



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:33 pm BST

PDB ID : 4G1B
Title : X-ray structure of yeast flavohemoglobin in complex with econazole
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Deposited on : 2012-07-10
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

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 : 2.11
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) : 2.11

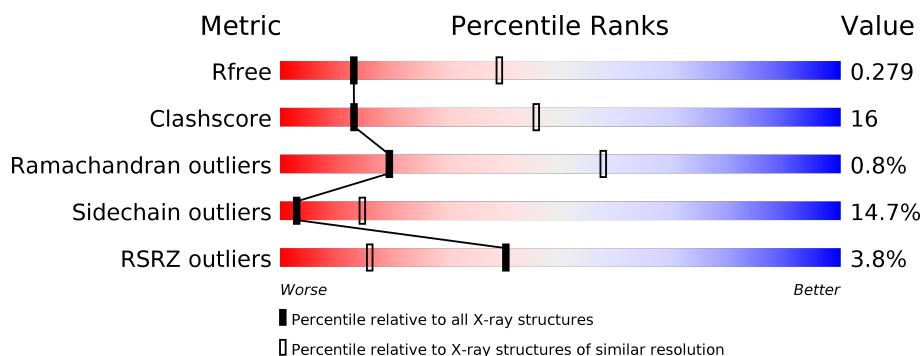
1 Overall quality at a glance

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 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	399	
1	B	399	
1	C	399	
1	D	399	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ECN	A	403	-	-	X	-
4	ECN	C	403	-	-	X	-
4	ECN	D	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13078 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 Flavohemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3123	1999	525	586	13			
1	B	398	Total	C	N	O	S	0	0	0
			3123	1999	525	586	13			
1	C	398	Total	C	N	O	S	0	0	0
			3123	1999	525	586	13			
1	D	398	Total	C	N	O	S	0	0	0
			3123	1999	525	586	13			

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



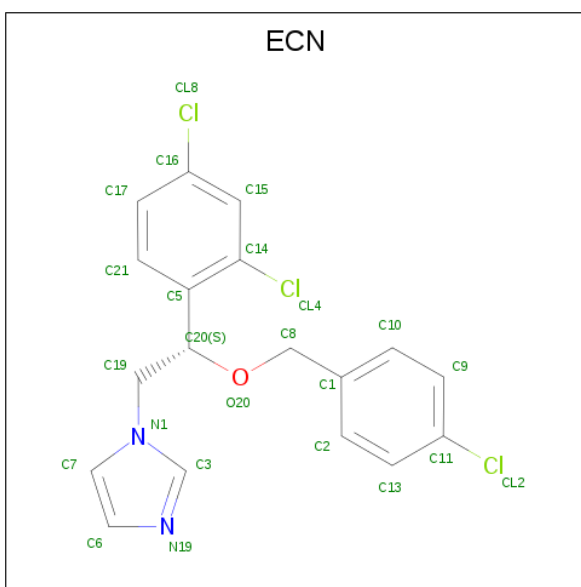
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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

- # FAD

- Molecule 4 is 1-[(2S)-2-[(4-CHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (three-letter code: ECN) (formula: C₁₈H₁₅Cl₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		
4	B	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		
4	C	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		
4	D	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		

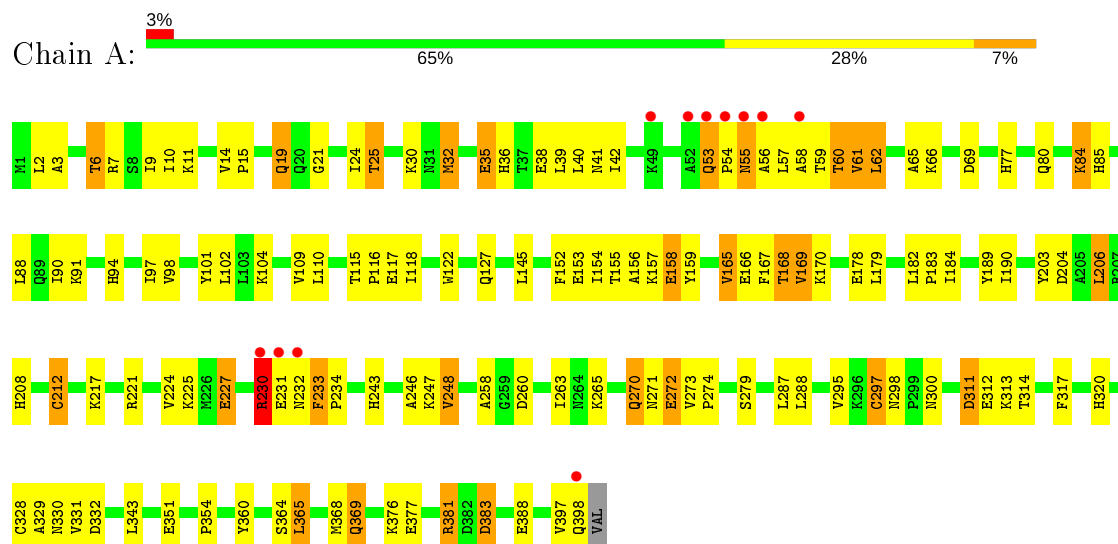
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	34	Total	O	0	0
			34	34		
5	C	19	Total	O	0	0
			19	19		
5	D	10	Total	O	0	0
			10	10		

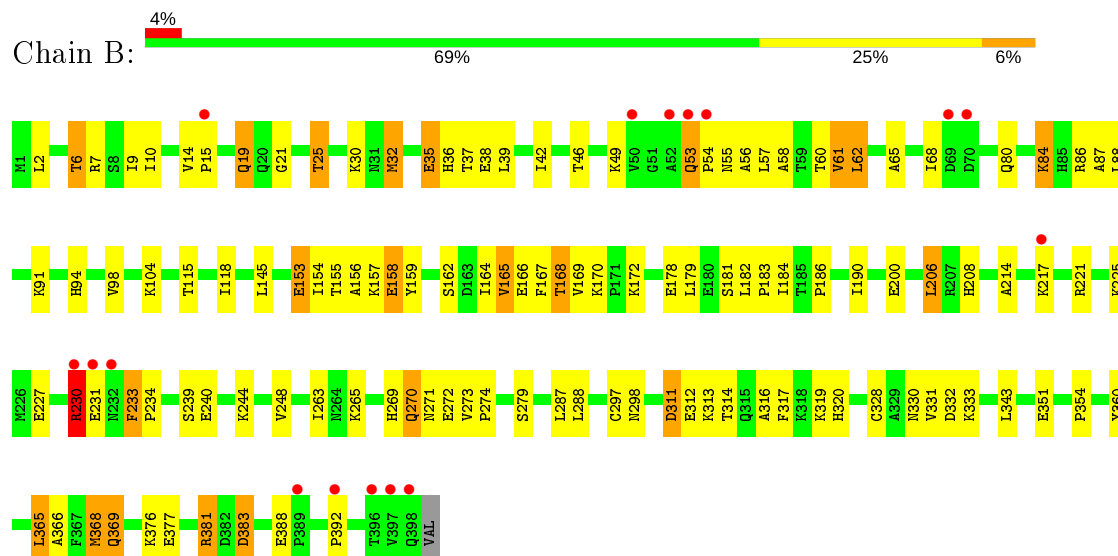
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Flavohemoglobin

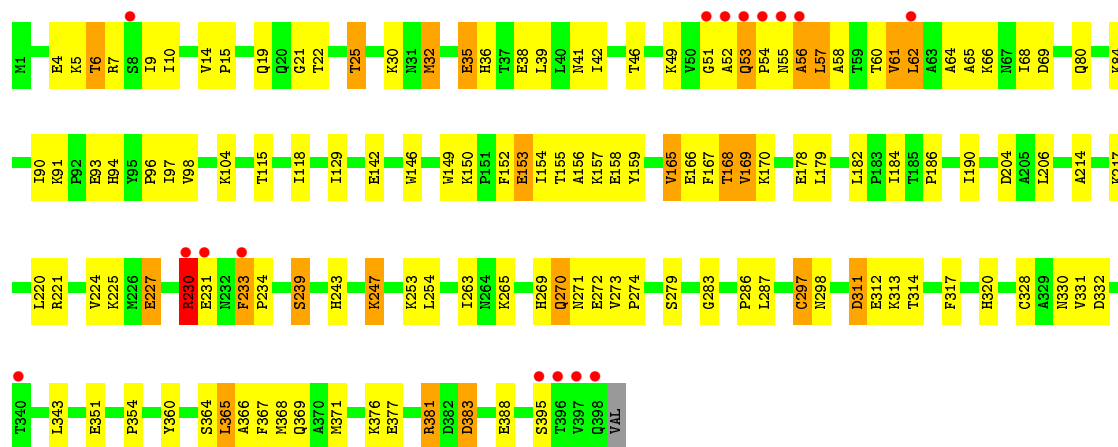


• Molecule 1: Flavohemoglobin

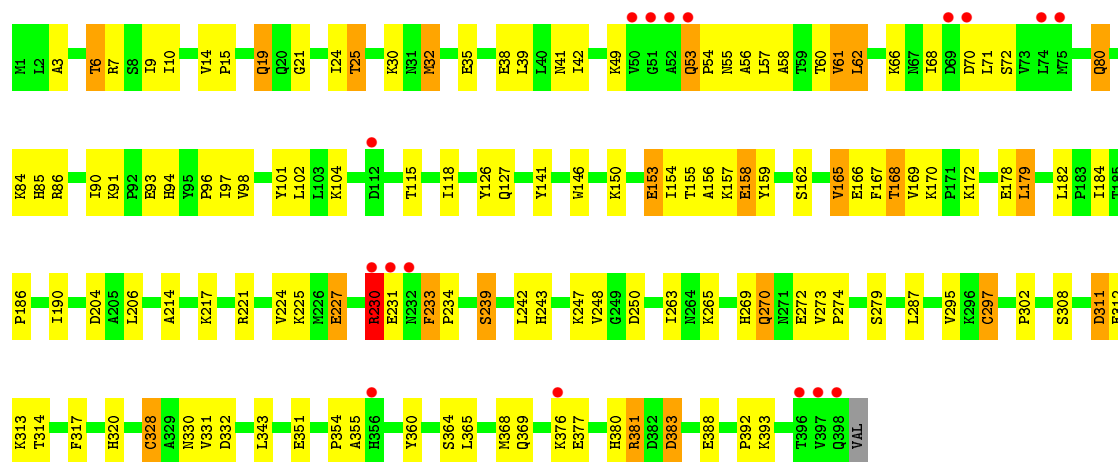


• Molecule 1: Flavohemoglobin





• Molecule 1: Flavohemoglobin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 93.83Å 111.02Å 90.00° 108.22° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.00-3.00) 95.8 (29.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.229 , 0.280 0.230 , 0.279	Depositor DCC
R_{free} test set	2722 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13078	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% 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, FAD, ECN

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	0.76	1/3193 (0.0%)	0.76	1/4337 (0.0%)
1	B	0.69	0/3193	0.72	1/4337 (0.0%)
1	C	0.60	0/3193	0.69	1/4337 (0.0%)
1	D	0.60	0/3193	0.67	1/4337 (0.0%)
All	All	0.67	1/12772 (0.0%)	0.71	4/17348 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	CYS	CB-SG	-5.07	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-CB-CG	6.09	129.31	115.30
1	B	182	LEU	CA-CB-CG	6.05	129.22	115.30
1	D	182	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	182	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3123	0	3124	131	1
1	B	3123	0	3124	96	0
1	C	3123	0	3124	110	2
1	D	3123	0	3124	92	0
2	A	43	0	30	7	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
2	D	43	0	30	9	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
3	C	53	0	31	3	0
3	D	53	0	31	2	0
4	A	24	0	15	17	0
4	B	24	0	15	2	0
4	C	24	0	15	10	0
4	D	24	0	15	7	0
5	A	43	0	0	8	0
5	B	34	0	0	6	1
5	C	19	0	0	8	0
5	D	10	0	0	3	0
All	All	13078	0	12800	421	2

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 16.

