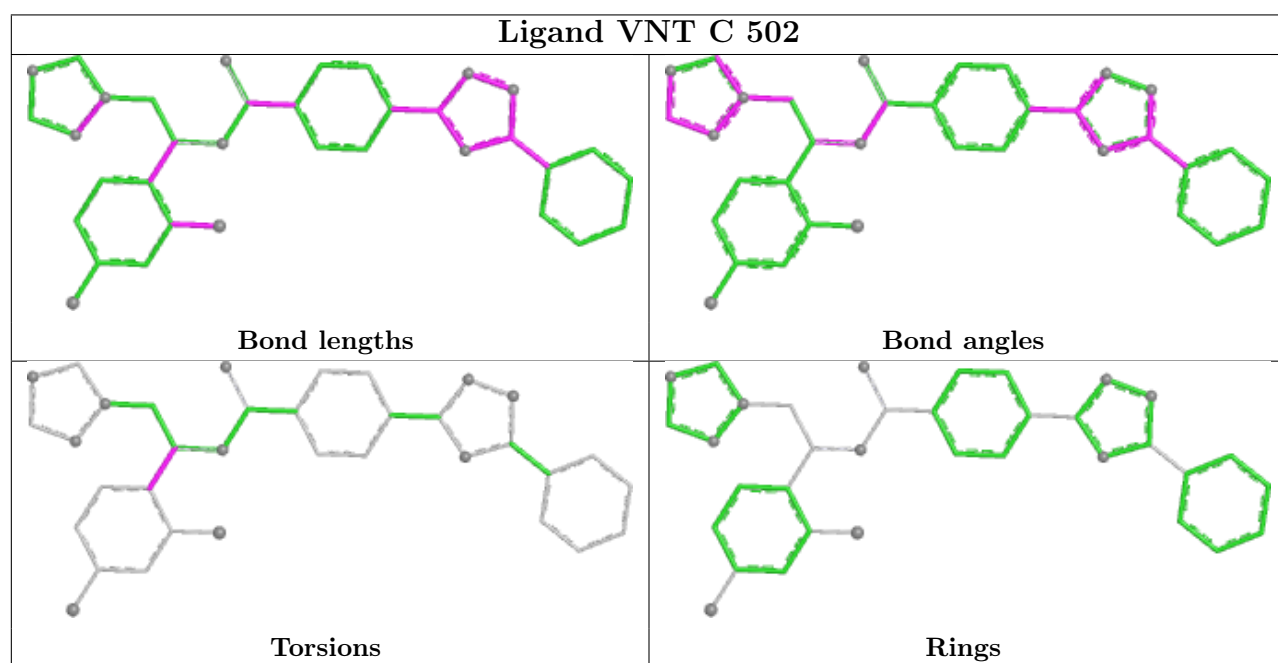
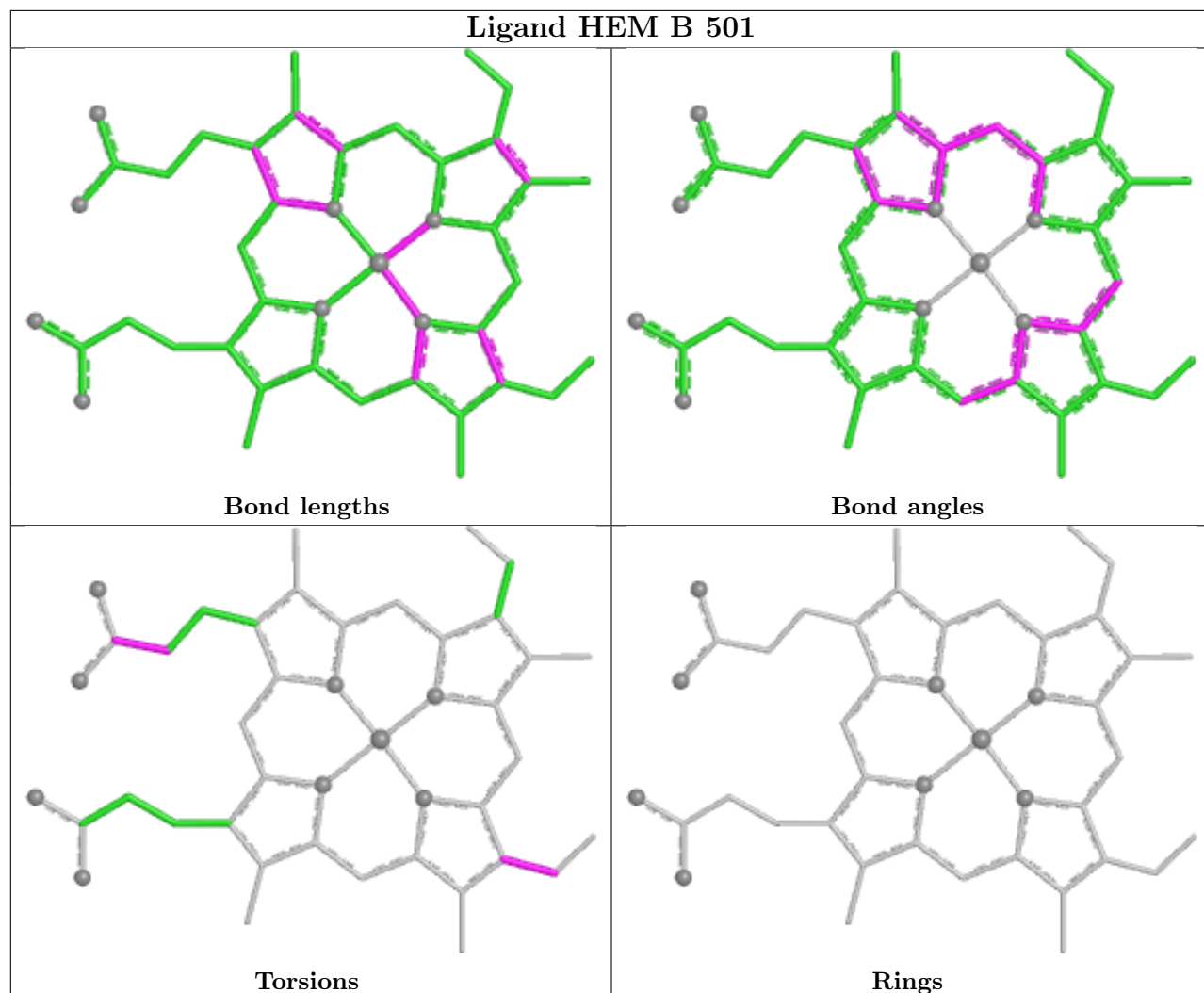
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

