



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 03:26 PM EDT

PDB ID : 7JJ1  
Title : Crystal structure of the sterol 14alpha-demethylase-ferredoxin (CYP51-fx) heme domain and architectural comparison to the whole fusion protein  
Authors : Zhao, B.; Lamb, D.C.  
Deposited on : 2020-07-24  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

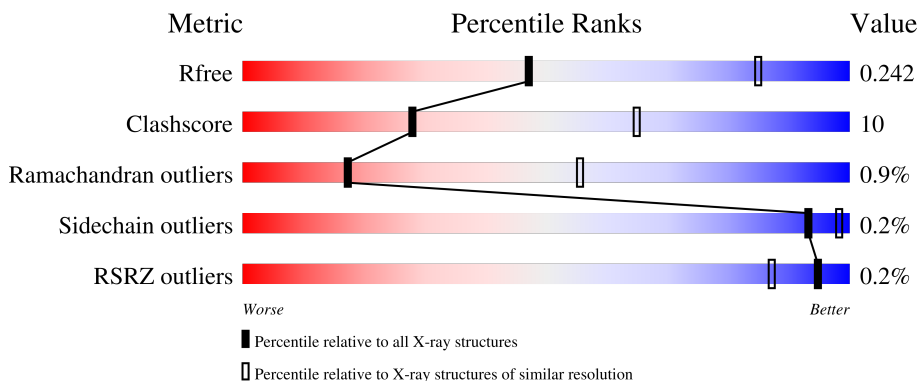
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



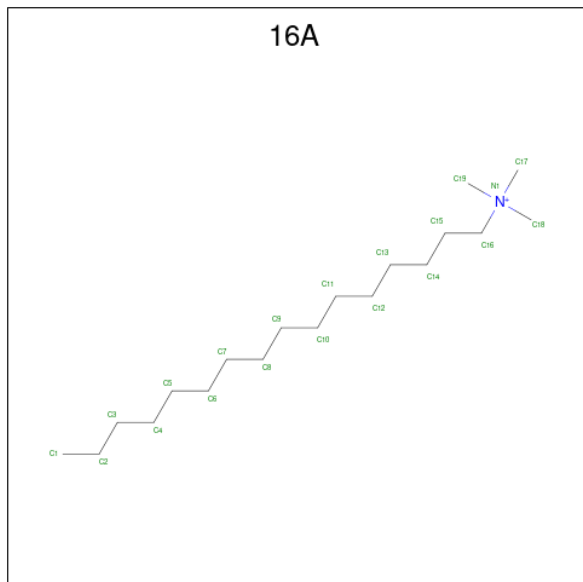
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	450	76% 22% .
1	B	450	75% 21% .
1	C	450	73% 25% .

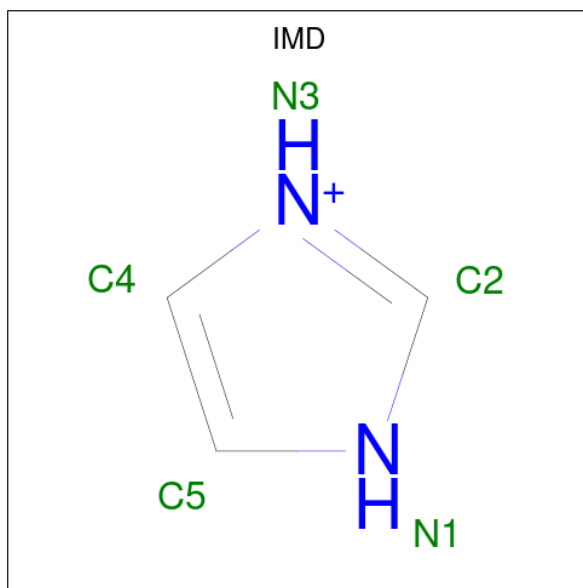


- Molecule 3 is CETYL-TRIMETHYL-AMMONIUM (three-letter code: 16A) (formula:  $C_{19}H_{42}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			20	19	1		
3	B	1	Total	C	N	0	0
			20	19	1		
3	C	1	Total	C	N	0	0
			20	19	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	C	1	Total C N 5 3 2	0	0
4	C	1	Total C N 5 3 2	0	0

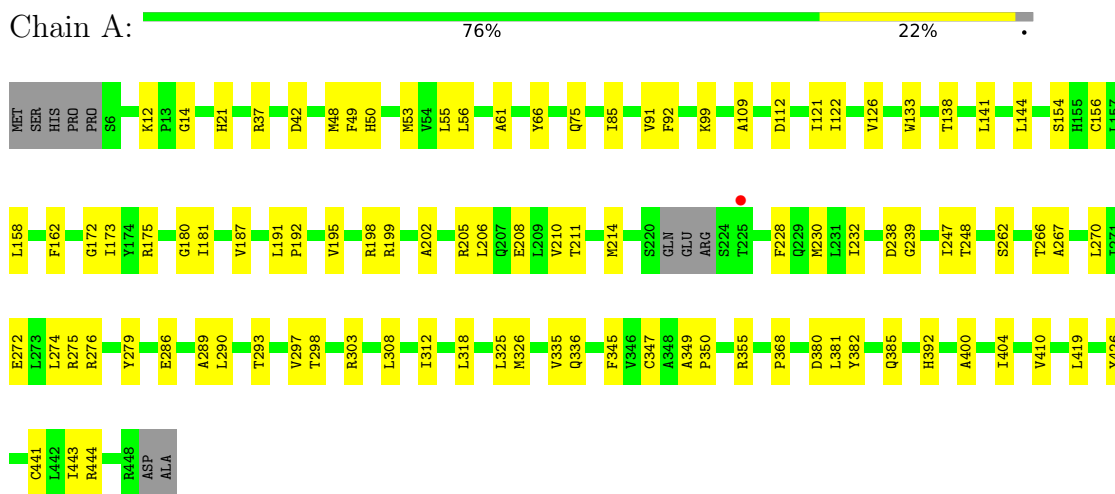
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	14	Total O 14 14	0	0
5	C	9	Total O 9 9	0	0