All (421) 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:A:57:LEU:HD13	4:A:403:ECN:CL8	1.72	1.24
1:A:57:LEU:HB2	4:A:403:ECN:C15	1.73	1.17
1:A:57:LEU:HD13	4:A:403:ECN:C16	1.79	1.12
1:C:7:ARG:HG2	1:C:68:ILE:HG23	1.30	1.11
1:A:57:LEU:HB2	4:A:403:ECN:H15	1.11	1.09
1:A:60:THR:HB	4:A:403:ECN:H2	1.35	1.08
1:C:69:ASP:OD1	5:C:506:HOH:O	1.75	1.04
1:C:41:ASN:ND2	1:C:204:ASP:H	1.55	1.03
1:C:69:ASP:CG	5:C:506:HOH:O	1.98	1.01
1:A:14:VAL:HG22	1:A:65:ALA:HB1	1.44	0.98
1:C:61:VAL:HA	4:C:403:ECN:CL2	2.03	0.94
1:C:56:ALA:O	1:C:58:ALA:N	2.05	0.90
1:C:41:ASN:HD22	1:C:204:ASP:N	1.69	0.89
1:B:156:ALA:HB3	1:B:168:THR:HG23	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ALA:HB3	1:D:168:THR:HG23	1.57	0.86
1:A:156:ALA:HB3	1:A:168:THR:HG23	1.56	0.85
1:B:233:PHE:HB2	1:B:234:PRO:HD2	1.58	0.85
1:A:25:THR:HB	1:A:57:LEU:HB3	1.57	0.85
1:A:25:THR:HB	1:A:57:LEU:CB	2.06	0.85
1:C:233:PHE:HB2	1:C:234:PRO:HD2	1.59	0.85
1:D:233:PHE:HB2	1:D:234:PRO:HD2	1.57	0.85
1:A:91:LYS:H	1:A:94:HIS:HD2	1.25	0.85
1:A:398:GLN:HB3	5:A:509:HOH:O	1.77	0.84
1:B:270:GLN:HE22	1:B:273:VAL:H	1.26	0.83
1:D:270:GLN:HE22	1:D:273:VAL:H	1.25	0.82
1:C:53:GLN:H	1:C:54:PRO:CD	1.92	0.82
1:D:53:GLN:H	1:D:54:PRO:CD	1.93	0.82
1:B:53:GLN:H	1:B:54:PRO:CD	1.93	0.82
1:B:53:GLN:H	1:B:54:PRO:HD3	1.45	0.82
1:C:69:ASP:HA	5:C:506:HOH:O	1.80	0.81
1:A:77:HIS:CE1	1:A:397:VAL:HG21	2.14	0.81
1:C:41:ASN:HD22	1:C:204:ASP:H	0.84	0.81
1:C:32:MET:CE	1:C:98:VAL:HA	2.10	0.81
1:A:57:LEU:CD1	4:A:403:ECN:CL8	2.61	0.81
1:A:58:ALA:O	1:A:62:LEU:HB2	1.80	0.81
1:B:58:ALA:O	1:B:62:LEU:HB2	1.81	0.81
2:B:401:HEM:HMD2	2:B:401:HEM:HBD2	1.63	0.81
1:C:53:GLN:H	1:C:54:PRO:HD3	1.46	0.81
1:A:53:GLN:H	1:A:54:PRO:CD	1.93	0.81
1:B:91:LYS:H	1:B:94:HIS:HD2	1.27	0.81
1:D:91:LYS:H	1:D:94:HIS:HD2	1.29	0.81
1:D:53:GLN:H	1:D:54:PRO:HD3	1.46	0.80
1:A:233:PHE:HB2	1:A:234:PRO:HD2	1.63	0.80
1:A:3:ALA:O	1:A:7:ARG:HB2	1.81	0.80
1:C:58:ALA:O	1:C:62:LEU:HB2	1.82	0.79
1:C:7:ARG:HG2	1:C:68:ILE:CG2	2.11	0.79
1:A:168:THR:HG22	5:A:522:HOH:O	1.81	0.79
1:A:53:GLN:H	1:A:54:PRO:HD3	1.48	0.79
1:D:58:ALA:O	1:D:62:LEU:HB2	1.83	0.79
1:C:91:LYS:H	1:C:94:HIS:HD2	1.31	0.78
1:D:32:MET:CE	1:D:98:VAL:HA	2.13	0.78
1:C:61:VAL:HG23	4:C:403:ECN:CL2	2.21	0.78
1:A:329:ALA:HB1	1:B:181:SER:CB	2.14	0.77
1:A:270:GLN:HE22	1:A:273:VAL:H	1.32	0.77
1:A:157:LYS:HD2	1:A:167:PHE:CE1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ALA:HB3	1:C:168:THR:HG23	1.67	0.76
1:C:61:VAL:CG2	4:C:403:ECN:CL2	2.70	0.76
1:C:7:ARG:CG	1:C:68:ILE:HG23	2.13	0.76
1:A:60:THR:HB	4:A:403:ECN:C2	2.15	0.76
1:A:55:ASN:O	1:A:59:THR:N	2.18	0.76
1:C:270:GLN:HE22	1:C:273:VAL:H	1.31	0.76
1:C:64:ALA:HB1	1:C:129:ILE:HD11	1.67	0.76
1:A:14:VAL:CG2	1:A:65:ALA:HB1	2.14	0.75
1:C:22:THR:HG23	1:C:54:PRO:O	1.86	0.75
1:B:158:GLU:CG	1:C:158:GLU:HG3	2.16	0.75
1:C:57:LEU:HD13	4:C:403:ECN:CL8	2.22	0.75
1:B:159:TYR:CE1	1:B:165:VAL:HG13	2.22	0.75
1:A:300:ASN:OD1	1:B:183:PRO:HA	1.86	0.74
1:D:311:ASP:HB2	1:D:314:THR:HG23	1.69	0.74
2:A:401:HEM:HBD2	2:A:401:HEM:HMD1	1.70	0.74
1:B:158:GLU:HG3	1:C:158:GLU:HG3	1.68	0.74
1:A:32:MET:CE	1:A:98:VAL:HA	2.19	0.73
1:B:158:GLU:HG3	1:C:158:GLU:CG	2.21	0.71
1:C:157:LYS:HD2	1:C:167:PHE:CE1	2.25	0.71
1:C:21:GLY:O	1:C:25:THR:HG22	1.90	0.71
1:A:57:LEU:CD1	4:A:403:ECN:C16	2.67	0.70
1:A:311:ASP:HB2	1:A:314:THR:HG23	1.72	0.70
1:D:233:PHE:HB2	1:D:234:PRO:CD	2.20	0.70
1:D:159:TYR:CE1	1:D:165:VAL:HG13	2.26	0.70
1:B:279:SER:HB3	1:B:287:LEU:HD12	1.74	0.70
1:C:152:PHE:CD1	1:C:169:VAL:HG13	2.27	0.70
1:B:21:GLY:O	1:B:25:THR:HG22	1.92	0.70
1:C:142:GLU:O	5:C:511:HOH:O	2.10	0.69
1:A:57:LEU:CB	4:A:403:ECN:H15	2.06	0.69
1:B:233:PHE:HB2	1:B:234:PRO:CD	2.21	0.69
1:A:297:CYS:SG	1:B:269:HIS:NE2	2.66	0.69
2:C:401:HEM:HBD2	2:C:401:HEM:HMD2	1.75	0.69
1:A:21:GLY:O	1:A:25:THR:HG22	1.94	0.68
1:C:53:GLN:HA	1:C:56:ALA:HB2	1.75	0.68
2:D:401:HEM:HMD2	2:D:401:HEM:HBD2	1.74	0.68
1:C:32:MET:HE3	1:C:98:VAL:HA	1.76	0.68
1:D:279:SER:HB3	1:D:287:LEU:HD12	1.74	0.67
1:B:32:MET:CE	1:B:98:VAL:HA	2.24	0.67
1:D:6:THR:O	1:D:10:ILE:HG12	1.95	0.67
1:B:145:LEU:HD22	1:B:183:PRO:HD2	1.75	0.67
1:C:153:GLU:O	1:C:169:VAL:HA	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:403:ECN:C5	4:C:403:ECN:H10	2.25	0.67
1:A:57:LEU:CB	4:A:403:ECN:C15	2.64	0.66
1:C:233:PHE:HB2	1:C:234:PRO:CD	2.24	0.66
1:C:311:ASP:HB2	1:C:314:THR:HG23	1.76	0.66
1:A:329:ALA:CB	1:B:181:SER:HA	2.25	0.66
1:B:311:ASP:HB2	1:B:314:THR:HG23	1.77	0.66
1:D:157:LYS:HD2	1:D:167:PHE:CE1	2.31	0.66
1:C:7:ARG:NE	5:C:506:HOH:O	2.11	0.66
1:B:6:THR:O	1:B:10:ILE:HG12	1.96	0.65
1:A:88:LEU:HD22	1:A:206:LEU:HD23	1.79	0.65
1:B:61:VAL:HG23	4:B:403:ECN:H13	1.78	0.65
1:C:154:ILE:HD13	1:C:167:PHE:CD1	2.31	0.65
1:B:162:SER:O	1:C:247:LYS:HD2	1.95	0.65
1:A:53:GLN:HA	1:A:56:ALA:HB2	1.78	0.65
1:A:297:CYS:SG	1:B:269:HIS:CE1	2.90	0.65
1:C:6:THR:O	1:C:10:ILE:HG12	1.96	0.65
1:A:159:TYR:CE1	1:A:165:VAL:HG13	2.32	0.64
1:B:263:ILE:HA	1:B:360:TYR:CE1	2.33	0.64
1:C:159:TYR:CE1	1:C:165:VAL:HG13	2.32	0.64
1:A:233:PHE:HB2	1:A:234:PRO:CD	2.26	0.64
1:A:158:GLU:HG3	1:D:158:GLU:CG	2.28	0.64
1:A:279:SER:HB3	1:A:287:LEU:HD12	1.78	0.64
1:C:41:ASN:ND2	1:C:204:ASP:N	2.38	0.64
1:C:227:GLU:HG3	3:C:402:FAD:O3B	1.99	0.63
1:A:158:GLU:CG	1:D:158:GLU:HG3	2.29	0.63
1:C:317:PHE:HD1	1:C:320:HIS:CD2	2.17	0.62
1:D:32:MET:HE3	1:D:98:VAL:HA	1.81	0.61
1:C:279:SER:HB3	1:C:287:LEU:HD12	1.82	0.61
1:A:329:ALA:HB1	1:B:181:SER:HA	1.82	0.61
1:B:53:GLN:N	1:B:54:PRO:CD	2.64	0.60
1:D:190:ILE:C	1:D:190:ILE:HD12	2.22	0.60
2:A:401:HEM:HBD2	2:A:401:HEM:CMD	2.29	0.60
1:C:154:ILE:HD13	1:C:167:PHE:CE1	2.35	0.60
1:D:102:LEU:HD13	4:D:403:ECN:H17	1.83	0.60
1:D:53:GLN:N	1:D:54:PRO:CD	2.64	0.60
1:C:57:LEU:HB2	4:C:403:ECN:H15	1.83	0.59
1:A:329:ALA:HB1	1:B:181:SER:CA	2.32	0.59
1:A:53:GLN:N	1:A:54:PRO:CD	2.65	0.59
1:A:247:LYS:HD2	1:D:162:SER:O	2.02	0.59
1:C:149:TRP:HB3	1:C:253:LYS:HB3	1.82	0.59
1:D:263:ILE:HA	1:D:360:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:THR:HB	4:D:403:ECN:H15	1.85	0.59
1:A:317:PHE:HD1	1:A:320:HIS:CD2	2.21	0.58
1:A:156:ALA:HB3	1:A:168:THR:CG2	2.29	0.58
3:A:402:FAD:H8A	5:A:508:HOH:O	2.03	0.58
1:A:166:GLU:OE1	1:A:221:ARG:NH1	2.36	0.58
1:B:381:ARG:NH1	1:B:383:ASP:HB2	2.19	0.58
1:A:25:THR:CB	1:A:57:LEU:HB3	2.33	0.57
2:C:401:HEM:CAB	4:C:403:ECN:H2	2.34	0.57
1:C:53:GLN:N	1:C:54:PRO:CD	2.64	0.57
1:A:57:LEU:HD13	4:A:403:ECN:C15	2.34	0.57
1:B:157:LYS:HD2	1:B:167:PHE:CE1	2.39	0.57
1:C:90:ILE:HD12	2:C:401:HEM:HAC	1.87	0.57
1:D:153:GLU:HG3	1:D:172:LYS:HE3	1.86	0.57
1:D:166:GLU:OE1	1:D:221:ARG:NH1	2.38	0.57
1:A:25:THR:HB	1:A:57:LEU:HB2	1.86	0.57
1:D:381:ARG:NH1	1:D:383:ASP:HB2	2.20	0.57
1:D:392:PRO:HA	2:D:401:HEM:O2A	2.05	0.57
1:A:10:ILE:O	1:A:14:VAL:HG23	2.05	0.57
1:D:317:PHE:HD1	1:D:320:HIS:CD2	2.23	0.56
1:D:41:ASN:HD22	1:D:204:ASP:H	1.54	0.56
1:B:156:ALA:HB3	1:B:168:THR:CG2	2.32	0.56
1:A:227:GLU:HG3	3:A:402:FAD:O3B	2.05	0.56
1:A:11:LYS:NZ	1:A:69:ASP:OD2	2.33	0.56
1:C:10:ILE:O	1:C:14:VAL:HG23	2.06	0.56
1:A:381:ARG:NH1	1:A:383:ASP:HB2	2.21	0.56
1:A:6:THR:O	1:A:10:ILE:HG12	2.05	0.55
1:C:263:ILE:HA	1:C:360:TYR:CE1	2.41	0.55
1:B:14:VAL:HG21	1:B:65:ALA:HB1	1.88	0.55
1:D:10:ILE:O	1:D:14:VAL:HG23	2.07	0.55
1:D:227:GLU:HG3	3:D:402:FAD:O3B	2.07	0.55
1:B:10:ILE:O	1:B:14:VAL:HG23	2.07	0.55
1:C:224:VAL:O	1:C:243:HIS:HE1	1.89	0.55
1:A:158:GLU:HG2	1:D:158:GLU:HG3	1.89	0.55
1:A:85:HIS:HE1	2:A:401:HEM:NB	2.05	0.55
1:B:190:ILE:HD12	1:B:190:ILE:C	2.27	0.55
1:B:53:GLN:HA	1:B:56:ALA:HB2	1.88	0.55
1:D:53:GLN:HA	1:D:56:ALA:HB2	1.89	0.55
1:B:154:ILE:HG22	1:B:248:VAL:HA	1.89	0.55
1:D:3:ALA:HB3	1:D:6:THR:HG23	1.90	0.54
1:A:224:VAL:O	1:A:243:HIS:HE1	1.90	0.54
4:A:403:ECN:H21	4:A:403:ECN:H10	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HB	4:B:403:ECN:H15	1.89	0.54
1:C:61:VAL:CA	4:C:403:ECN:CL2	2.85	0.54
1:C:155:THR:HG21	1:C:170:LYS:HD2	1.90	0.54
1:C:69:ASP:CA	5:C:506:HOH:O	2.42	0.54
1:A:42:ILE:CG2	2:A:401:HEM:HMD2	2.38	0.54
1:B:186:PRO:HG3	1:B:214:ALA:HB2	1.90	0.54
1:B:166:GLU:OE1	1:B:221:ARG:NH1	2.40	0.53
1:C:297:CYS:SG	1:D:269:HIS:CE1	3.01	0.53
1:A:116:PRO:N	5:A:518:HOH:O	2.41	0.53
1:D:61:VAL:HG23	4:D:403:ECN:H13	1.90	0.53
1:D:7:ARG:HG2	1:D:68:ILE:HG23	1.91	0.53
1:B:168:THR:HG22	5:B:524:HOH:O	2.09	0.53
1:C:381:ARG:NH1	1:C:383:ASP:HB2	2.23	0.53
1:D:93:GLU:O	1:D:96:PRO:HD2	2.09	0.53
1:C:14:VAL:HG11	1:C:62:LEU:HD23	1.90	0.53
1:D:355:ALA:HA	5:D:504:HOH:O	2.07	0.53
1:A:155:THR:HG21	1:A:170:LYS:HD2	1.91	0.53
1:A:168:THR:HB	1:A:221:ARG:HG2	1.91	0.53
1:A:271:ASN:ND2	1:A:298:ASN:HD21	2.07	0.53
1:D:159:TYR:CD1	1:D:165:VAL:HG13	2.44	0.53
1:B:7:ARG:HG2	1:B:68:ILE:HG23	1.91	0.52
1:C:269:HIS:CE1	1:D:297:CYS:SG	3.03	0.52
1:B:227:GLU:HG3	3:B:402:FAD:O3B	2.09	0.52
1:D:21:GLY:O	1:D:25:THR:HG22	2.09	0.52
1:A:270:GLN:NE2	1:A:272:GLU:H	2.07	0.52
1:A:6:THR:HA	1:A:9:ILE:HD12	1.91	0.52
1:C:168:THR:HB	1:C:221:ARG:HG2	1.92	0.52
1:B:21:GLY:HA2	1:B:57:LEU:HD23	1.92	0.52
1:A:102:LEU:HD13	4:A:403:ECN:H17	1.92	0.52
1:D:90:ILE:HD12	2:D:401:HEM:HAC	1.90	0.52
1:A:263:ILE:HA	1:A:360:TYR:CE1	2.45	0.52
1:A:62:LEU:HD22	1:A:66:LYS:HD2	1.92	0.52
1:B:368:MET:HE2	1:B:368:MET:HA	1.90	0.52
1:C:166:GLU:OE1	1:C:221:ARG:NH1	2.39	0.52