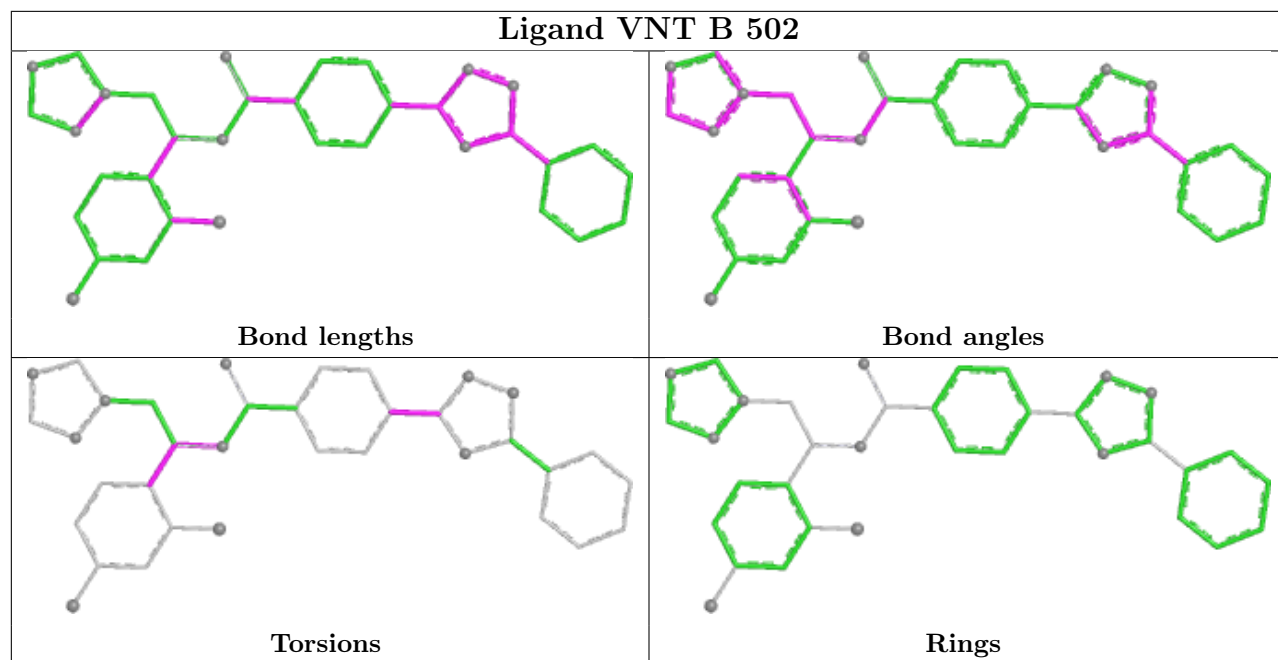












5.7 Other polymers [i](#)

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	11 (2%) 58 64	18, 31, 54, 119	0
1	B	448/448 (100%)	-0.31	5 (1%) 78 84	18, 30, 48, 107	0
1	C	448/448 (100%)	0.03	5 (1%) 78 84	23, 38, 62, 104	0
1	D	448/448 (100%)	-0.03	1 (0%) 91 94	21, 36, 57, 76	0
All	All	1792/1792 (100%)	-0.10	22 (1%) 76 82	18, 34, 57, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ILE	7.0
1	A	43	GLY	6.7
1	D	29	GLY	5.7
1	A	253	ASN	4.9
1	C	29	GLY	4.3
1	C	254	LYS	4.1
1	A	42	LEU	3.7
1	A	254	LYS	3.5
1	A	252	VAL	3.3
1	A	255	ASP	3.2
1	B	256	SER	3.1
1	C	256	SER	2.7
1	B	254	LYS	2.7
1	B	29	GLY	2.6
1	C	257	SER	2.6
1	A	30	LYS	2.5
1	A	40	PRO	2.5
1	A	29	GLY	2.4
1	B	255	ASP	2.4
1	A	256	SER	2.3
1	B	30	LYS	2.2
1	C	258	THR	2.2

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](#)

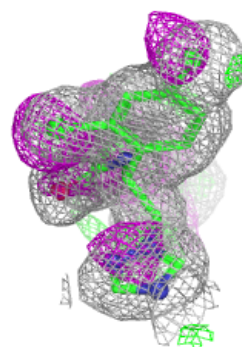
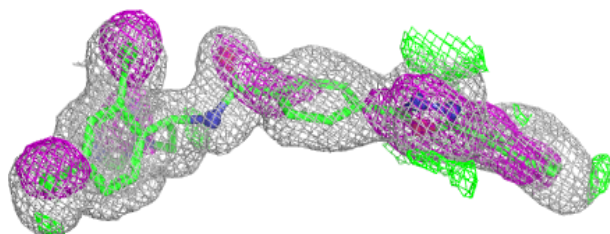
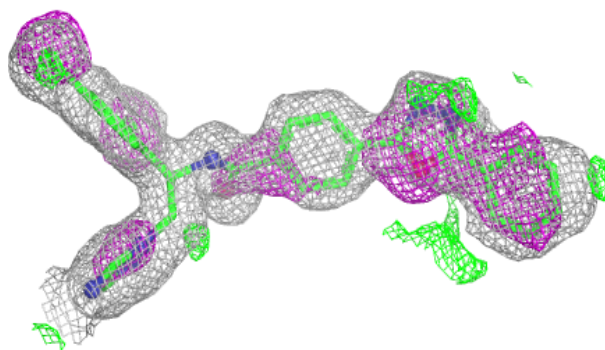
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VNT	D	502	35/35	0.88	0.10	21,23,26,27	0
3	VNT	C	502	35/35	0.92	0.09	21,22,24,27	0
3	VNT	B	502	35/35	0.92	0.09	20,22,25,26	0
3	VNT	A	502	35/35	0.94	0.08	19,22,25,25	0
2	HEM	A	501	43/43	0.98	0.06	17,20,28,33	0
2	HEM	B	501	43/43	0.98	0.05	16,20,26,37	0
2	HEM	C	501	43/43	0.98	0.07	23,28,41,50	0
2	HEM	D	501	43/43	0.98	0.06	18,23,32,42	0