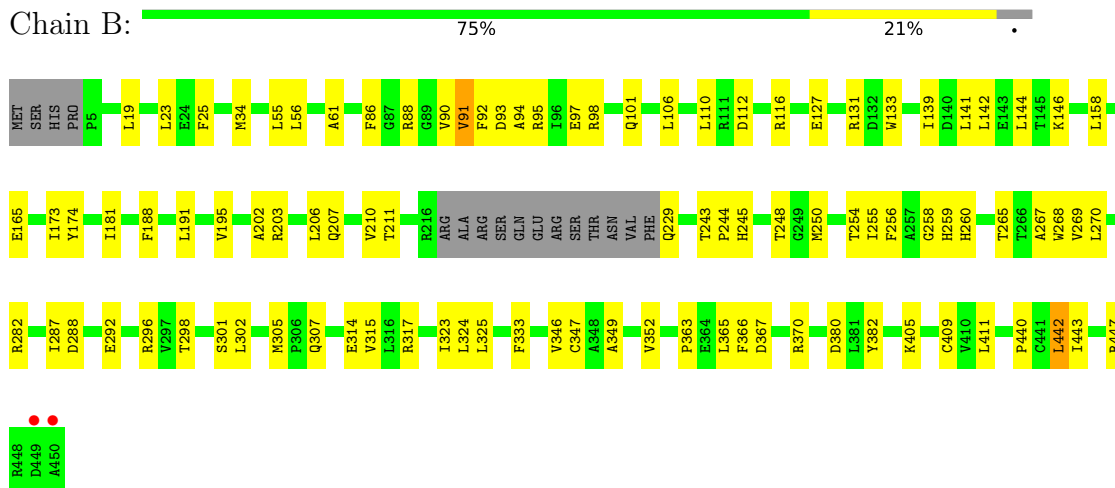
### 3 Residue-property plots

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: Cytochrome P450 51



- Molecule 1: Cytochrome P450 51



- Molecule 1: Cytochrome P450 51



MET	V126	G238	Q403
SER	E127	S240	I404
HIS	A128	F241	K405
PRO	M129	L242	L411
PRO	L130	T248	L412
SER	R131	G249	R413
Y7	D132	M250	R414
T8	W133	L251	R415
P9	K134	L275	Y416
L33	D135	R275	F417
V43	D140	R284	Y426
M48	L141	T298	P437
M53	L142	F299	I443
V54	E143	L302	R444
L55	L144	E309	R447
L56	T145	M310	R448
A61	T149	V311	ASP
S62	T152	I312	ALA
E63	F170	K313	
A64	L173	F314	
F65	L176	V315	
V72	D176	L318	
L73	I181	L324	
D74	A185	L325	
I81	Y186	V329	
M82	P189	M330	
F86	M190	K331	
V91	L191	D332	
F92	P192	F333	
R95	L193	E334	
R98	F196	V335	
K99	K197	A342	
M100	R198	F345	
Q104	R199	V346	
A109	D200	C347	
L110	Q201	A348	
R111	A202	R355	
D112	R203	E364	
K113	L206	D378	
P114	V210	Y382	
T117	F228	G383	
Y118	Q229	R384	
I121	M230	Q385	
I122	Y236	G396	
V123	D237		
	D238		

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.68Å 164.75Å 187.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 3.00 46.92 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.52-3.00) 98.2 (46.92-2.98)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.81 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.196 , 0.237 0.197 , 0.242	Depositor DCC
$R_{free}$ test set	5354 reflections (10.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.792	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 16A, IMD, 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	0/3550	0.51	0/4810
1	B	0.28	0/3485	0.53	0/4724
1	C	0.29	0/3622	0.55	0/4904
All	All	0.28	0/10657	0.53	0/14438

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	3465	0	3384	58	0
1	B	3400	0	3300	60	0
1	C	3535	0	3515	83	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
2	C	43	0	30	2	0
3	A	20	0	42	3	0
3	B	20	0	42	2	0
3	C	20	0	42	4	0
4	A	15	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	5	0	0
4	C	10	0	10	0	0
5	A	19	0	0	0	0
5	B	14	0	0	0	0
5	C	9	0	0	0	0
All	All	10661	0	10445	208	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 10.