1:A:190:ILE:C	1:A:190:ILE:HD12	2.30	0.51
1:B:84:LYS:HD3	1:B:208:HIS:HE2	1.75	0.51
1:B:333:LYS:HE3	5:B:516:HOH:O	2.10	0.51
1:A:329:ALA:HB1	1:B:181:SER:HB3	1.93	0.51
1:A:90:ILE:HD12	2:A:401:HEM:HAC	1.93	0.51
1:C:52:ALA:CB	1:C:395:SER:HB3	2.41	0.51
1:D:71:LEU:N	5:D:505:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:O	1:D:243:HIS:HE1	1.93	0.51
1:A:117:GLU:N	5:A:518:HOH:O	2.33	0.51
1:D:380:HIS:CE1	5:D:504:HOH:O	2.65	0.51
1:C:190:ILE:C	1:C:190:ILE:HD12	2.31	0.50
1:A:158:GLU:HG3	1:D:158:GLU:HG2	1.93	0.50
1:B:392:PRO:HA	2:B:401:HEM:O2A	2.12	0.50
1:C:61:VAL:HG22	4:C:403:ECN:CL2	2.47	0.50
1:A:329:ALA:CB	1:B:181:SER:CA	2.89	0.50
1:A:329:ALA:HB2	1:B:181:SER:HA	1.93	0.50
1:A:77:HIS:HE1	1:A:397:VAL:HG21	1.72	0.50
1:C:69:ASP:CB	5:C:506:HOH:O	2.47	0.50
1:D:91:LYS:H	1:D:94:HIS:CD2	2.20	0.50
1:A:158:GLU:CG	1:D:158:GLU:CG	2.90	0.49
1:B:311:ASP:HB3	1:B:314:THR:H	1.77	0.49
2:B:401:HEM:CMD	2:B:401:HEM:HBD2	2.37	0.49
1:A:115:THR:OG1	1:A:118:ILE:HG12	2.13	0.49
1:A:60:THR:CB	4:A:403:ECN:H2	2.24	0.49
1:C:231:GLU:HG3	1:C:231:GLU:O	2.13	0.49
1:A:85:HIS:HE1	2:A:401:HEM:C4B	2.31	0.49
1:C:170:LYS:HG2	1:C:179:LEU:HD11	1.95	0.49
1:B:14:VAL:N	1:B:15:PRO:CD	2.76	0.49
1:A:57:LEU:O	1:A:61:VAL:HB	2.13	0.48
1:C:42:ILE:HG22	2:C:401:HEM:HMD1	1.95	0.48
1:D:115:THR:OG1	1:D:118:ILE:HG12	2.13	0.48
1:D:230:ARG:NE	1:D:230:ARG:HA	2.28	0.48
1:B:270:GLN:NE2	5:B:529:HOH:O	2.37	0.48
1:B:383:ASP:N	1:B:383:ASP:OD1	2.46	0.48
1:A:42:ILE:HG22	2:A:401:HEM:HMD2	1.96	0.48
1:D:393:LYS:N	2:D:401:HEM:O2A	2.46	0.48
1:D:6:THR:HA	1:D:9:ILE:HD12	1.95	0.48
1:A:145:LEU:HD22	1:A:183:PRO:HD2	1.96	0.48
1:A:368:MET:HA	1:A:368:MET:CE	2.43	0.48
1:B:159:TYR:CD1	1:B:165:VAL:HG13	2.47	0.48
1:C:150:LYS:O	1:C:253:LYS:HA	2.14	0.48
1:A:32:MET:HE3	1:A:98:VAL:HA	1.95	0.48
1:B:115:THR:OG1	1:B:118:ILE:HG12	2.13	0.48
1:C:4:GLU:O	1:C:5:LYS:CB	2.61	0.48
1:A:230:ARG:NE	1:A:230:ARG:HA	2.29	0.48
1:A:57:LEU:N	4:A:403:ECN:CL4	2.84	0.48
1:C:21:GLY:HA2	1:C:57:LEU:HD23	1.96	0.48
1:B:14:VAL:CG2	1:B:65:ALA:HB1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD22	1:B:206:LEU:HD23	1.95	0.48
1:C:271:ASN:ND2	1:C:298:ASN:HD21	2.12	0.48
1:B:153:GLU:HG3	1:B:172:LYS:HE3	1.96	0.47
1:C:10:ILE:HG22	1:C:65:ALA:HB1	1.95	0.47
1:D:170:LYS:HG2	1:D:179:LEU:HD11	1.95	0.47
1:B:157:LYS:HB3	1:C:159:TYR:CD2	2.49	0.47
1:B:91:LYS:H	1:B:94:HIS:CD2	2.19	0.47
1:A:94:HIS:HA	1:A:97:ILE:HD12	1.95	0.47
1:B:230:ARG:NE	1:B:230:ARG:HA	2.29	0.47
1:A:116:PRO:HB2	5:A:518:HOH:O	2.13	0.47
1:C:230:ARG:NE	1:C:230:ARG:HA	2.30	0.47
1:A:91:LYS:H	1:A:94:HIS:CD2	2.16	0.47
1:B:231:GLU:O	1:B:231:GLU:HG3	2.15	0.47
1:A:2:LEU:O	1:A:7:ARG:NH1	2.38	0.47
1:A:231:GLU:O	1:A:231:GLU:HG3	2.14	0.47
1:D:7:ARG:HG2	1:D:68:ILE:CG2	2.45	0.47
1:A:56:ALA:HA	1:A:59:THR:HB	1.97	0.47
1:B:155:THR:HG21	1:B:170:LYS:HD2	1.97	0.47
1:D:186:PRO:HG3	1:D:214:ALA:HB2	1.97	0.46
1:B:164:ILE:HD12	1:B:316:ALA:HB2	1.97	0.46
1:C:94:HIS:HA	1:C:97:ILE:HD12	1.97	0.46
1:D:274:PRO:HG3	1:D:354:PRO:HG2	1.96	0.46
1:A:109:VAL:HG12	1:A:110:LEU:HD12	1.97	0.46
1:D:311:ASP:HB3	1:D:314:THR:H	1.80	0.46
1:A:165:VAL:HG22	1:A:243:HIS:CE1	2.51	0.46
1:C:115:THR:OG1	1:C:118:ILE:HG12	2.15	0.46
1:D:155:THR:HG21	1:D:170:LYS:HD2	1.98	0.46
1:A:41:ASN:HD22	1:A:204:ASP:H	1.63	0.46
1:D:19:GLN:HE21	1:D:19:GLN:HB3	1.52	0.46
1:D:231:GLU:HG3	1:D:231:GLU:O	2.16	0.46
1:A:159:TYR:CD1	1:A:165:VAL:HG13	2.49	0.46
1:B:42:ILE:HG22	2:B:401:HEM:HMD1	1.98	0.46
1:B:288:LEU:HG	5:B:518:HOH:O	2.16	0.46
1:A:32:MET:HG3	1:A:101:TYR:CD2	2.51	0.46
1:B:317:PHE:HD1	1:B:320:HIS:CD2	2.34	0.46
1:C:283:GLY:O	1:C:286:PRO:HD2	2.16	0.46
1:D:224:VAL:HG21	1:D:242:LEU:HD13	1.97	0.46
1:D:24:ILE:HG22	4:D:403:ECN:CL8	2.53	0.46
1:A:189:TYR:CE1	1:A:258:ALA:HB3	2.50	0.45
1:D:14:VAL:N	1:D:15:PRO:CD	2.79	0.45
1:D:156:ALA:HB3	1:D:168:THR:CG2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HG2	1:A:179:LEU:HD11	1.98	0.45
1:C:35:GLU:HB3	1:C:36:HIS:HD2	1.80	0.45
1:D:146:TRP:CD1	1:D:150:LYS:HG3	2.52	0.45
1:A:274:PRO:HG3	1:A:354:PRO:HG2	1.98	0.45
1:D:41:ASN:ND2	1:D:204:ASP:H	2.15	0.45
1:D:270:GLN:HE22	1:D:273:VAL:N	2.04	0.45
1:D:311:ASP:CB	1:D:314:THR:HG23	2.45	0.45
2:D:401:HEM:CBD	2:D:401:HEM:HMD2	2.46	0.45
1:A:271:ASN:HD21	1:A:298:ASN:HD21	1.65	0.45
1:D:247:LYS:O	1:D:250:ASP:HB2	2.16	0.45
1:A:368:MET:HA	1:A:368:MET:HE2	1.97	0.45
1:A:260:ASP:OD2	5:A:539:HOH:O	2.21	0.45
1:A:295:VAL:HG22	1:A:328:CYS:SG	2.57	0.45
1:B:6:THR:HA	1:B:9:ILE:HD12	1.98	0.45
1:D:42:ILE:HG22	2:D:401:HEM:HMD1	1.99	0.45
1:A:19:GLN:HB3	1:A:19:GLN:HE21	1.55	0.45
2:B:401:HEM:HMD2	2:B:401:HEM:CBD	2.40	0.45
1:C:274:PRO:HG3	1:C:354:PRO:HG2	1.99	0.45
1:C:64:ALA:HB1	1:C:129:ILE:CD1	2.42	0.45
1:B:32:MET:HE3	1:B:98:VAL:HA	1.98	0.45
1:B:57:LEU:O	1:B:61:VAL:HB	2.17	0.44
1:C:159:TYR:CD1	1:C:165:VAL:HG13	2.52	0.44
1:B:14:VAL:HG21	1:B:65:ALA:CB	2.47	0.44
1:B:200:GLU:N	5:B:520:HOH:O	2.11	0.44
1:D:94:HIS:HA	1:D:97:ILE:HD12	1.98	0.44
1:A:116:PRO:CB	5:A:518:HOH:O	2.66	0.44
1:A:65:ALA:HB2	1:A:122:TRP:HH2	1.82	0.44
1:A:14:VAL:N	1:A:15:PRO:CD	2.80	0.44
1:A:152:PHE:CD1	1:A:169:VAL:HG13	2.53	0.44
1:C:186:PRO:HG3	1:C:214:ALA:HB2	1.98	0.44
1:C:93:GLU:O	1:C:96:PRO:HD2	2.17	0.44
1:A:232:ASN:HB3	1:A:233:PHE:H	1.65	0.44
1:B:271:ASN:ND2	1:B:298:ASN:HD21	2.15	0.44
1:D:80:GLN:OE1	1:D:393:LYS:HD3	2.18	0.44
1:C:169:VAL:HG12	1:C:220:LEU:HB2	1.99	0.44
1:D:168:THR:HB	1:D:221:ARG:HG2	2.00	0.44
1:B:170:LYS:HG2	1:B:179:LEU:HD11	1.99	0.43
1:C:317:PHE:HA	1:C:320:HIS:HD2	1.83	0.43
1:C:239:SER:HB3	3:C:402:FAD:O2P	2.18	0.43
1:C:10:ILE:HG22	1:C:65:ALA:CB	2.48	0.43
4:D:403:ECN:H20	4:D:403:ECN:H7	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:CYS:HB2	1:B:331:VAL:HG13	2.01	0.43
1:C:271:ASN:HD21	1:C:298:ASN:HD21	1.66	0.43
1:C:57:LEU:HB2	4:C:403:ECN:C15	2.48	0.43
1:A:317:PHE:HA	1:A:320:HIS:HD2	1.82	0.43
1:C:233:PHE:HE1	5:C:512:HOH:O	2.01	0.43
1:A:364:SER:HB2	1:A:365:LEU:HD12	2.00	0.43
1:D:190:ILE:C	1:D:190:ILE:CD1	2.87	0.43
1:A:311:ASP:HB3	1:A:314:THR:H	1.84	0.43
1:A:328:CYS:HB2	1:A:331:VAL:HG13	1.99	0.43
1:A:56:ALA:O	1:A:57:LEU:C	2.56	0.43
1:A:84:LYS:HD3	1:A:208:HIS:NE2	2.34	0.43
1:D:32:MET:HG3	1:D:101:TYR:CD2	2.54	0.43
1:A:84:LYS:HD3	1:A:208:HIS:HE2	1.84	0.43
1:C:146:TRP:CD1	1:C:150:LYS:HG3	2.53	0.43
1:B:274:PRO:HG3	1:B:354:PRO:HG2	2.01	0.42
1:B:365:LEU:CD1	1:B:366:ALA:H	2.32	0.42
1:D:86:ARG:HG2	1:D:141:TYR:CE1	2.54	0.42
1:A:154:ILE:HG22	1:A:248:VAL:HA	2.01	0.42
1:A:56:ALA:O	1:A:60:THR:OG1	2.35	0.42
1:C:381:ARG:HB3	1:C:381:ARG:HH11	1.85	0.42
1:D:154:ILE:HG22	1:D:248:VAL:HA	2.01	0.42
1:C:364:SER:HB2	1:C:365:LEU:HD12	2.01	0.42
1:C:91:LYS:H	1:C:94:HIS:CD2	2.22	0.42
2:D:401:HEM:HBD2	2:D:401:HEM:CMD	2.44	0.42
1:A:57:LEU:CD1	4:A:403:ECN:C15	2.96	0.42
1:B:2:LEU:O	1:B:7:ARG:NH1	2.52	0.42
1:C:6:THR:HA	1:C:9:ILE:HD12	2.02	0.42
1:B:368:MET:O	1:B:369:GLN:C	2.58	0.42
1:C:368:MET:HA	1:C:368:MET:CE	2.50	0.42
1:B:317:PHE:HA	1:B:320:HIS:HD2	1.85	0.42
1:C:157:LYS:HD2	1:C:167:PHE:HE1	1.80	0.42
1:D:368:MET:CE	1:D:368:MET:HA	2.50	0.42
1:C:152:PHE:CD2	1:C:254:LEU:HD13	2.54	0.42
1:D:383:ASP:N	1:D:383:ASP:OD1	2.53	0.42
1:D:62:LEU:HD22	1:D:66:LYS:HD2	2.00	0.42
1:A:212:CYS:HB3	1:A:288:LEU:HD23	2.02	0.42
1:B:19:GLN:HB3	1:B:19:GLN:HE21	1.49	0.42
1:D:328:CYS:HB2	1:D:331:VAL:HG13	2.02	0.42
1:B:157:LYS:HB3	1:C:159:TYR:HD2	1.85	0.41
1:B:240:GLU:HG3	1:B:244:LYS:HD2	2.02	0.41
1:C:14:VAL:N	1:C:15:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:HEM:ND	4:D:403:ECN:N19	2.67	0.41
1:B:368:MET:HA	1:B:368:MET:CE	2.50	0.41
1:B:84:LYS:HD3	1:B:208:HIS:NE2	2.34	0.41
1:C:14:VAL:CG2	1:C:65:ALA:HB1	2.51	0.41
1:D:70:ASP:OD1	1:D:72:SER:OG	2.38	0.41
1:B:145:LEU:CD2	1:B:183:PRO:HD2	2.48	0.41
1:B:365:LEU:HD13	1:B:366:ALA:H	1.84	0.41
1:D:85:HIS:HE1	2:D:401:HEM:C4B	2.38	0.41
1:A:40:LEU:HD12	1:A:203:TYR:CZ	2.56	0.41
1:B:168:THR:HB	1:B:221:ARG:HG2	2.02	0.41
1:B:35:GLU:HB3	1:B:36:HIS:HD2	1.83	0.41
3:C:402:FAD:H1'1	3:C:402:FAD:H9	1.86	0.41
1:B:311:ASP:CB	1:B:314:THR:HG23	2.48	0.41
1:A:270:GLN:HE22	1:A:273:VAL:N	2.08	0.41
1:C:328:CYS:HB2	1:C:331:VAL:HG13	2.01	0.41
1:D:360:TYR:CD2	1:D:360:TYR:N	2.88	0.41
1:D:263:ILE:HA	1:D:360:TYR:CZ	2.55	0.41
2:C:401:HEM:HBD2	2:C:401:HEM:CMD	2.46	0.41
1:D:21:GLY:HA2	1:D:57:LEU:HD23	2.02	0.41
1:B:158:GLU:HG2	1:C:158:GLU:HG3	1.98	0.41
1:D:126:TYR:CD1	4:D:403:ECN:H9	2.56	0.41
1:B:319:LYS:HE2	5:B:505:HOH:O	2.21	0.41
1:C:311:ASP:HB3	1:C:314:THR:H	1.85	0.41
1:C:62:LEU:HD22	1:C:66:LYS:HD2	2.02	0.41
1:B:179:LEU:HA	1:B:179:LEU:HD23	1.89	0.41
1:B:86:ARG:O	1:B:87:ALA:C	2.59	0.41
1:C:365:LEU:CD1	1:C:366:ALA:H	2.34	0.41
1:D:364:SER:O	1:D:368:MET:HG2	2.21	0.41
1:D:274:PRO:HB3	1:D:302:PRO:HB2	2.02	0.40
1:D:295:VAL:HG22	1:D:328:CYS:SG	2.60	0.40
1:A:35:GLU:HB3	1:A:36:HIS:HD2	1.87	0.40
1:A:11:LYS:HD2	1:A:69:ASP:OD1	2.21	0.40
1:C:367:PHE:O	1:C:371:MET:HG2	2.21	0.40
1:A:154:ILE:CG2	1:A:248:VAL:HA	2.52	0.40
1:A:368:MET:O	1:A:369:GLN:C	2.59	0.40
1:C:311:ASP:CB	1:C:314:THR:HG23	2.49	0.40
1:D:239:SER:HB3	3:D:402:FAD:O2P	2.22	0.40
1:A:24:ILE:HG22	4:A:403:ECN:CL8	2.58	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:O	1:C:7:ARG:NH2[1_454]	1.80	0.40
1:C:311:ASP:OD2	5:B:526:HOH:O[2_756]	2.04	0.16