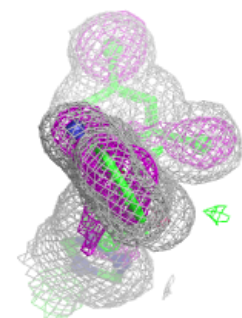
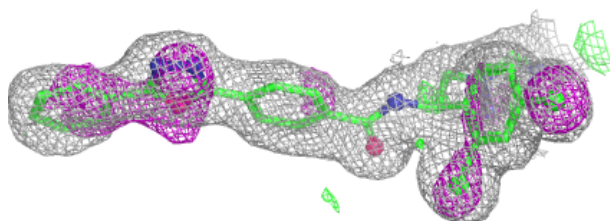
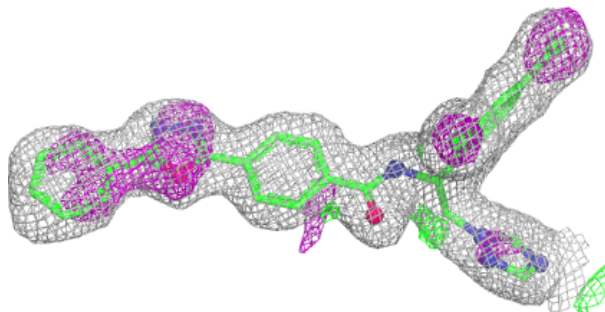
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

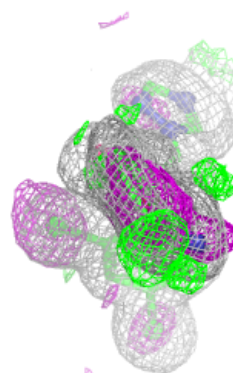
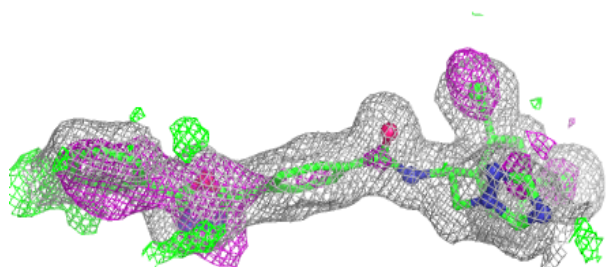
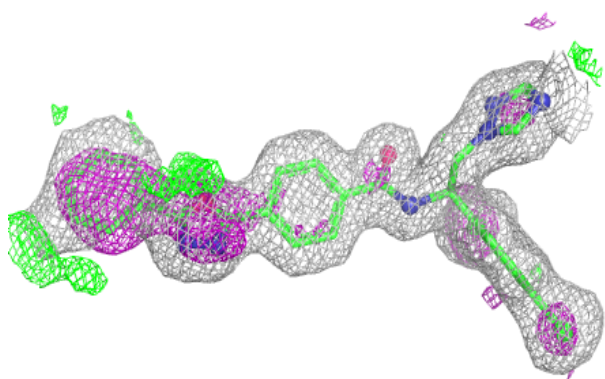
**Electron density around VNT C 502:**