All (208) 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:C:91:VAL:HG13	1:C:92:PHE:H	1.37	0.89
1:C:73:LEU:HD21	1:C:333:PHE:HE2	1.38	0.87
1:C:206:LEU:HD22	1:C:248:THR:HG23	1.61	0.83
1:B:207:GLN:HA	1:B:248:THR:HG21	1.63	0.80
1:A:138:THR:HG22	1:A:444:ARG:HG2	1.63	0.79
1:B:173:ILE:HG21	1:B:206:LEU:HG	1.65	0.78
1:B:250:MET:HB3	3:B:502:16A:H13	1.69	0.73
1:B:298:THR:H	1:B:301:SER:HB3	1.52	0.73
1:C:135:ASP:HA	1:C:447:ARG:HE	1.52	0.72
1:C:95:ARG:HH11	1:C:98:ARG:HD3	1.55	0.72
1:C:142:LEU:HD21	1:C:437:PRO:HD2	1.72	0.72
1:C:199:ARG:NH1	1:C:200:ASP:OD1	2.24	0.69
1:C:242:LEU:HD22	1:C:250:MET:HE1	1.74	0.68
1:C:48:MET:HE3	1:C:53:MET:HG3	1.75	0.68
1:B:173:ILE:HG23	1:B:202:ALA:HB1	1.76	0.68
1:A:48:MET:HB2	1:A:53:MET:HE1	1.75	0.67
1:A:92:PHE:H	1:A:99:LYS:HG3	1.59	0.67
1:C:142:LEU:HA	1:C:145:THR:HG22	1.76	0.67
1:C:298:THR:HG22	1:C:299:PHE:H	1.58	0.66
1:C:81:ILE:HG13	1:C:185:ALA:HB3	1.78	0.65
1:C:100:ASN:O	1:C:104:GLN:HG2	1.99	0.63
1:C:189:PRO:O	1:C:199:ARG:NH2	2.30	0.63
1:C:228:PHE:CD1	1:C:251:LEU:HD11	2.33	0.63
1:A:326:MET:H	4:A:504:IMD:H2	1.64	0.62
1:B:141:LEU:HD12	1:B:443:ILE:HD13	1.80	0.62
1:A:48:MET:HB2	1:A:53:MET:CE	2.29	0.62
1:B:302:LEU:HD12	1:B:405:LYS:HB3	1.82	0.62
1:C:170:PHE:HA	1:C:173:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HD12	1:C:443:ILE:HG21	1.80	0.62
1:A:50[B]:HIS:CD2	1:B:195:VAL:HG21	2.34	0.62
2:A:501:HEM:HMD3	3:A:502:16A:H13	1.81	0.62
1:B:142:LEU:HG	1:B:146:LYS:HE3	1.82	0.61
1:C:109:ALA:HA	1:C:230:MET:SD	2.41	0.61
1:A:56:LEU:HB3	1:A:61:ALA:HB1	1.83	0.60
1:B:90:VAL:HG12	1:B:91:VAL:HG23	1.84	0.60
1:A:272:GLU:OE1	1:A:276:ARG:NH1	2.35	0.60
1:C:82:MET:HE1	3:C:502:16A:H102	1.84	0.59
1:B:181:ILE:HD11	1:B:256[B]:PHE:HE2	1.68	0.59
1:A:266:THR:HG22	1:A:404:ILE:HG23	1.84	0.59
1:B:255:ILE:O	1:B:259:HIS:HB3	2.03	0.58
1:A:350:PRO:HA	1:A:385:GLN:HE21	1.69	0.57
1:C:284:ARG:NH1	1:C:412:LEU:O	2.37	0.57
1:B:250:MET:O	1:B:254:THR:HG23	2.04	0.57
1:A:228:PHE:O	1:A:232:ILE:HG12	2.04	0.57
1:A:419:LEU:HA	1:A:443:ILE:HD12	1.87	0.57
1:B:34:MET:HG2	1:B:352:VAL:HG22	1.86	0.57
2:C:501:HEM:HMD2	3:C:502:16A:H13	1.87	0.57
1:B:56:LEU:HB3	1:B:61:ALA:HB1	1.87	0.56
2:B:501:HEM:HMD3	3:B:502:16A:H61	1.87	0.56
1:C:236:TYR:HB2	1:C:240:SER:HB2	1.87	0.56
1:C:332:ASP:OD1	1:C:342:ALA:N	2.38	0.55
1:C:133:TRP:HZ2	1:C:144:LEU:HD13	1.71	0.55
1:B:244:PRO:O	1:B:248:THR:HG23	2.06	0.55
1:C:81:ILE:HB	1:C:186:TYR:CE1	2.42	0.55
1:C:86:PHE:O	1:C:203:ARG:NH2	2.33	0.55
1:A:158:LEU:HB3	1:A:162:PHE:CD2	2.42	0.55
1:C:140:ASP:HB3	1:C:143:GLU:HB2	1.88	0.54
1:B:325:LEU:HD22	2:B:501:HEM:HBA2	1.89	0.54
1:C:112:ASP:O	1:C:114:PRO:HD2	2.08	0.54
1:A:121:ILE:HD11	1:A:156:CYS:SG	2.48	0.54
1:C:196:PHE:HA	1:C:199:ARG:HG2	1.88	0.54
1:A:279:TYR:CZ	1:A:368:PRO:HD2	2.43	0.54
1:A:173:ILE:HG23	1:A:202:ALA:HB1	1.89	0.53
1:B:365:LEU:HD22	1:B:367:ASP:HB2	1.89	0.53
1:C:236:TYR:CE2	1:C:242:LEU:HD23	2.44	0.53
1:B:94:ALA:HB3	1:B:98:ARG:HB2	1.90	0.53
1:B:367:ASP:O	1:B:370:ARG:HG3	2.09	0.53
1:C:110:LEU:HD13	1:C:396:GLY:HA2	1.91	0.52
1:A:133:TRP:HZ2	1:A:144:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:NH2	1:B:363:PRO:O	2.38	0.52
1:C:197:LYS:O	1:C:201:GLN:HG3	2.08	0.52
1:C:206:LEU:CD2	1:C:248:THR:HG23	2.36	0.52
1:B:265:THR:O	1:B:269:VAL:HG23	2.09	0.52
1:B:447:ARG:HG3	1:B:447:ARG:HH11	1.74	0.52
1:B:19:LEU:HD13	1:B:23:LEU:HD11	1.91	0.52
1:C:91:VAL:HG13	1:C:92:PHE:N	2.16	0.52
1:C:56:LEU:HD12	1:C:65:PHE:HB2	1.91	0.51
1:A:55:LEU:HD11	1:A:349:ALA:HB2	1.92	0.51
1:A:335:VAL:HG12	1:A:336:GLN:HG3	1.91	0.51
1:A:205:ARG:NH1	1:A:208:GLU:OE1	2.44	0.51
1:A:37:ARG:NH1	1:A:42:ASP:OD1	2.43	0.51
1:C:383:GLY:O	1:C:385:GLN:HG3	2.11	0.51
1:B:25:PHE:CZ	1:B:324:LEU:HD11	2.45	0.51
1:B:127:GLU:O	1:B:131:ARG:HG3	2.11	0.51
1:C:56:LEU:HB3	1:C:61:ALA:HB1	1.92	0.51
1:C:43:VAL:HG22	1:C:56:LEU:HD22	1.93	0.51
1:A:180:GLY:HA3	1:A:199:ARG:HD3	1.93	0.50
1:C:309:GLU:HG2	1:C:405:LYS:HE2	1.93	0.50
1:A:49:PHE:CZ	1:A:187:VAL:HG22	2.45	0.50
1:C:173:ILE:HD12	1:C:206:LEU:HB2	1.93	0.50
1:A:262:SER:O	1:A:266:THR:HG23	2.11	0.50
1:A:286:GLU:O	1:A:290:LEU:HD23	2.11	0.50
1:A:266:THR:HG22	1:A:404:ILE:HA	1.94	0.50
1:B:258:GLY:HA2	2:B:501:HEM:HMC2	1.95	0.49
1:C:126:VAL:O	1:C:130:LEU:HD13	2.13	0.49
1:B:207:GLN:O	1:B:211:THR:HG23	2.12	0.48
1:C:122:ILE:HD13	1:C:403:GLN:HA	1.95	0.48
2:C:501:HEM:CMD	3:C:502:16A:H13	2.43	0.48
1:A:232:ILE:HD13	1:A:247:ILE:HD13	1.95	0.48
1:B:243:THR:HG22	1:B:245:HIS:H	1.79	0.48
1:A:109:ALA:HB2	1:A:230:MET:HG3	1.96	0.48
1:C:122:ILE:HG12	1:C:152:THR:OG1	2.14	0.48
1:A:289:ALA:O	1:A:293:THR:HG22	2.14	0.48
1:B:112:ASP:O	1:B:116:ARG:HG3	2.14	0.48
1:B:282:ARG:NE	1:B:307:GLN:OE1	2.42	0.48
1:C:236:TYR:O	1:C:238:ASP:N	2.43	0.48
1:A:210:VAL:HG13	1:A:228:PHE:CZ	2.49	0.48
1:A:274:LEU:HD13	1:A:443:ILE:HD11	1.95	0.47
1:B:86:PHE:O	1:B:203:ARG:NE	2.44	0.47
1:B:380:ASP:O	1:B:382:TYR:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:TYR:O	1:C:122:ILE:HG13	2.15	0.47
1:C:117:THR:O	1:C:121:ILE:HG13	2.15	0.47
1:A:12:LYS:HD3	1:A:21:HIS:CD2	2.49	0.47
1:A:195:VAL:HG12	1:A:198:ARG:HH21	1.79	0.47
1:A:75:GLN:NE2	1:A:392:HIS:CG	2.82	0.47
1:B:288:ASP:O	1:B:292:GLU:HG2	2.14	0.47
1:C:149:THR:HA	1:C:152:THR:HG22	1.97	0.47
1:C:275:ARG:NH2	1:C:426:TYR:O	2.47	0.47
1:A:297:VAL:HG21	1:A:410:VAL:HG22	1.97	0.47
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.45	0.46
1:C:112:ASP:C	1:C:114:PRO:HD2	2.36	0.46
1:A:318:LEU:O	1:A:355:ARG:NH2	2.44	0.46
1:B:141:LEU:CD2	1:B:267:ALA:HA	2.45	0.46
1:C:413:ARG:HD2	1:C:413:ARG:O	2.16	0.46
1:B:106:LEU:O	1:B:110:LEU:HG	2.16	0.46
1:B:333:PHE:HZ	1:B:346:VAL:HG11	1.81	0.45
1:A:419:LEU:HD22	1:A:426:TYR:CE2	2.51	0.45
1:B:287:ILE:HD13	1:B:409:CYS:HA	1.97	0.45
1:C:63:GLU:HG3	1:C:382:TYR:CE2	2.51	0.45
1:C:95:ARG:HH11	1:C:98:ARG:CD	2.27	0.45
1:C:298:THR:HG22	1:C:299:PHE:N	2.29	0.45
1:C:329:VAL:HG12	1:C:342:ALA:HA	1.98	0.45
1:A:275:ARG:NH2	1:A:426:TYR:O	2.50	0.45
1:B:97:GLU:O	1:B:101:GLN:HG3	2.17	0.45
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.99	0.45
1:C:33:LEU:HD22	1:C:55:LEU:HD22	1.99	0.44
1:C:318:LEU:O	1:C:355:ARG:NH2	2.48	0.44
1:A:238:ASP:OD1	1:A:239:GLY:N	2.51	0.44
1:B:88:ARG:O	1:B:93:ASP:HB3	2.17	0.44
1:A:141:LEU:HD22	1:A:267:ALA:HA	1.99	0.44
1:B:158:LEU:HA	1:B:229:GLN:OE1	2.16	0.44
1:B:55:LEU:HA	1:B:347:CYS:HB2	1.99	0.44
1:C:206:LEU:O	1:C:210:VAL:HG23	2.17	0.44
1:C:313:LYS:NZ	1:C:378:ASP:OD2	2.42	0.44
1:A:53:MET:SD	1:A:345:PHE:HB2	2.58	0.44
1:B:91:VAL:HG12	1:B:92:PHE:N	2.32	0.44
1:B:188:PHE:HB3	1:B:191:LEU:HG	1.99	0.44
1:C:228:PHE:HD1	1:C:251:LEU:HD11	1.81	0.44
1:C:325:LEU:O	1:C:347:CYS:HA	2.18	0.44
1:C:123:VAL:O	1:C:127:GLU:HG2	2.17	0.44
1:A:400:ALA:O	1:A:404:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HB3	1:C:43:VAL:HG12	2.00	0.44
1:C:309:GLU:CG	1:C:405:LYS:HE2	2.48	0.43
1:A:141:LEU:HD21	1:A:270:LEU:HD12	2.00	0.43
1:B:110:LEU:HD21	2:B:501:HEM:HBC1	1.99	0.43
3:A:502:16A:H192	3:A:502:16A:H151	1.73	0.43
1:C:355:ARG:HD3	1:C:364:GLU:OE2	2.18	0.43
1:A:308:LEU:O	1:A:312:ILE:HG13	2.18	0.43
1:B:258:GLY:HA2	2:B:501:HEM:CMC	2.48	0.43
1:B:365:LEU:HD23	1:B:366:PHE:N	2.34	0.43
1:B:133:TRP:HZ2	1:B:144:LEU:HD13	1.83	0.43
1:A:66:TYR:HE2	1:A:385:GLN:OE1	2.01	0.43
1:B:174:TYR:HH	1:B:260:HIS:CD2	2.36	0.43
1:C:72:VAL:CG1	1:C:333:PHE:HD2	2.32	0.43
1:C:126:VAL:HG12	1:C:130:LEU:HD13	2.01	0.43
1:B:270:LEU:HD11	1:B:411:LEU:HD23	1.99	0.43
1:C:53:MET:SD	1:C:345:PHE:HB2	2.59	0.43
1:C:210:VAL:HG13	1:C:228:PHE:CE1	2.54	0.43
1:A:325:LEU:O	1:A:347:CYS:HA	2.18	0.43
1:B:25:PHE:HZ	1:B:324:LEU:HD11	1.84	0.43
1:A:50[B]:HIS:HD2	1:B:195:VAL:HG21	1.81	0.42
1:B:323:ILE:O	1:B:349:ALA:HA	2.19	0.42
1:C:130:LEU:HG	1:C:415:TYR:CE2	2.54	0.42
1:C:128:ALA:O	1:C:131:ARG:HG2	2.19	0.42
3:C:502:16A:H22	3:C:502:16A:H51	1.83	0.42
1:B:305:MET:HE2	1:B:405:LYS:HE3	2.02	0.42
1:C:122:ILE:O	1:C:126:VAL:HG23	2.20	0.42
1:A:14:GLY:O	1:A:21:HIS:NE2	2.53	0.42
1:C:228:PHE:HA	1:C:251:LEU:HD21	2.01	0.42
1:C:333:PHE:CE1	1:C:335:VAL:HG23	2.54	0.42
1:B:210:VAL:HB	1:B:248:THR:HG22	2.02	0.42
1:C:74:ASP:HB2	1:C:330:MET:SD	2.60	0.42
1:C:311:VAL:O	1:C:315:VAL:HG23	2.20	0.42
1:A:191:LEU:HD12	1:A:192:PRO:HD2	2.02	0.42
1:A:154:SER:O	1:A:158:LEU:HB2	2.20	0.41
1:B:142:LEU:O	1:B:146:LYS:HG3	2.20	0.41
1:A:122:ILE:O	1:A:126:VAL:HG23	2.20	0.41
1:A:172:GLY:HA2	1:A:175:ARG:NH1	2.35	0.41
1:C:81:ILE:HB	1:C:186:TYR:CD1	2.56	0.41
1:C:191:LEU:C	1:C:193:LEU:H	2.24	0.41
1:C:324:LEU:HA	1:C:348:ALA:O	2.20	0.41
1:C:82:MET:HE1	1:C:181:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:O	1:B:442:LEU:HA	2.20	0.41
1:B:380:ASP:C	1:B:382:TYR:H	2.23	0.41
1:A:206:LEU:HD22	1:A:248:THR:OG1	2.21	0.41
1:A:211:THR:HA	1:A:214:MET:HE2	2.03	0.41
1:C:130:LEU:HD11	1:C:411:LEU:HD23	2.03	0.41
1:C:176:ASP:OD2	1:C:198:ARG:HG2	2.21	0.41
3:A:502:16A:H81	4:A:505:IMD:H5	2.03	0.40
1:A:380:ASP:C	1:A:382:TYR:H	2.25	0.40
1:B:268:TRP:HB3	1:B:315:VAL:HG13	2.04	0.40
1:C:95:ARG:N	1:C:95:ARG:HD3	2.36	0.40
1:C:298:THR:O	1:C:302:LEU:HG	2.21	0.40
1:C:417:PHE:HA	1:C:444:ARG:O	2.21	0.40
1:A:85:ILE:CD1	1:A:181:ILE:HG12	2.51	0.40
1:A:380:ASP:O	1:A:381:LEU:HB2	2.20	0.40
1:B:314:GLU:HA	1:B:314:GLU:OE2	2.20	0.40
1:A:326:MET:HG2	1:A:347:CYS:SG	2.62	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	437/450 (97%)	415 (95%)	17 (4%)	5 (1%)	14	50
1	B	431/450 (96%)	404 (94%)	22 (5%)	5 (1%)	13	48
1	C	441/450 (98%)	425 (96%)	14 (3%)	2 (0%)	29	68
All	All	1309/1350 (97%)	1244 (95%)	53 (4%)	12 (1%)	17	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	VAL