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	396/399 (99%)	371 (94%)	22 (6%)	3 (1%)	19	57
1	B	396/399 (99%)	367 (93%)	27 (7%)	2 (0%)	29	68
1	C	396/399 (99%)	369 (93%)	22 (6%)	5 (1%)	12	45
1	D	396/399 (99%)	371 (94%)	22 (6%)	3 (1%)	19	57
All	All	1584/1596 (99%)	1478 (93%)	93 (6%)	13 (1%)	19	57

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	B	53	GLN
1	C	53	GLN
1	C	56	ALA
1	C	57	LEU
1	D	53	GLN
1	A	246	ALA
1	B	230	ARG
1	A	230	ARG
1	C	51	GLY
1	C	230	ARG
1	D	230	ARG
1	D	179	LEU

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	336/341 (98%)	288 (86%)	48 (14%)	3	15
1	B	336/341 (98%)	286 (85%)	50 (15%)	3	14
1	C	336/341 (98%)	287 (85%)	49 (15%)	3	15
1	D	336/341 (98%)	285 (85%)	51 (15%)	3	14
All	All	1344/1364 (98%)	1146 (85%)	198 (15%)	3	15

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	19	GLN
1	A	25	THR
1	A	30	LYS
1	A	32	MET
1	A	35	GLU
1	A	38	GLU
1	A	39	LEU
1	A	55	ASN
1	A	60	THR
1	A	61	VAL
1	A	62	LEU
1	A	80	GLN
1	A	84	LYS
1	A	104	LYS
1	A	127	GLN
1	A	153	GLU
1	A	158	GLU
1	A	165	VAL
1	A	168	THR
1	A	169	VAL
1	A	178	GLU
1	A	184	ILE
1	A	206	LEU

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Mol	Chain	Res	Type
1	A	217	LYS
1	A	225	LYS
1	A	227	GLU
1	A	230	ARG
1	A	233	PHE
1	A	248	VAL
1	A	265	LYS
1	A	270	GLN
1	A	272	GLU
1	A	297	CYS
1	A	311	ASP
1	A	312	GLU
1	A	313	LYS
1	A	330	ASN
1	A	332	ASP
1	A	343	LEU
1	A	351	GLU
1	A	365	LEU
1	A	369	GLN
1	A	376	LYS
1	A	377	GLU
1	A	381	ARG
1	A	383	ASP
1	A	388	GLU
1	B	6	THR
1	B	19	GLN
1	B	25	THR
1	B	30	LYS
1	B	32	MET
1	B	35	GLU
1	B	37	THR
1	B	38	GLU
1	B	39	LEU
1	B	46	THR
1	B	49	LYS
1	B	55	ASN
1	B	60	THR
1	B	61	VAL
1	B	62	LEU
1	B	80	GLN
1	B	84	LYS
1	B	104	LYS