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

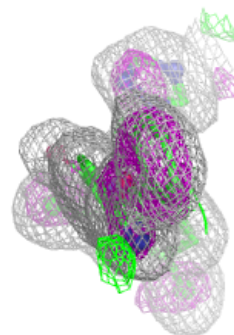
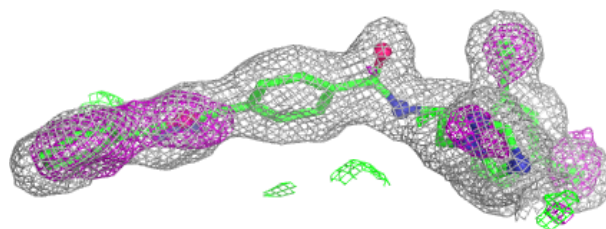
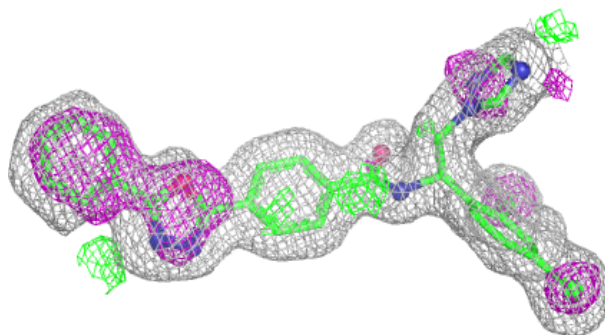


Electron density around VNT B 502:

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

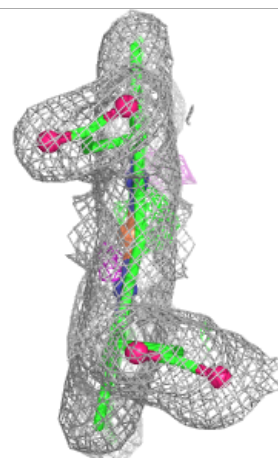
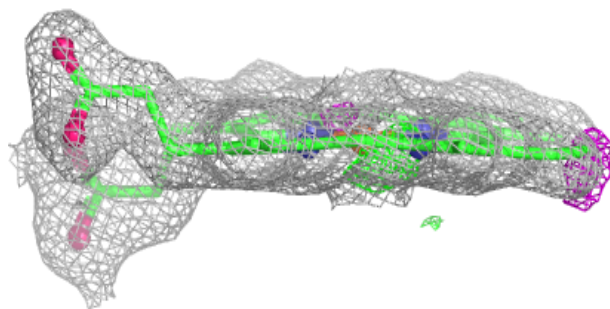
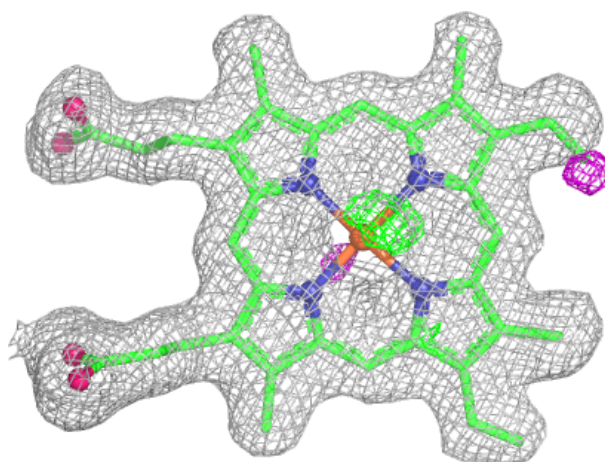
**Electron density around VNT A 502:**