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Mol	Chain	Res	Type
1	A	303	ARG
1	B	95	ARG
1	B	165	GLU
1	C	113	LYS
1	A	441	CYS
1	B	91	VAL
1	B	440	PRO
1	C	91	VAL
1	B	442	LEU
1	A	112	ASP
1	A	298	THR

### 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	357/389 (92%)	357 (100%)	0	100	100
1	B	341/389 (88%)	340 (100%)	1 (0%)	92	97
1	C	369/389 (95%)	368 (100%)	1 (0%)	92	97
All	All	1067/1167 (91%)	1065 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	296	ARG
1	C	95	ARG

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

Mol	Chain	Res	Type
1	B	102	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 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
4	IMD	A	504	-	3,5,5	0.59	0	4,5,5	0.72	0
4	IMD	B	503	2	3,5,5	0.63	0	4,5,5	0.77	0
4	IMD	A	503	-	3,5,5	0.62	0	4,5,5	0.76	0
3	16A	C	502	-	19,19,19	0.53	0	21,21,21	0.53	0
4	IMD	C	504	-	3,5,5	0.59	0	4,5,5	0.70	0
3	16A	B	502	-	19,19,19	0.53	0	21,21,21	0.66	0
2	HEM	B	501	4	41,50,50	1.72	5 (12%)	45,82,82	1.42	8 (17%)
3	16A	A	502	-	19,19,19	0.52	0	21,21,21	0.66	0
4	IMD	C	503	-	3,5,5	0.60	0	4,5,5	0.65	0
2	HEM	C	501	-	41,50,50	1.70	5 (12%)	45,82,82	1.38	7 (15%)
4	IMD	A	505	-	3,5,5	0.61	0	4,5,5	0.67	0
2	HEM	A	501	-	41,50,50	1.70	6 (14%)	45,82,82	1.44	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	A	504	-	-	-	0/1/1/1
4	IMD	B	503	2	-	-	0/1/1/1
4	IMD	A	503	-	-	-	0/1/1/1
3	16A	C	502	-	-	2/17/17/17	-
4	IMD	C	504	-	-	-	0/1/1/1
3	16A	B	502	-	-	2/17/17/17	-
2	HEM	B	501	4	-	0/12/54/54	-
3	16A	A	502	-	-	3/17/17/17	-
4	IMD	C	503	-	-	-	0/1/1/1
2	HEM	C	501	-	-	2/12/54/54	-
4	IMD	A	505	-	-	-	0/1/1/1
2	HEM	A	501	-	-	3/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CBB-CAB	4.81	1.54	1.30
2	A	501	HEM	CBB-CAB	4.81	1.54	1.30
2	C	501	HEM	CBB-CAB	4.77	1.54	1.30
2	B	501	HEM	C3C-C2C	-4.41	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.10	1.34	1.40
2	C	501	HEM	C3C-C2C	-4.04	1.34	1.40
2	C	501	HEM	CBC-CAC	3.62	1.53	1.29
2	B	501	HEM	CBC-CAC	3.61	1.53	1.29
2	A	501	HEM	CBC-CAC	3.60	1.53	1.29
2	C	501	HEM	C3C-CAC	3.34	1.54	1.47
2	A	501	HEM	C3C-CAC	3.25	1.54	1.47
2	B	501	HEM	C3C-CAC	3.21	1.54	1.47
2	B	501	HEM	CAB-C3B	2.89	1.55	1.47
2	C	501	HEM	CAB-C3B	2.88	1.55	1.47
2	A	501	HEM	CAB-C3B	2.87	1.55	1.47
2	A	501	HEM	O2A-CGA	-2.01	1.24	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4C-CHD-C1D	4.81	128.90	122.56
2	C	501	HEM	C4C-CHD-C1D	4.77	128.86	122.56
2	B	501	HEM	C4C-CHD-C1D	4.69	128.75	122.56
2	B	501	HEM	C4B-CHC-C1C	3.15	126.71	122.56
2	A	501	HEM	CMC-C2C-C3C	3.10	130.47	124.68
2	C	501	HEM	C4B-CHC-C1C	3.04	126.57	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4B-CHC-C1C	3.01	126.53	122.56
2	C	501	HEM	CMC-C2C-C3C	2.70	129.74	124.68
2	A	501	HEM	O1A-CGA-CBA	-2.66	114.52	123.08
2	B	501	HEM	C1B-NB-C4B	2.63	107.79	105.07
2	B	501	HEM	CBA-CAA-C2A	2.60	117.06	112.62
2	C	501	HEM	O1A-CGA-CBA	-2.56	114.86	123.08
2	B	501	HEM	CMC-C2C-C3C	2.50	129.35	124.68
2	C	501	HEM	C1B-NB-C4B	2.49	107.65	105.07
2	A	501	HEM	C1B-NB-C4B	2.46	107.61	105.07
2	B	501	HEM	O1A-CGA-CBA	-2.42	115.31	123.08
2	A	501	HEM	CBB-CAB-C3B	-2.39	115.75	127.62
2	A	501	HEM	CMA-C3A-C4A	-2.29	124.95	128.46
2	C	501	HEM	CBB-CAB-C3B	-2.26	116.39	127.62
2	A	501	HEM	CAD-C3D-C4D	2.25	128.59	124.66
2	C	501	HEM	CMA-C3A-C4A	-2.25	125.01	128.46
2	B	501	HEM	CBB-CAB-C3B	-2.24	116.48	127.62
2	B	501	HEM	CMA-C3A-C4A	-2.19	125.10	128.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	16A	C14-C15-C16-N1
3	A	502	16A	C12-C13-C14-C15
3	C	502	16A	C10-C11-C12-C13
2	C	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
3	C	502	16A	C15-C16-N1-C18
3	B	502	16A	C4-C5-C6-C7
2	C	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O2A
3	B	502	16A	C2-C3-C4-C5
3	A	502	16A	C9-C10-C11-C12