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Mol	Chain	Res	Type
1	B	153	GLU
1	B	158	GLU
1	B	165	VAL
1	B	168	THR
1	B	169	VAL
1	B	178	GLU
1	B	184	ILE
1	B	206	LEU
1	B	217	LYS
1	B	225	LYS
1	B	230	ARG
1	B	233	PHE
1	B	239	SER
1	B	265	LYS
1	B	270	GLN
1	B	272	GLU
1	B	297	CYS
1	B	311	ASP
1	B	312	GLU
1	B	313	LYS
1	B	330	ASN
1	B	332	ASP
1	B	343	LEU
1	B	351	GLU
1	B	365	LEU
1	B	368	MET
1	B	369	GLN
1	B	376	LYS
1	B	377	GLU
1	B	381	ARG
1	B	383	ASP
1	B	388	GLU
1	C	6	THR
1	C	19	GLN
1	C	25	THR
1	C	30	LYS
1	C	32	MET
1	C	35	GLU
1	C	38	GLU
1	C	39	LEU
1	C	46	THR
1	C	49	LYS

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Mol	Chain	Res	Type
1	C	55	ASN
1	C	60	THR
1	C	61	VAL
1	C	62	LEU
1	C	80	GLN
1	C	84	LYS
1	C	104	LYS
1	C	153	GLU
1	C	165	VAL
1	C	168	THR
1	C	169	VAL
1	C	178	GLU
1	C	184	ILE
1	C	206	LEU
1	C	217	LYS
1	C	225	LYS
1	C	227	GLU
1	C	230	ARG
1	C	233	PHE
1	C	239	SER
1	C	247	LYS
1	C	265	LYS
1	C	270	GLN
1	C	272	GLU
1	C	297	CYS
1	C	311	ASP
1	C	312	GLU
1	C	313	LYS
1	C	330	ASN
1	C	332	ASP
1	C	343	LEU
1	C	351	GLU
1	C	365	LEU
1	C	369	GLN
1	C	376	LYS
1	C	377	GLU
1	C	381	ARG
1	C	383	ASP
1	C	388	GLU
1	D	6	THR
1	D	19	GLN
1	D	25	THR

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Mol	Chain	Res	Type
1	D	30	LYS
1	D	32	MET
1	D	35	GLU
1	D	38	GLU
1	D	39	LEU
1	D	49	LYS
1	D	55	ASN
1	D	60	THR
1	D	61	VAL
1	D	62	LEU
1	D	80	GLN
1	D	84	LYS
1	D	104	LYS
1	D	127	GLN
1	D	153	GLU
1	D	158	GLU
1	D	165	VAL
1	D	168	THR
1	D	169	VAL
1	D	178	GLU
1	D	184	ILE
1	D	206	LEU
1	D	217	LYS
1	D	225	LYS
1	D	227	GLU
1	D	230	ARG
1	D	233	PHE
1	D	239	SER
1	D	265	LYS
1	D	270	GLN
1	D	272	GLU
1	D	297	CYS
1	D	308	SER
1	D	311	ASP
1	D	312	GLU
1	D	313	LYS
1	D	328	CYS
1	D	330	ASN
1	D	332	ASP
1	D	343	LEU
1	D	351	GLU
1	D	365	LEU

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Mol	Chain	Res	Type
1	D	369	GLN
1	D	376	LYS
1	D	377	GLU
1	D	381	ARG
1	D	383	ASP
1	D	388	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	36	HIS
1	A	41	ASN
1	A	77	HIS
1	A	94	HIS
1	A	218	ASN
1	A	243	HIS
1	A	270	GLN
1	A	271	ASN
1	A	320	HIS
1	B	19	GLN
1	B	36	HIS
1	B	41	ASN
1	B	94	HIS
1	B	202	GLN
1	B	218	ASN
1	B	243	HIS
1	B	270	GLN
1	B	271	ASN
1	B	320	HIS
1	C	19	GLN
1	C	36	HIS
1	C	41	ASN
1	C	89	GLN
1	C	94	HIS
1	C	218	ASN
1	C	243	HIS
1	C	270	GLN
1	C	271	ASN
1	C	320	HIS
1	D	19	GLN
1	D	36	HIS

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Mol	Chain	Res	Type
1	D	41	ASN
1	D	94	HIS
1	D	202	GLN
1	D	243	HIS
1	D	270	GLN
1	D	271	ASN
1	D	300	ASN
1	D	320	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
2	HEM	B	401	1,4	27,50,50	2.13	6 (22%)	17,82,82	1.01	0
2	HEM	D	401	1,4	27,50,50	2.09	6 (22%)	17,82,82	1.22	1 (5%)
4	ECN	D	403	2	24,26,26	1.42	5 (20%)	32,35,35	1.89	5 (15%)
2	HEM	C	401	1,4	27,50,50	2.13	5 (18%)	17,82,82	1.22	1 (5%)
4	ECN	C	403	2	24,26,26	1.45	6 (25%)	32,35,35	2.52	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	402	-	51,58,58	1.60	8 (15%)	60,89,89	1.88	9 (15%)
2	HEM	A	401	1,4	27,50,50	2.00	7 (25%)	17,82,82	1.53	2 (11%)
3	FAD	A	402	-	51,58,58	1.84	9 (17%)	60,89,89	2.18	12 (20%)
4	ECN	A	403	2	24,26,26	1.09	2 (8%)	32,35,35	2.03	11 (34%)
3	FAD	C	402	-	51,58,58	1.49	6 (11%)	60,89,89	1.92	12 (20%)
3	FAD	D	402	-	51,58,58	1.62	7 (13%)	60,89,89	1.95	11 (18%)
4	ECN	B	403	2	24,26,26	1.34	4 (16%)	32,35,35	1.68	4 (12%)

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
2	HEM	B	401	1,4	-	2/6/54/54	-
2	HEM	D	401	1,4	-	2/6/54/54	-
4	ECN	D	403	2	-	3/13/13/13	0/3/3/3
2	HEM	C	401	1,4	-	2/6/54/54	-
4	ECN	C	403	2	-	5/13/13/13	0/3/3/3
3	FAD	B	402	-	-	5/30/50/50	0/6/6/6
2	HEM	A	401	1,4	-	2/6/54/54	-
3	FAD	A	402	-	-	4/30/50/50	0/6/6/6
4	ECN	A	403	2	-	3/13/13/13	0/3/3/3
3	FAD	C	402	-	-	6/30/50/50	0/6/6/6
3	FAD	D	402	-	-	5/30/50/50	0/6/6/6
4	ECN	B	403	2	-	1/13/13/13	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3D-C2D	5.42	1.53	1.37
3	A	402	FAD	C10-N1	5.34	1.40	1.33
2	D	401	HEM	C3D-C2D	5.20	1.53	1.37
3	A	402	FAD	C4X-N5	5.17	1.40	1.33
2	A	401	HEM	C3C-C2C	-5.15	1.33	1.40
2	B	401	HEM	C3D-C2D	4.98	1.52	1.37
3	D	402	FAD	C10-N1	4.96	1.39	1.33
2	B	401	HEM	C3C-C2C	-4.92	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C3D-C2D	4.86	1.52	1.37
3	A	402	FAD	C4-N3	4.85	1.41	1.33
3	A	402	FAD	C4X-C10	4.41	1.43	1.38
3	B	402	FAD	C2A-N3A	4.23	1.38	1.32
3	D	402	FAD	C2A-N3A	4.20	1.38	1.32
2	D	401	HEM	C3C-C2C	-4.19	1.34	1.40
2	C	401	HEM	C3B-C2B	-4.17	1.34	1.40
2	B	401	HEM	C3B-C2B	-4.14	1.34	1.40
2	D	401	HEM	C3B-C2B	-4.08	1.34	1.40
3	C	402	FAD	C2A-N3A	4.06	1.38	1.32
3	B	402	FAD	C10-N1	4.03	1.38	1.33
3	D	402	FAD	C4X-N5	4.00	1.39	1.33
3	B	402	FAD	C4-N3	3.99	1.40	1.33
3	D	402	FAD	C1'-N10	3.99	1.52	1.48
3	A	402	FAD	C2A-N3A	3.97	1.38	1.32
2	C	401	HEM	C3C-C2C	-3.95	1.34	1.40
3	C	402	FAD	C1'-N10	3.94	1.52	1.48
3	B	402	FAD	C4X-N5	3.93	1.38	1.33
3	C	402	FAD	C10-N1	3.87	1.38	1.33
2	C	401	HEM	C3B-CAB	3.80	1.55	1.47
2	C	401	HEM	C3C-CAC	3.63	1.55	1.47
2	A	401	HEM	C3B-CAB	3.39	1.54	1.47
3	D	402	FAD	C4-N3	3.37	1.38	1.33
3	C	402	FAD	C4-N3	3.27	1.38	1.33
2	A	401	HEM	C3B-C2B	-3.25	1.35	1.40
4	D	403	ECN	C19-N1	-3.20	1.44	1.48
2	D	401	HEM	C3C-CAC	3.18	1.54	1.47
2	D	401	HEM	C3B-CAB	3.16	1.54	1.47
4	D	403	ECN	C14-CL4	3.14	1.81	1.73
3	D	402	FAD	C2A-N1A	3.12	1.39	1.33
4	B	403	ECN	C14-CL4	3.11	1.81	1.73
2	B	401	HEM	C3C-CAC	3.09	1.54	1.47
4	C	403	ECN	C14-CL4	3.08	1.81	1.73
3	A	402	FAD	C5X-N5	3.00	1.40	1.35
4	C	403	ECN	C16-CL8	2.97	1.81	1.74
2	B	401	HEM	C3B-CAB	2.96	1.54	1.47
3	B	402	FAD	C2A-N1A	2.86	1.39	1.33
4	A	403	ECN	C14-CL4	2.85	1.80	1.73
3	C	402	FAD	C2A-N1A	2.75	1.39	1.33
3	C	402	FAD	C4X-N5	2.72	1.37	1.33
4	B	403	ECN	C19-N1	-2.70	1.45	1.48
3	B	402	FAD	C5X-N5	2.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	ECN	C16-CL8	2.65	1.80	1.74
3	A	402	FAD	C2A-N1A	2.64	1.38	1.33
4	B	403	ECN	C7-N1	-2.55	1.33	1.37
4	B	403	ECN	C11-CL2	2.51	1.80	1.74
4	A	403	ECN	C5-C20	-2.50	1.45	1.52
3	D	402	FAD	O4B-C4B	-2.43	1.39	1.45
2	A	401	HEM	C3C-CAC	2.37	1.52	1.47
3	B	402	FAD	C9A-N10	2.37	1.41	1.38
2	D	401	HEM	CAA-C2A	2.36	1.55	1.52
3	B	402	FAD	C1'-N10	2.35	1.50	1.48
4	C	403	ECN	C11-CL2	2.31	1.79	1.74
4	C	403	ECN	C15-C16	2.27	1.42	1.38
2	A	401	HEM	C1A-CHA	-2.22	1.34	1.41
4	C	403	ECN	C7-N1	-2.20	1.33	1.37
4	C	403	ECN	C5-C20	-2.17	1.46	1.52
4	D	403	ECN	C7-N1	-2.12	1.33	1.37
2	B	401	HEM	CAA-C2A	2.12	1.55	1.52
4	D	403	ECN	C11-CL2	2.09	1.79	1.74
3	A	402	FAD	C1'-N10	2.07	1.50	1.48
2	A	401	HEM	CAA-C2A	2.05	1.55	1.52
3	A	402	FAD	C9A-N10	2.04	1.41	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FAD	C4-N3-C2	9.15	122.86	115.14
3	D	402	FAD	C4-N3-C2	8.36	122.20	115.14
3	B	402	FAD	C4-N3-C2	7.86	121.78	115.14
3	C	402	FAD	C4-N3-C2	7.73	121.67	115.14
4	C	403	ECN	O20-C20-C5	-7.56	100.66	112.08
3	A	402	FAD	N3A-C2A-N1A	-6.48	118.55	128.68
4	D	403	ECN	C21-C5-C14	5.95	122.74	116.81
3	C	402	FAD	N3A-C2A-N1A	-5.87	119.50	128.68
3	D	402	FAD	N3A-C2A-N1A	-5.71	119.76	128.68
3	B	402	FAD	N3A-C2A-N1A	-5.71	119.76	128.68
4	B	403	ECN	C14-C5-C20	-5.68	116.49	122.16
3	A	402	FAD	C4X-C4-N3	-5.15	116.39	123.43
4	C	403	ECN	C21-C5-C14	5.07	121.86	116.81
4	C	403	ECN	C5-C14-CL4	-4.93	115.31	120.41
4	B	403	ECN	C21-C5-C14	4.88	121.67	116.81
4	A	403	ECN	C21-C5-C14	4.87	121.66	116.81
4	C	403	ECN	C15-C14-CL4	4.73	126.13	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	ECN	C14-C5-C20	-4.68	117.49	122.16
4	C	403	ECN	C15-C16-CL8	4.51	124.78	119.15
3	C	402	FAD	C4X-C4-N3	-4.51	117.27	123.43
4	A	403	ECN	C8-O20-C20	-4.45	104.11	113.90
4	A	403	ECN	C14-C5-C20	-4.30	117.87	122.16
3	B	402	FAD	C1'-N10-C9A	4.19	121.59	118.29
3	D	402	FAD	C1'-N10-C9A	4.18	121.58	118.29
3	D	402	FAD	C4X-N5-C5X	4.16	120.92	116.77
3	C	402	FAD	C4X-N5-C5X	4.12	120.89	116.77
3	A	402	FAD	C1'-N10-C9A	3.98	121.43	118.29
3	A	402	FAD	C4X-N5-C5X	3.93	120.69	116.77
3	D	402	FAD	C4X-C4-N3	-3.81	118.22	123.43
4	A	403	ECN	C15-C14-C5	-3.58	118.13	122.41
4	D	403	ECN	O20-C20-C19	3.58	113.46	106.33
3	B	402	FAD	C4X-C4-N3	-3.40	118.78	123.43
4	C	403	ECN	O20-C20-C19	3.37	113.03	106.33
3	D	402	FAD	C5X-C9A-N10	3.31	120.11	117.72
4	C	403	ECN	C15-C14-C5	-3.23	118.56	122.41
3	A	402	FAD	C5X-C9A-N10	3.22	120.05	117.72
3	C	402	FAD	C1'-N10-C9A	3.19	120.80	118.29
3	B	402	FAD	C4X-N5-C5X	3.07	119.84	116.77
3	A	402	FAD	C10-C4X-N5	-3.02	119.17	121.26
3	C	402	FAD	C1'-C2'-C3'	3.01	118.19	109.79
3	B	402	FAD	O2'-C2'-C3'	-2.90	102.05	109.10
2	A	401	HEM	C4C-C3C-C2C	2.81	108.86	106.90
4	D	403	ECN	C15-C14-C5	-2.80	119.07	122.41
3	A	402	FAD	O3'-C3'-C4'	2.80	115.57	108.81
3	A	402	FAD	P-O3P-PA	-2.78	123.28	132.83
2	D	401	HEM	C4C-C3C-C2C	2.78	108.84	106.90
3	D	402	FAD	C1'-C2'-C3'	2.76	117.50	109.79
4	A	403	ECN	C13-C11-CL2	-2.74	115.07	119.35
4	C	403	ECN	C14-C5-C20	-2.74	119.43	122.16
3	A	402	FAD	C1'-C2'-C3'	2.73	117.42	109.79
3	C	402	FAD	C10-C4X-N5	-2.72	119.38	121.26
4	A	403	ECN	C10-C1-C2	2.67	122.36	118.17
3	D	402	FAD	C10-C4X-N5	-2.66	119.42	121.26
3	B	402	FAD	P-O3P-PA	-2.66	123.70	132.83
4	C	403	ECN	C17-C16-CL8	-2.64	115.22	119.35
3	B	402	FAD	C5X-C9A-N10	2.63	119.62	117.72
3	C	402	FAD	C5X-C9A-N10	2.62	119.61	117.72
4	C	403	ECN	O20-C8-C1	2.58	115.86	109.91
4	A	403	ECN	O20-C20-C5	-2.54	108.24	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C1D-C2D-C3D	-2.53	105.24	107.00
4	B	403	ECN	O20-C20-C19	2.50	111.30	106.33
3	D	402	FAD	P-O3P-PA	-2.43	124.48	132.83
3	A	402	FAD	O3'-C3'-C2'	-2.42	102.96	108.81
3	C	402	FAD	P-O3P-PA	-2.41	124.57	132.83
4	B	403	ECN	C15-C14-C5	-2.37	119.58	122.41
4	D	403	ECN	C15-C14-CL4	2.32	122.23	118.49
3	B	402	FAD	C1'-C2'-C3'	2.31	116.25	109.79
4	A	403	ECN	C9-C10-C1	-2.29	117.88	121.03
4	A	403	ECN	C8-C1-C2	-2.24	115.41	120.66
4	A	403	ECN	C13-C11-C9	2.18	124.07	121.24
3	D	402	FAD	C1B-N9A-C4A	-2.17	122.83	126.64
3	C	402	FAD	C5A-C6A-N6A	-2.15	117.09	120.35
2	C	401	HEM	C4C-C3C-C2C	2.13	108.39	106.90
3	C	402	FAD	C9A-N10-C10	-2.13	119.12	121.91
3	D	402	FAD	C9A-N10-C10	-2.10	119.16	121.91
3	C	402	FAD	N6A-C6A-N1A	2.07	122.88	118.57
4	A	403	ECN	C2-C13-C11	-2.04	117.08	119.24
3	A	402	FAD	C1B-N9A-C4A	-2.03	123.08	126.64