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



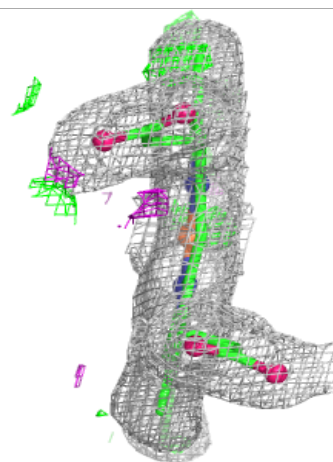
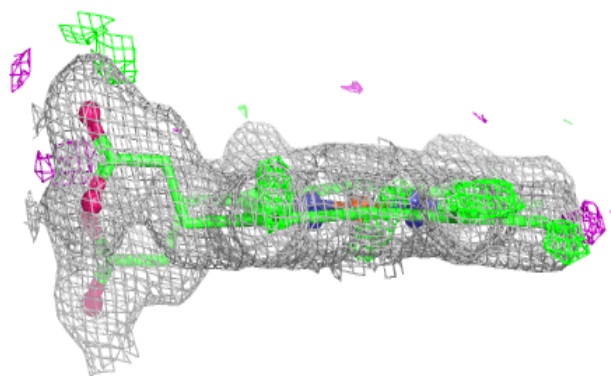
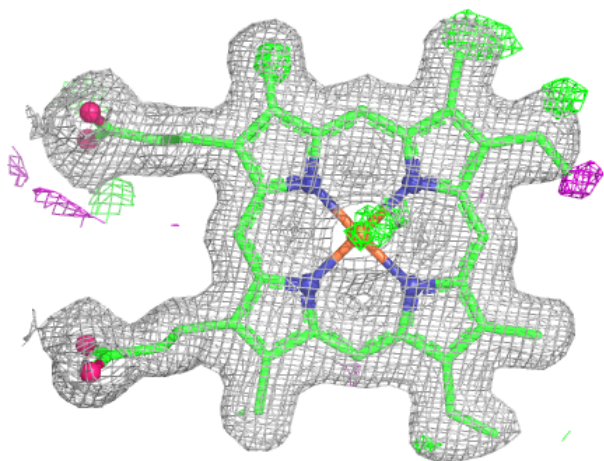
Electron density around HEM A 501:

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



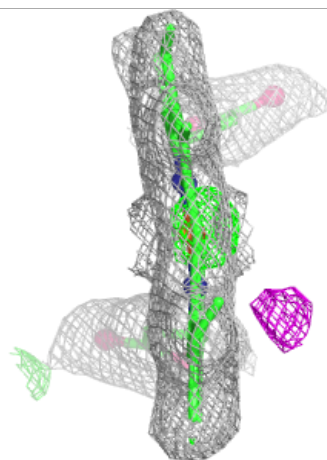
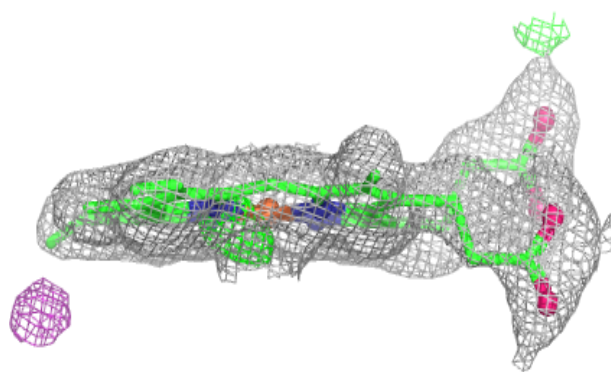
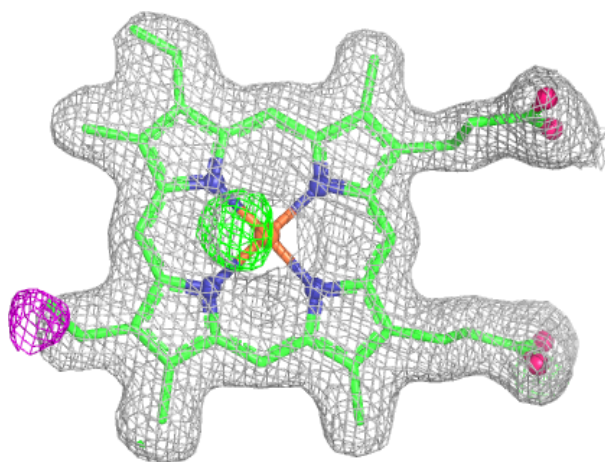
Electron density around HEM B 501:

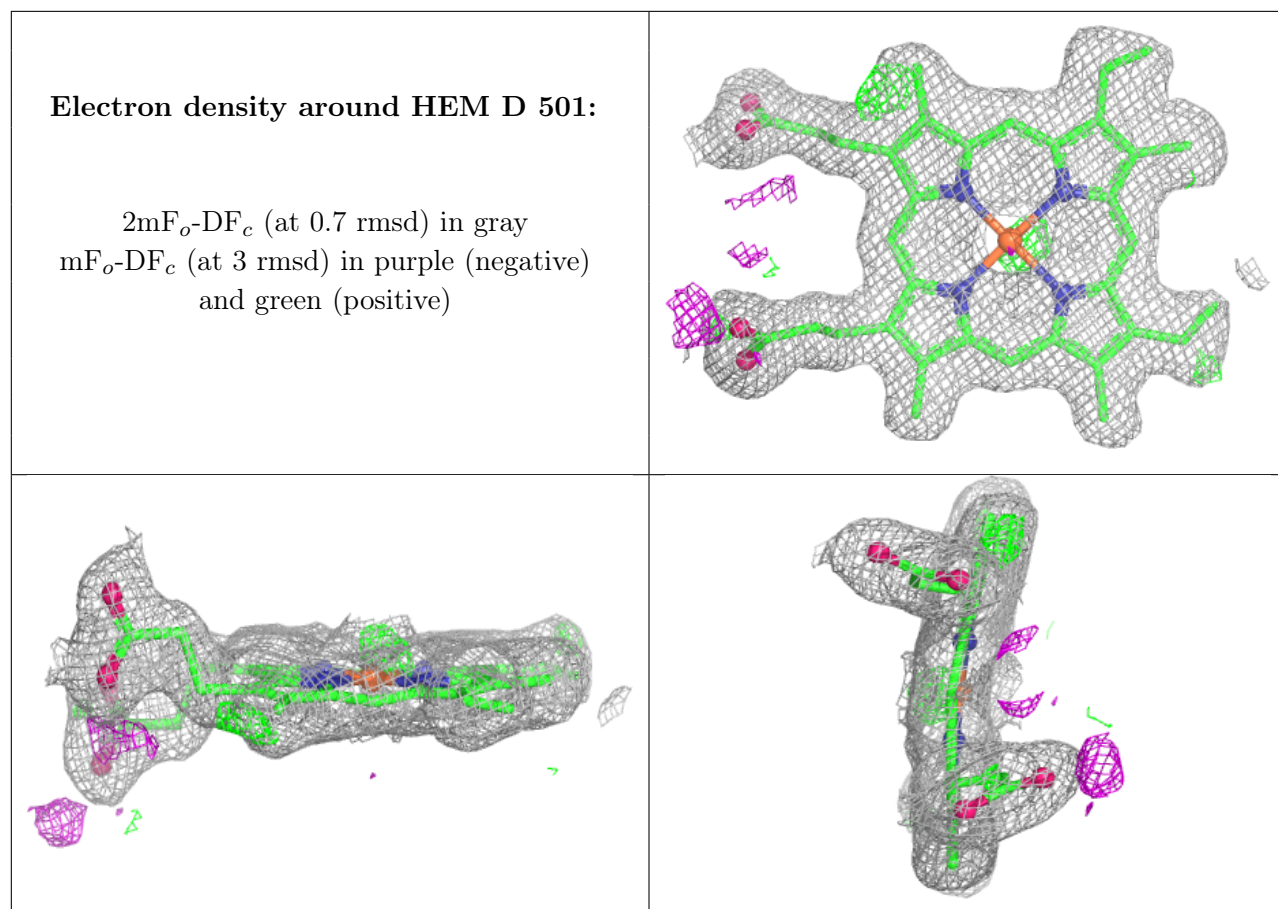
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 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 ⓘ

There are no such residues in this entry.