There are no ring outliers.

8 monomers are involved in 16 short contacts:

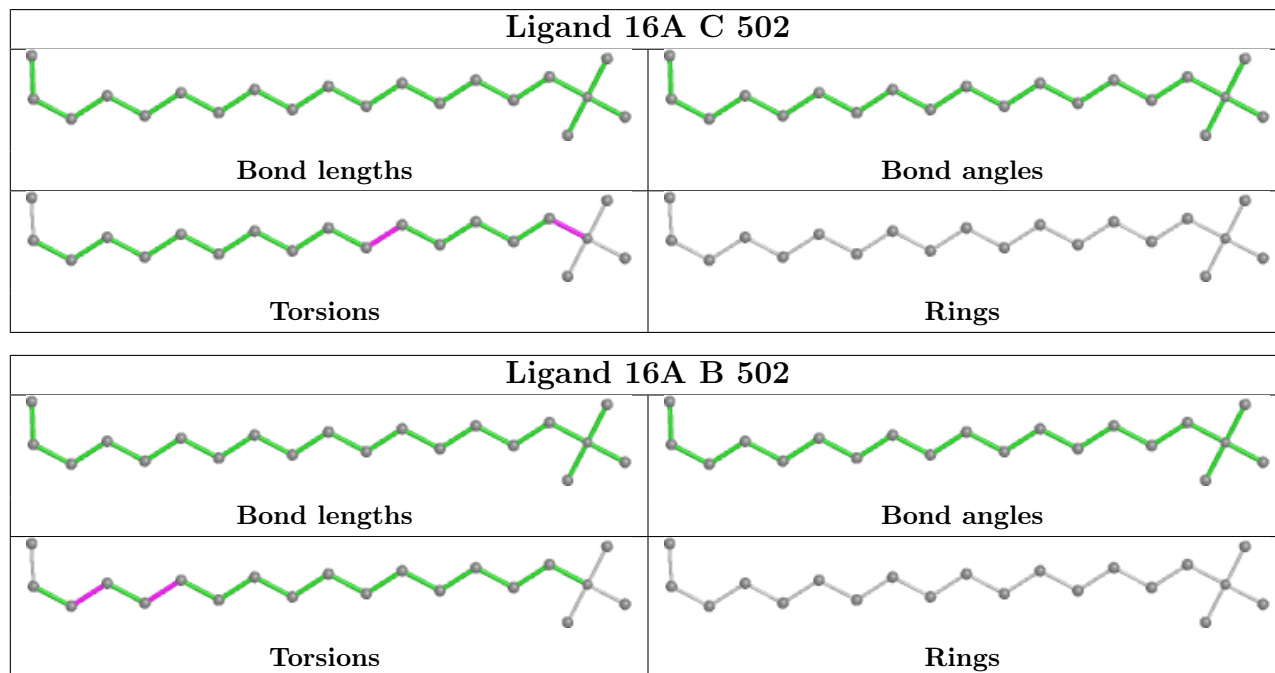
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	IMD	1	0
3	C	502	16A	4	0