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C4D-C3D-CAD-CBD
2	D	401	HEM	C2D-C3D-CAD-CBD
2	D	401	HEM	C4D-C3D-CAD-CBD
3	A	402	FAD	C1'-C2'-C3'-C4'
4	C	403	ECN	N1-C19-C20-O20
4	C	403	ECN	N1-C19-C20-C5
4	C	403	ECN	C19-C20-O20-C8
4	C	403	ECN	C5-C20-O20-C8
3	B	402	FAD	C1'-C2'-C3'-C4'
2	A	401	HEM	C2D-C3D-CAD-CBD
2	A	401	HEM	C4D-C3D-CAD-CBD
2	C	401	HEM	C2D-C3D-CAD-CBD
2	C	401	HEM	C4D-C3D-CAD-CBD
3	C	402	FAD	C1'-C2'-C3'-C4'
4	D	403	ECN	C20-C19-N1-C3
3	D	402	FAD	C1'-C2'-C3'-C4'
3	C	402	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
3	B	402	FAD	O2'-C2'-C3'-O3'
3	A	402	FAD	O2'-C2'-C3'-C4'
3	B	402	FAD	O2'-C2'-C3'-C4'
3	C	402	FAD	O2'-C2'-C3'-C4'
3	D	402	FAD	O2'-C2'-C3'-C4'
4	B	403	ECN	C1-C8-O20-C20
3	D	402	FAD	O2'-C2'-C3'-O3'
4	A	403	ECN	C1-C8-O20-C20
3	A	402	FAD	O2'-C2'-C3'-O3'
4	A	403	ECN	C5-C20-O20-C8
4	A	403	ECN	C19-C20-O20-C8
4	D	403	ECN	C1-C8-O20-C20
4	C	403	ECN	C1-C8-O20-C20
4	D	403	ECN	C20-C19-N1-C7
3	A	402	FAD	C5B-O5B-PA-O1A
3	B	402	FAD	C5B-O5B-PA-O1A
3	C	402	FAD	C5B-O5B-PA-O1A
3	D	402	FAD	C5B-O5B-PA-O1A
3	B	402	FAD	C1'-C2'-C3'-O3'
3	C	402	FAD	C1'-C2'-C3'-O3'
3	D	402	FAD	C1'-C2'-C3'-O3'
3	C	402	FAD	O4'-C4'-C5'-O5'

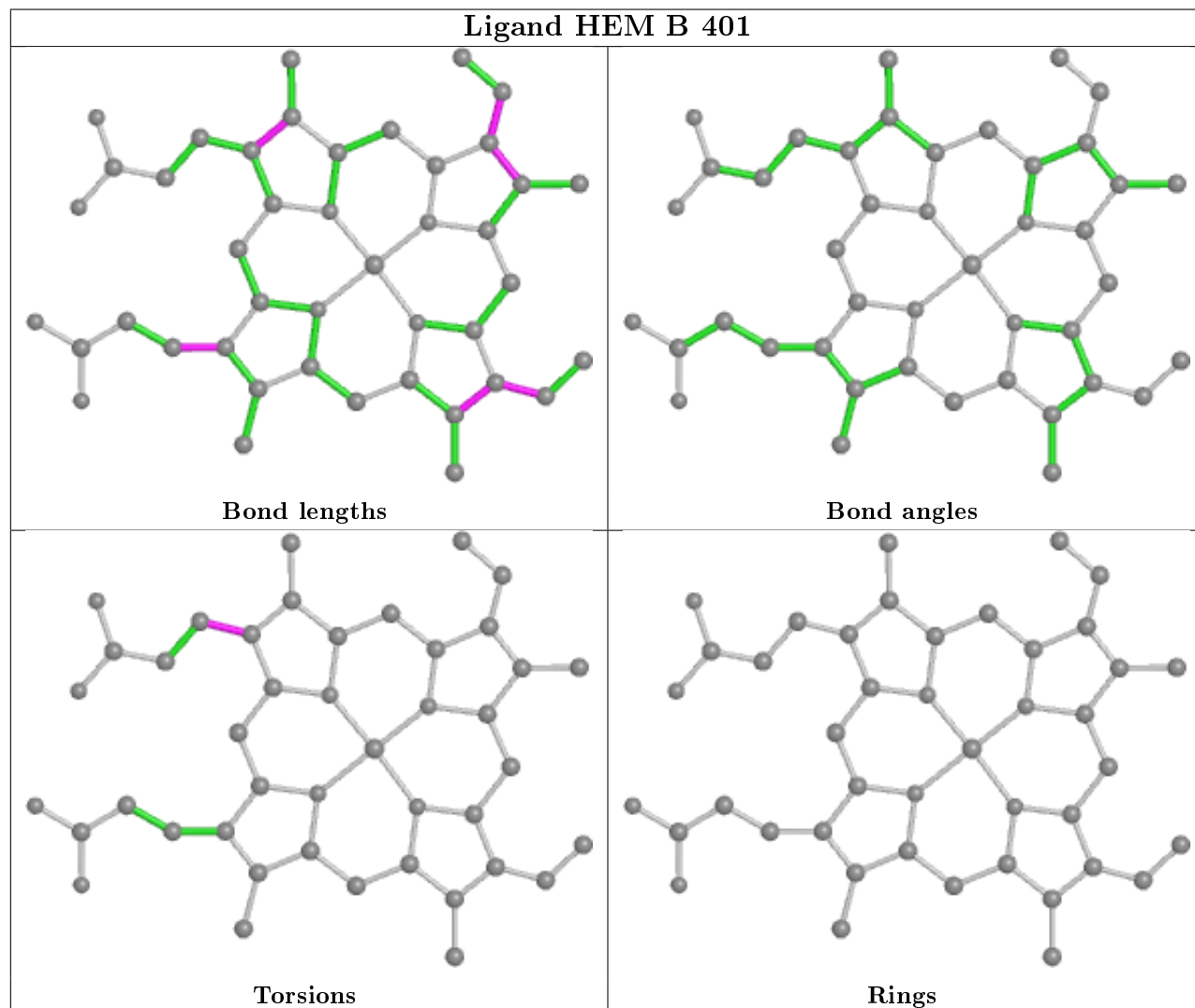
There are no ring outliers.