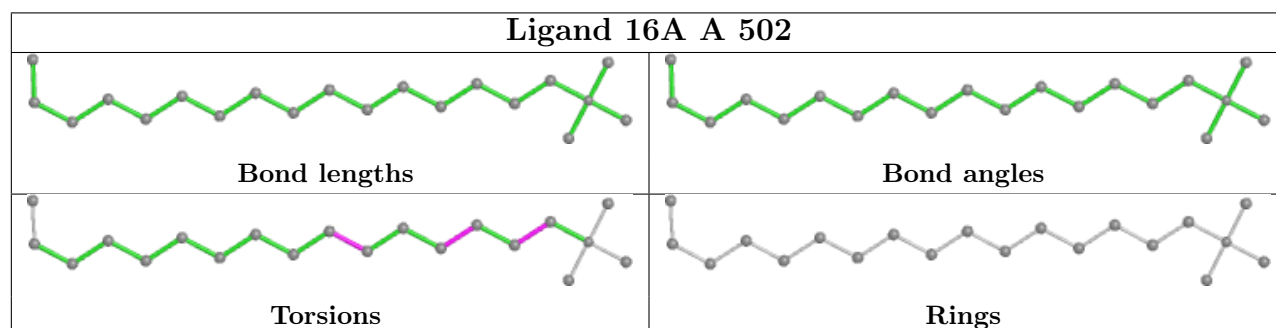
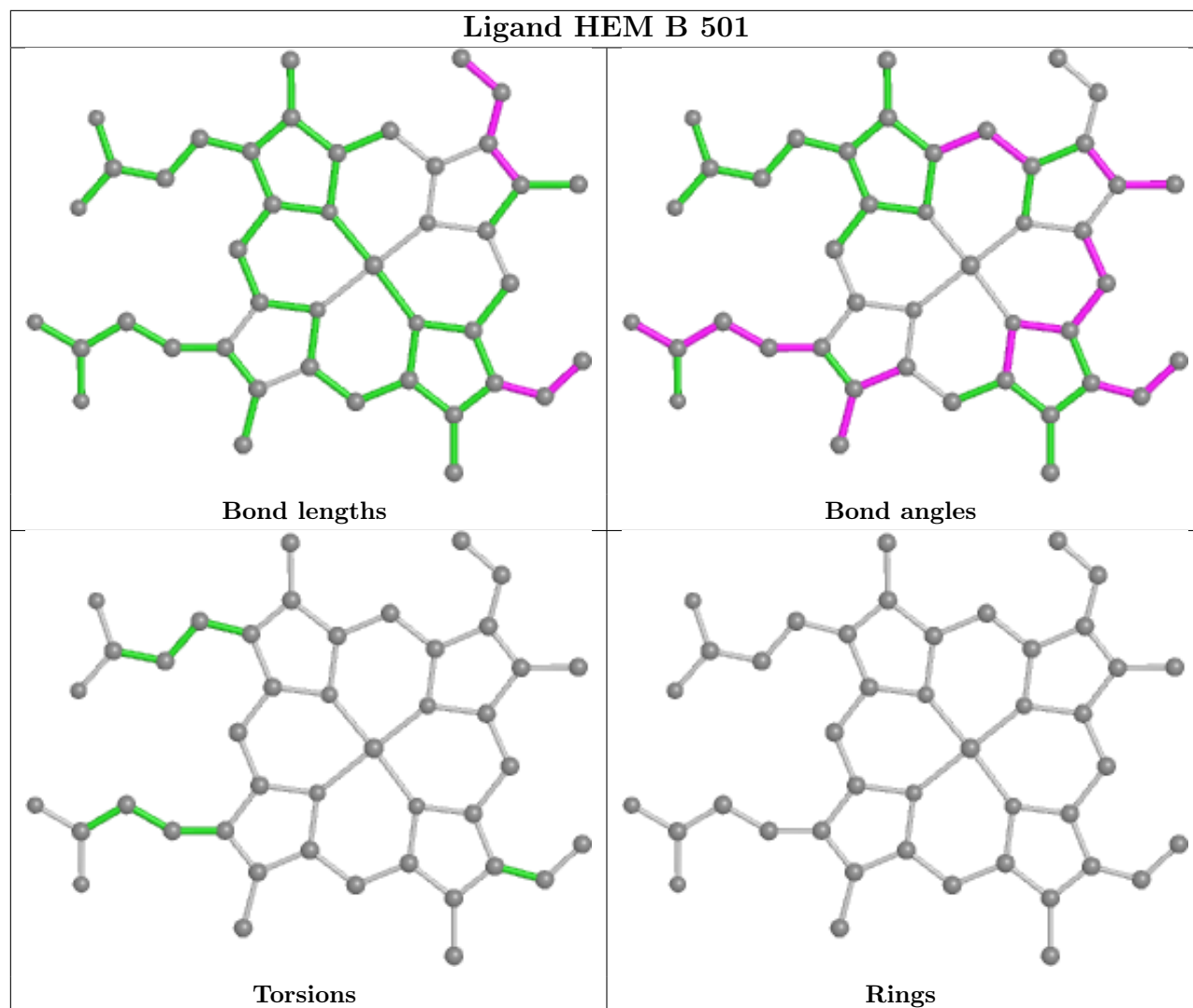
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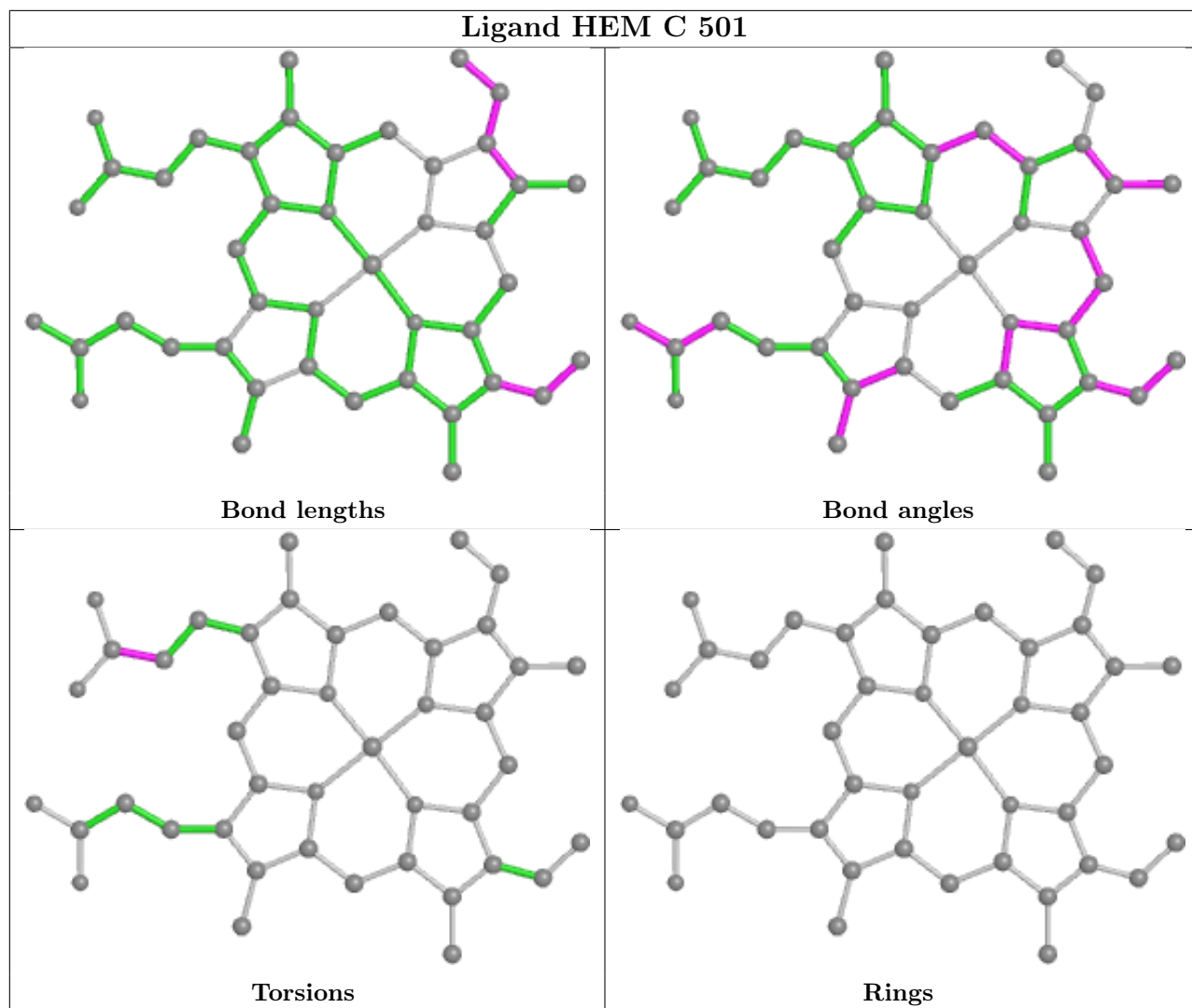
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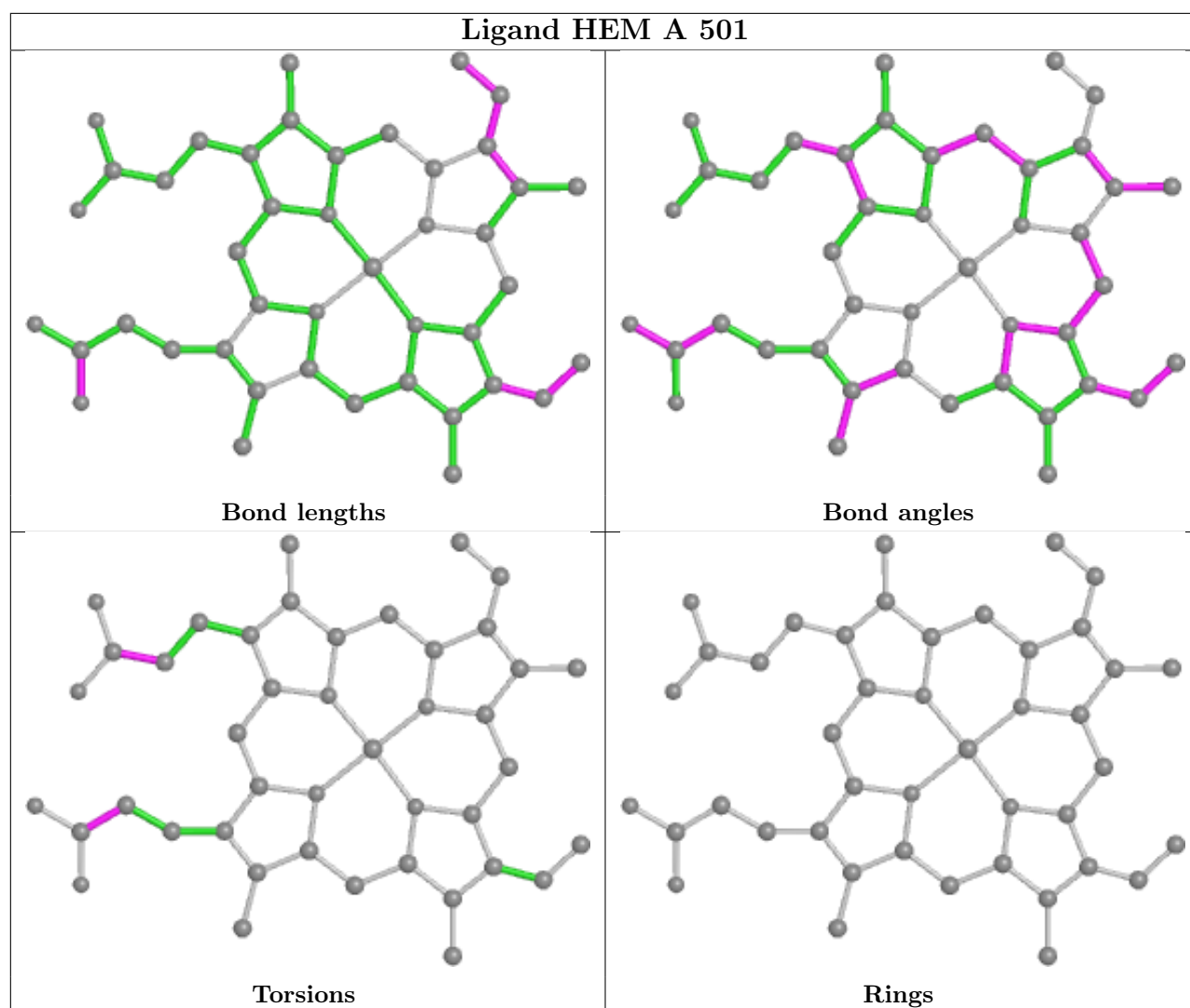
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	16A	2	0
2	B	501	HEM	5	0
3	A	502	16A	3	0
2	C	501	HEM	2	0
4	A	505	IMD	1	0
2	A	501	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	440/450 (97%)	-0.52	1 (0%) 95 87	24, 47, 79, 102	0
1	B	434/450 (96%)	-0.57	2 (0%) 91 75	22, 44, 79, 119	0
1	C	442/450 (98%)	-0.61	0 100 100	21, 39, 71, 91	0
All	All	1316/1350 (97%)	-0.57	3 (0%) 95 87	21, 43, 77, 119	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	ASP	2.7
1	A	225	THR	2.2
1	B	450	ALA	2.1

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	16A	B	502	20/20	0.89	0.33	36,56,75,77	0

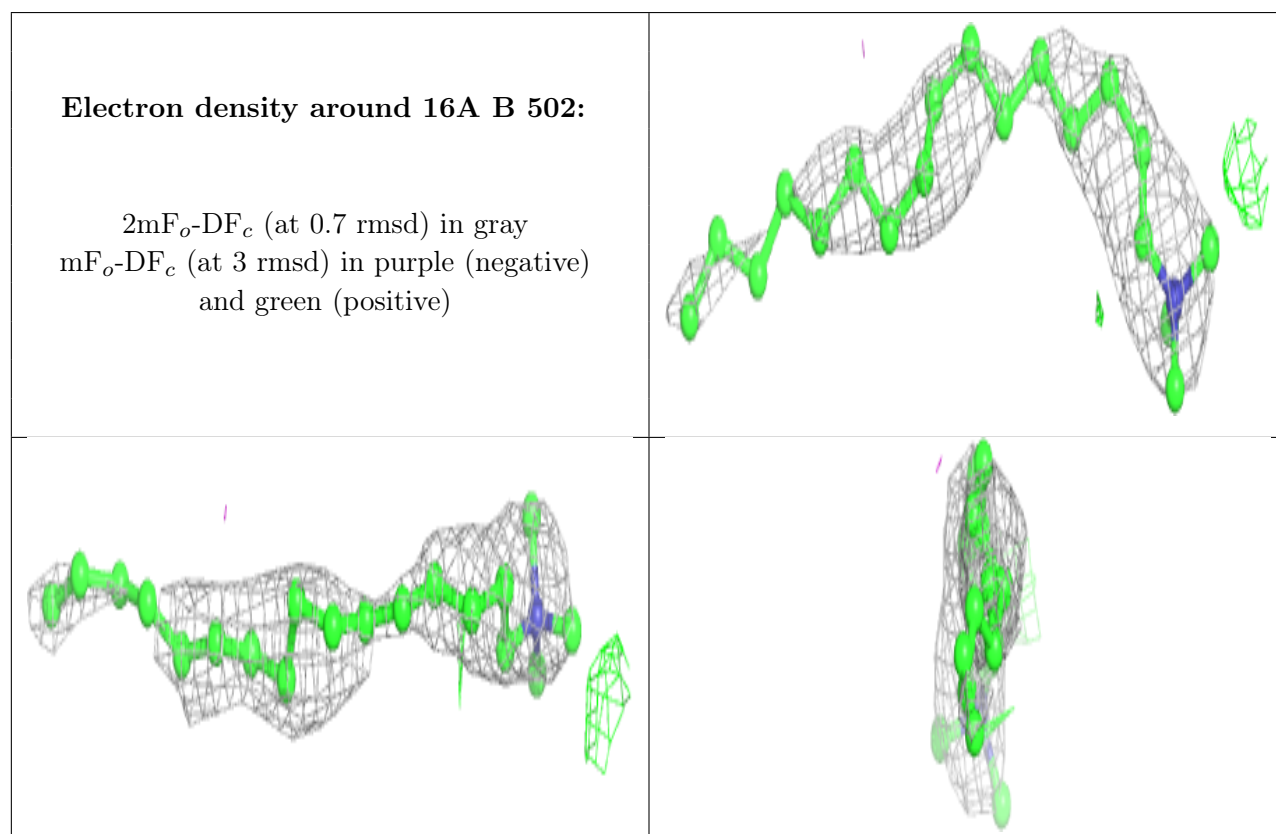
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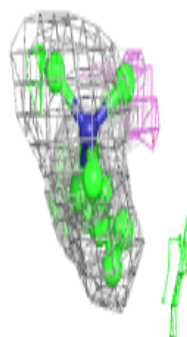
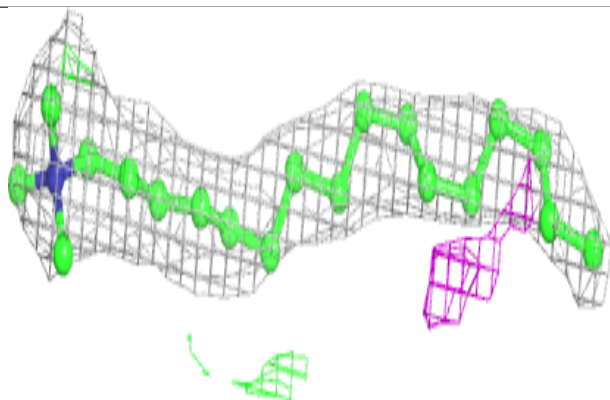
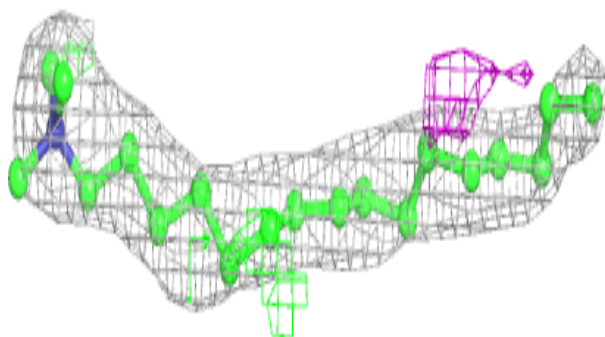
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IMD	A	505	5/5	0.90	0.27	71,73,75,82	0
4	IMD	C	504	5/5	0.91	0.20	64,67,78,83	0
3	16A	C	502	20/20	0.92	0.23	15,35,45,46	0
4	IMD	C	503	5/5	0.92	0.27	24,41,54,59	0
4	IMD	A	504	5/5	0.92	0.21	54,60,65,78	0
3	16A	A	502	20/20	0.95	0.21	29,35,49,50	0
4	IMD	A	503	5/5	0.96	0.17	40,41,42,59	0
2	HEM	B	501	43/43	0.97	0.19	19,31,43,60	0
2	HEM	C	501	43/43	0.97	0.16	18,27,37,48	0
2	HEM	A	501	43/43	0.98	0.19	26,41,52,57	0
4	IMD	B	503	5/5	0.99	0.17	29,38,47,53	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.