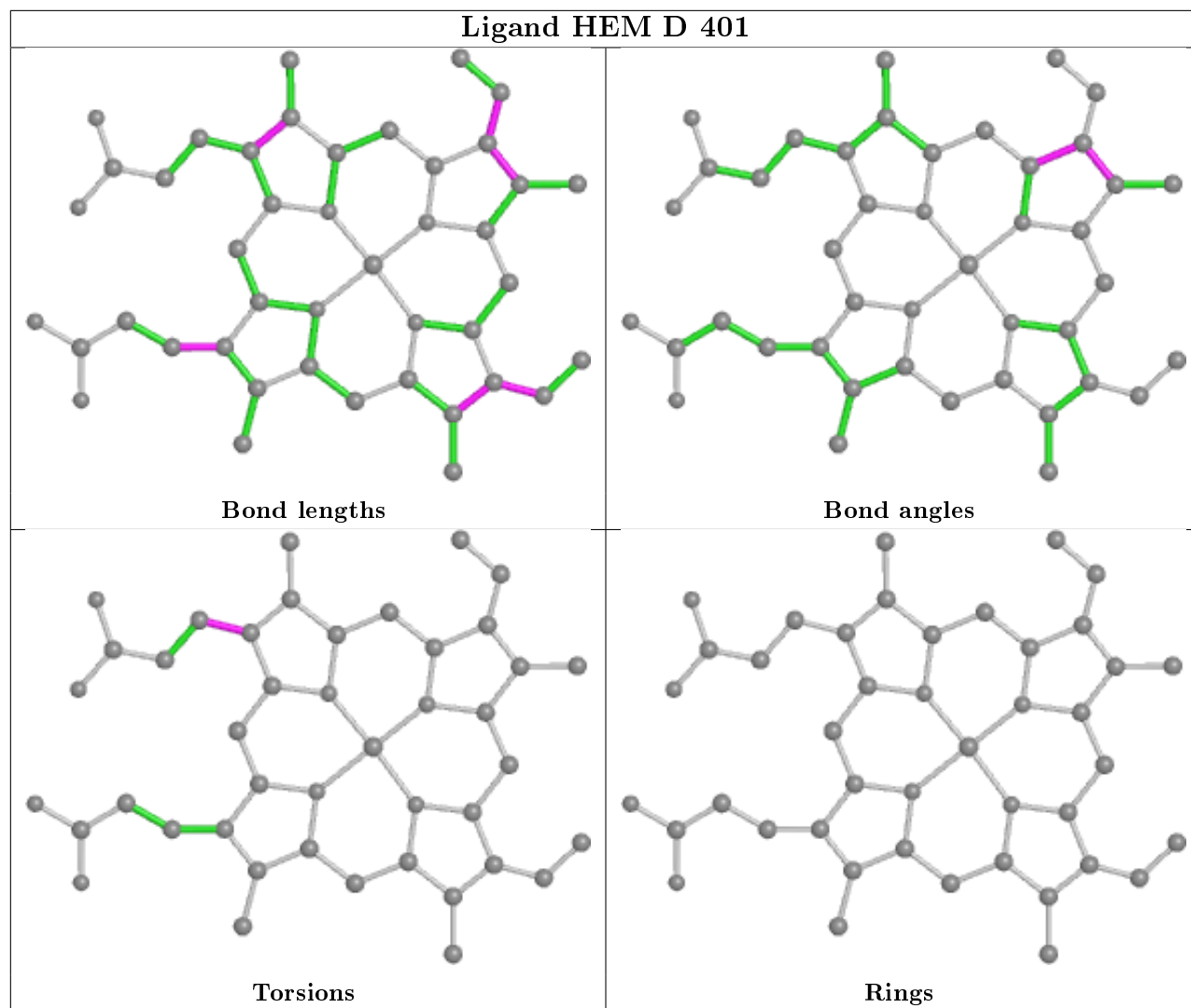
12 monomers are involved in 68 short contacts:

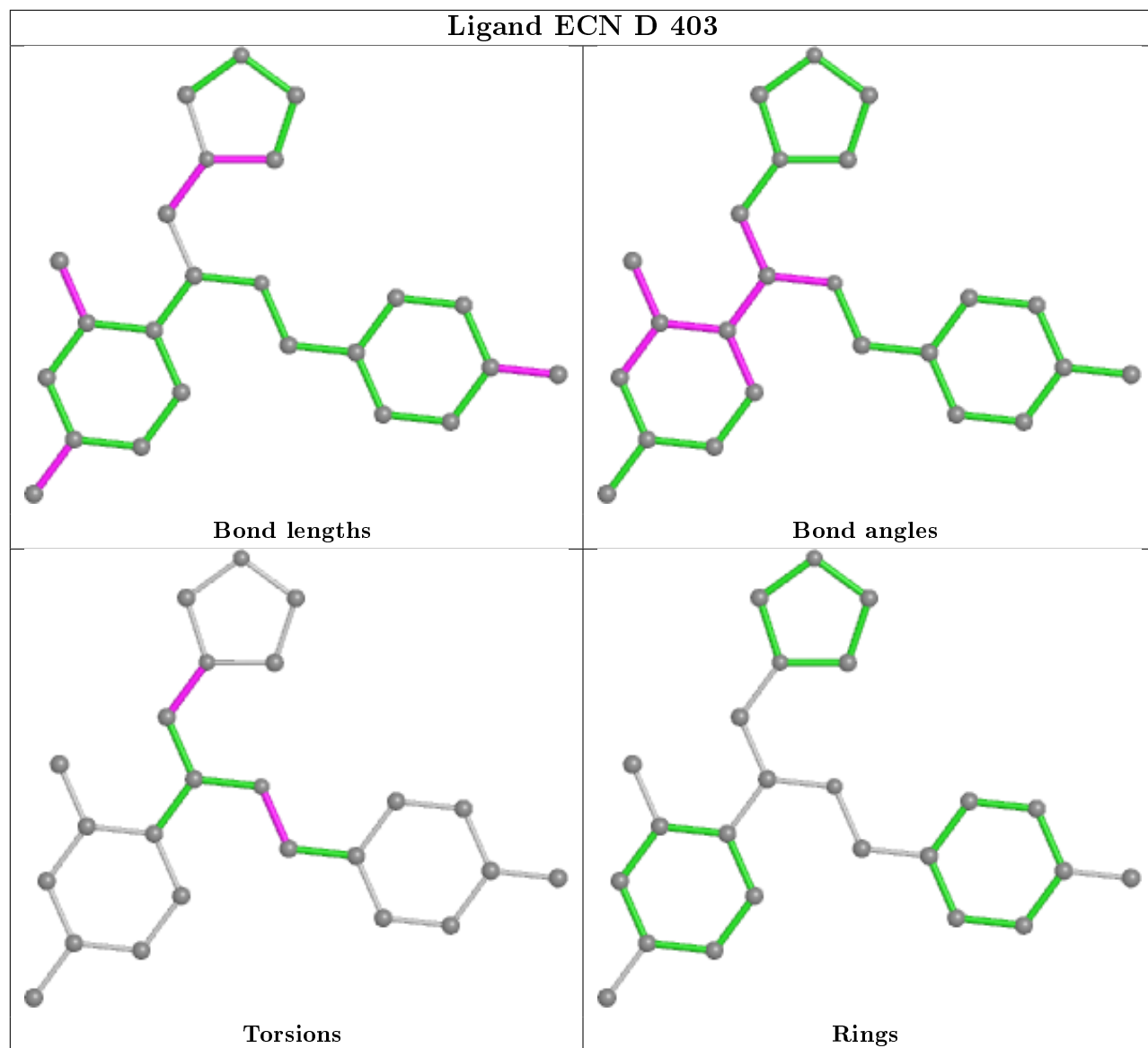
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	5	0
2	D	401	HEM	9	0
4	D	403	ECN	7	0
2	C	401	HEM	5	0
4	C	403	ECN	10	0
3	B	402	FAD	1	0
2	A	401	HEM	7	0
3	A	402	FAD	2	0
4	A	403	ECN	17	0
3	C	402	FAD	3	0
3	D	402	FAD	2	0
4	B	403	ECN	2	0

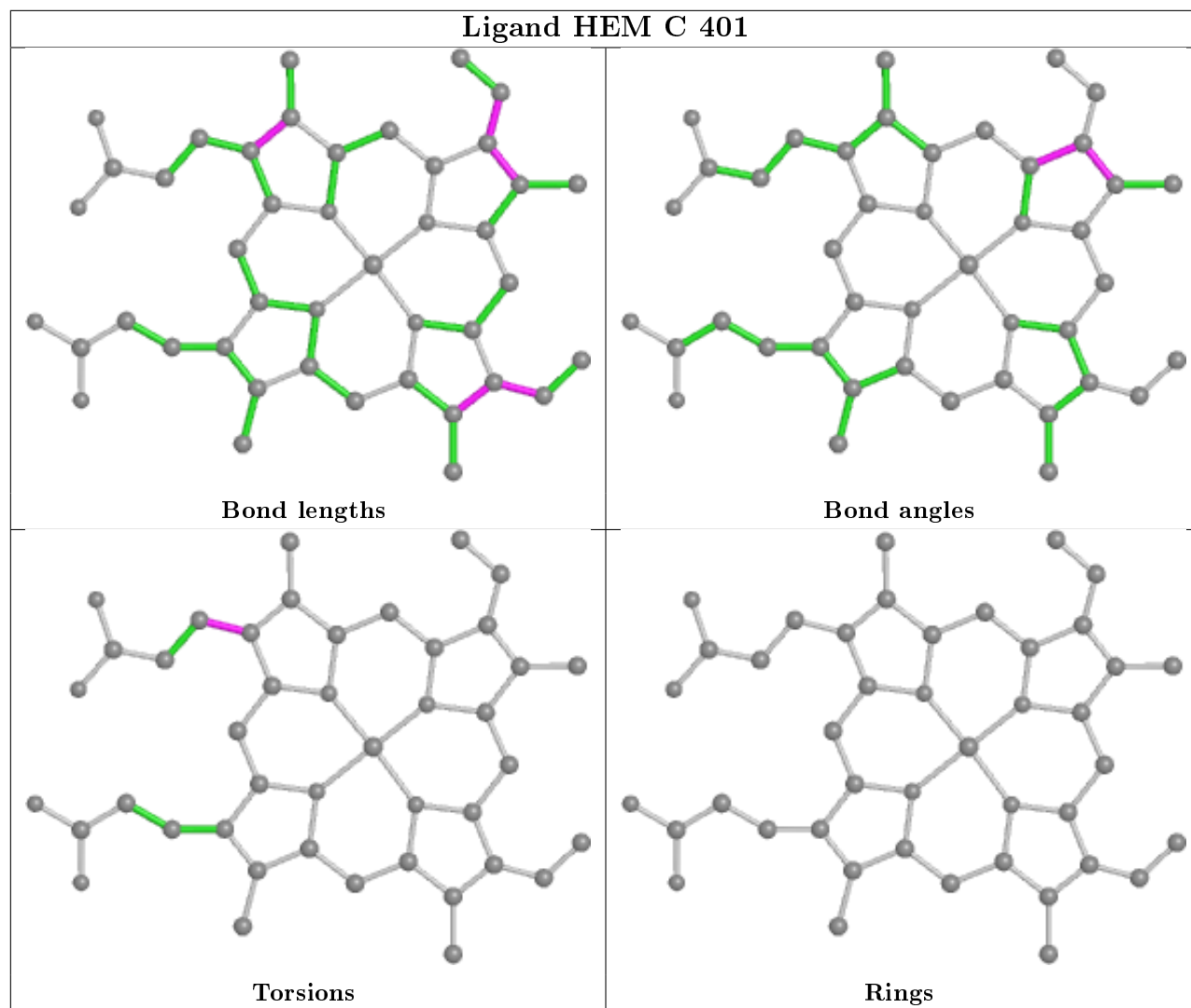
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