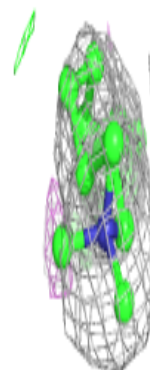
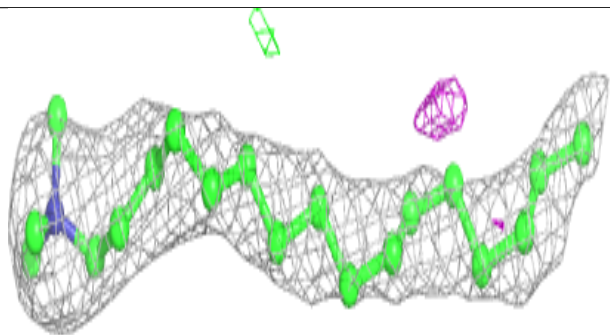
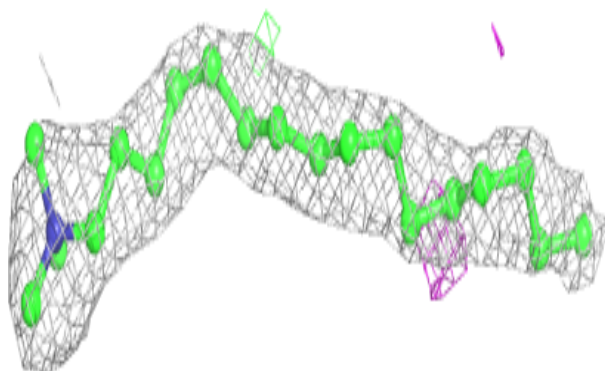


**Electron density around 16A C 502:**

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

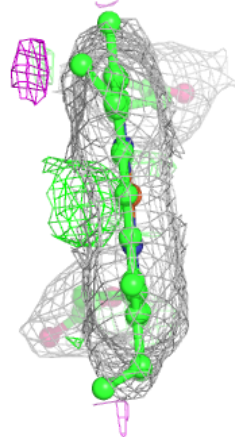
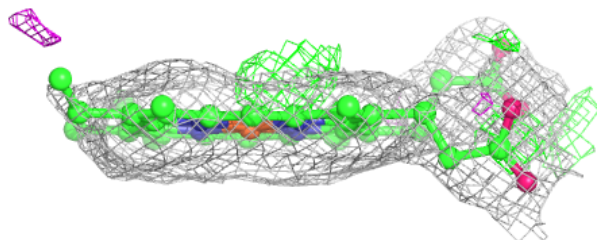
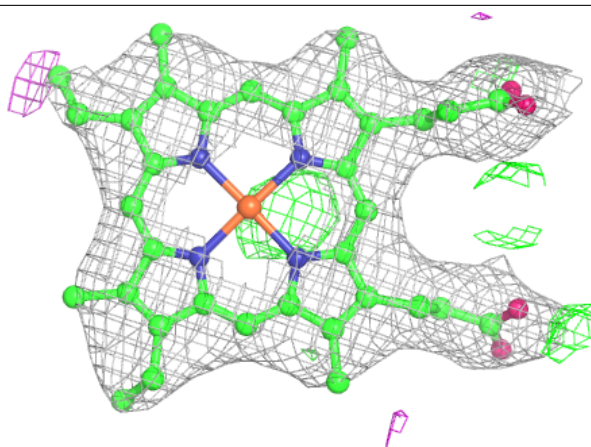
**Electron density around 16A A 502:**

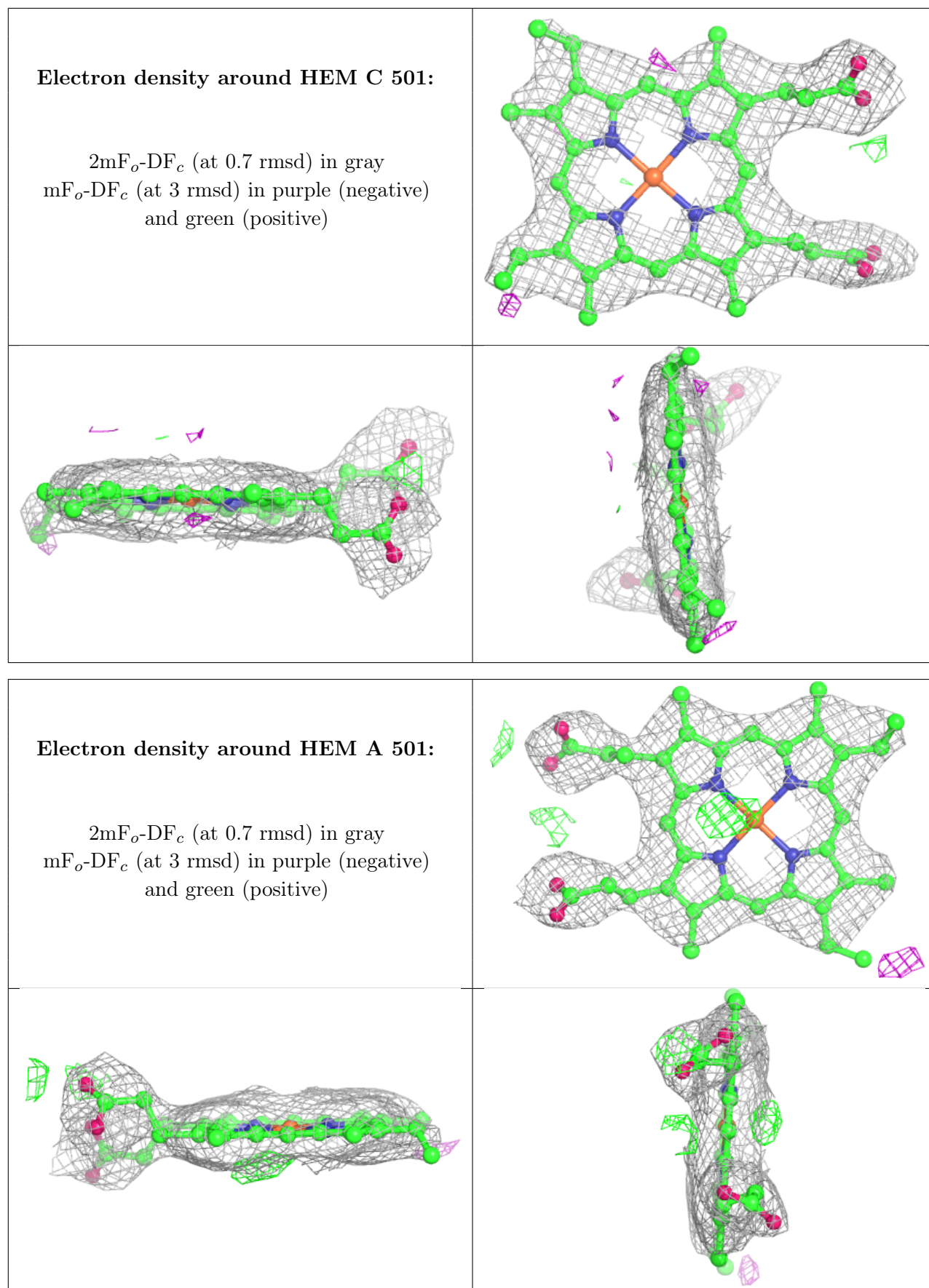
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.