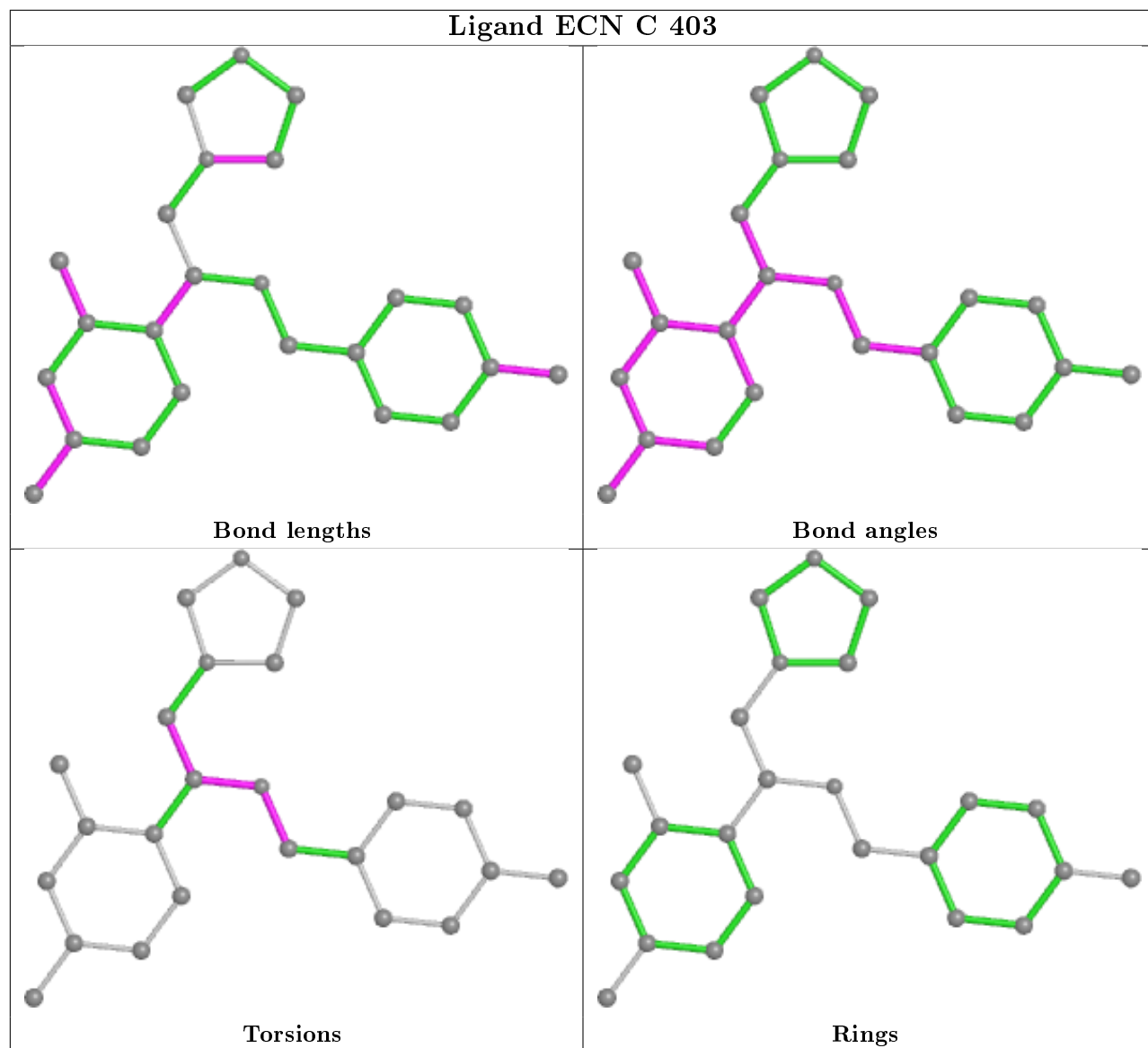
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



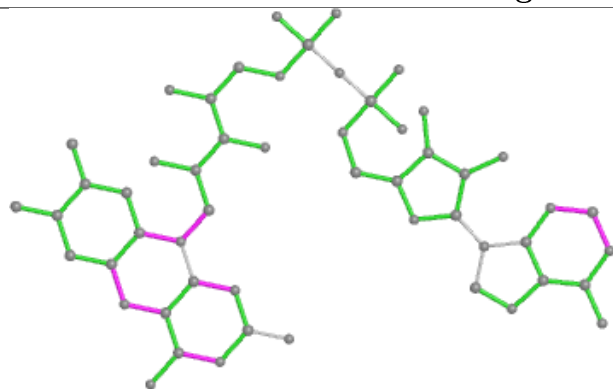




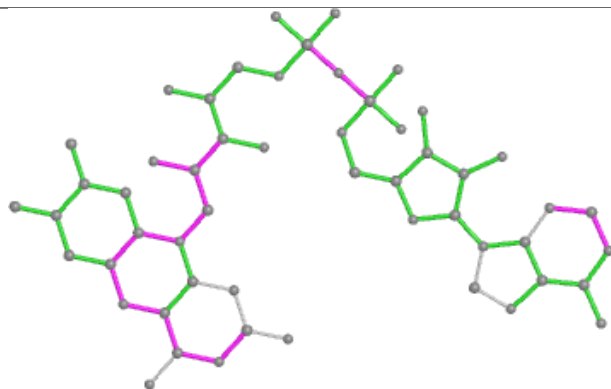




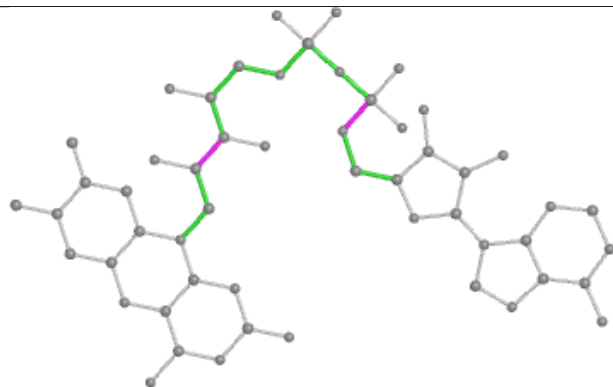
Ligand FAD B 402



Bond lengths



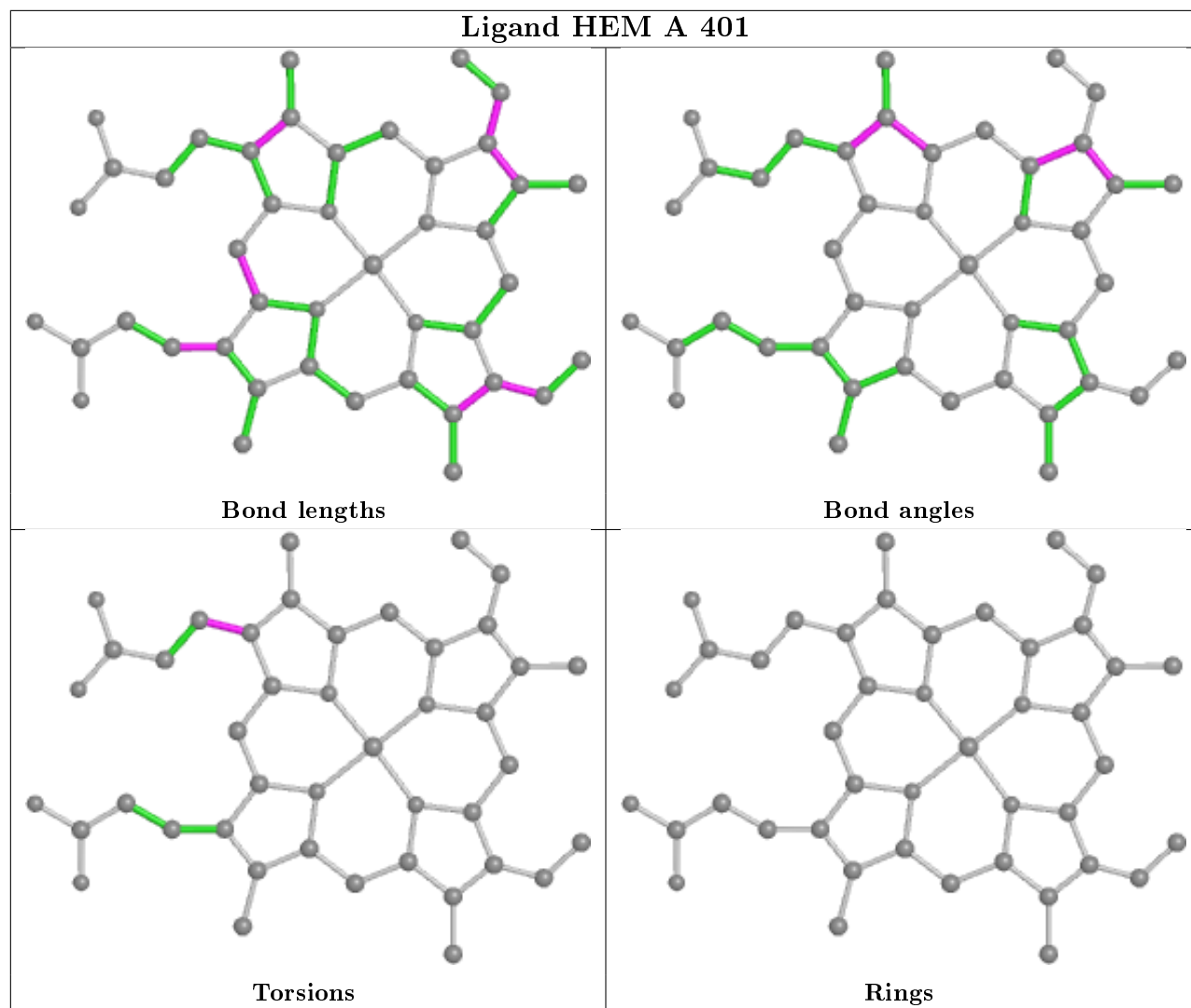
Bond angles

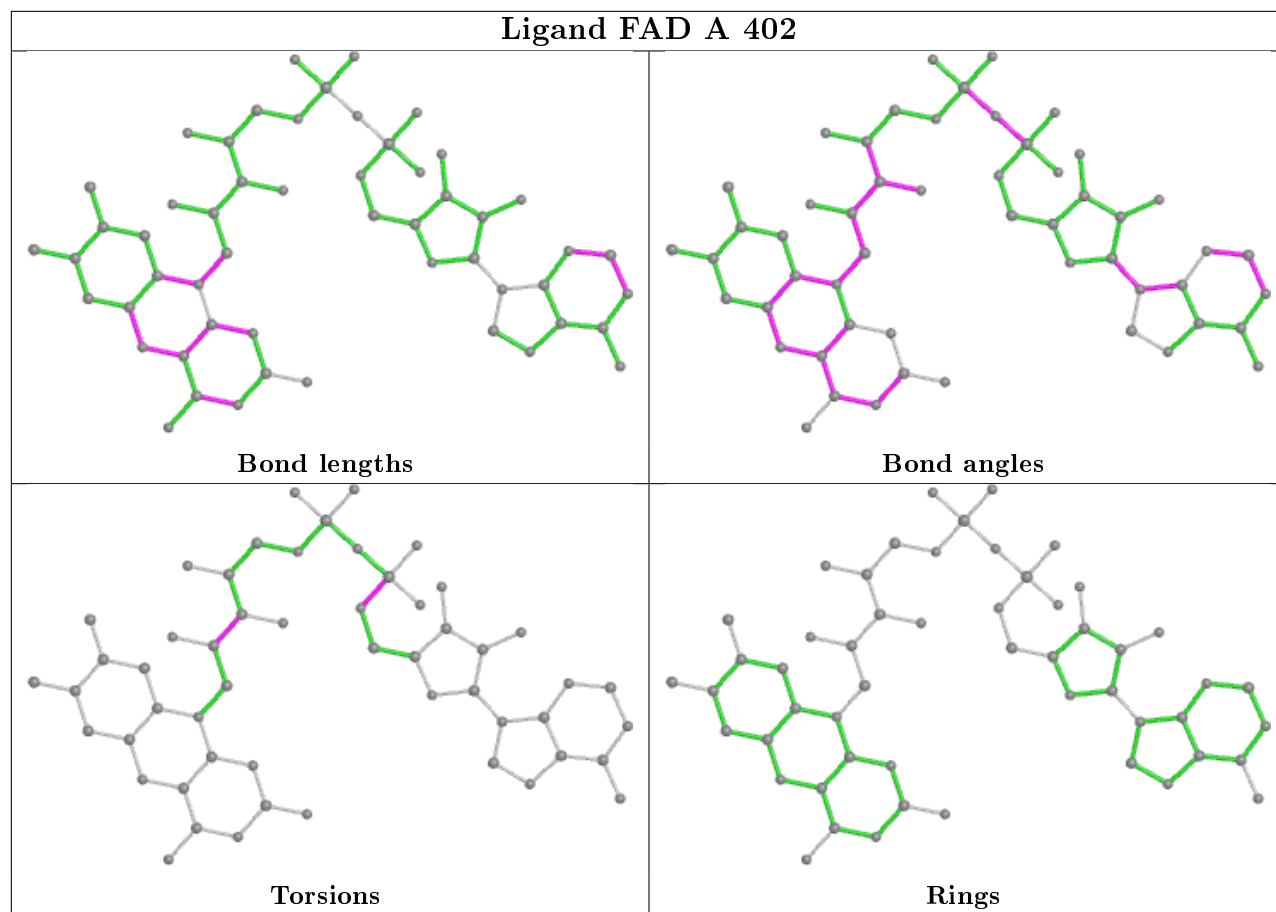


Torsions

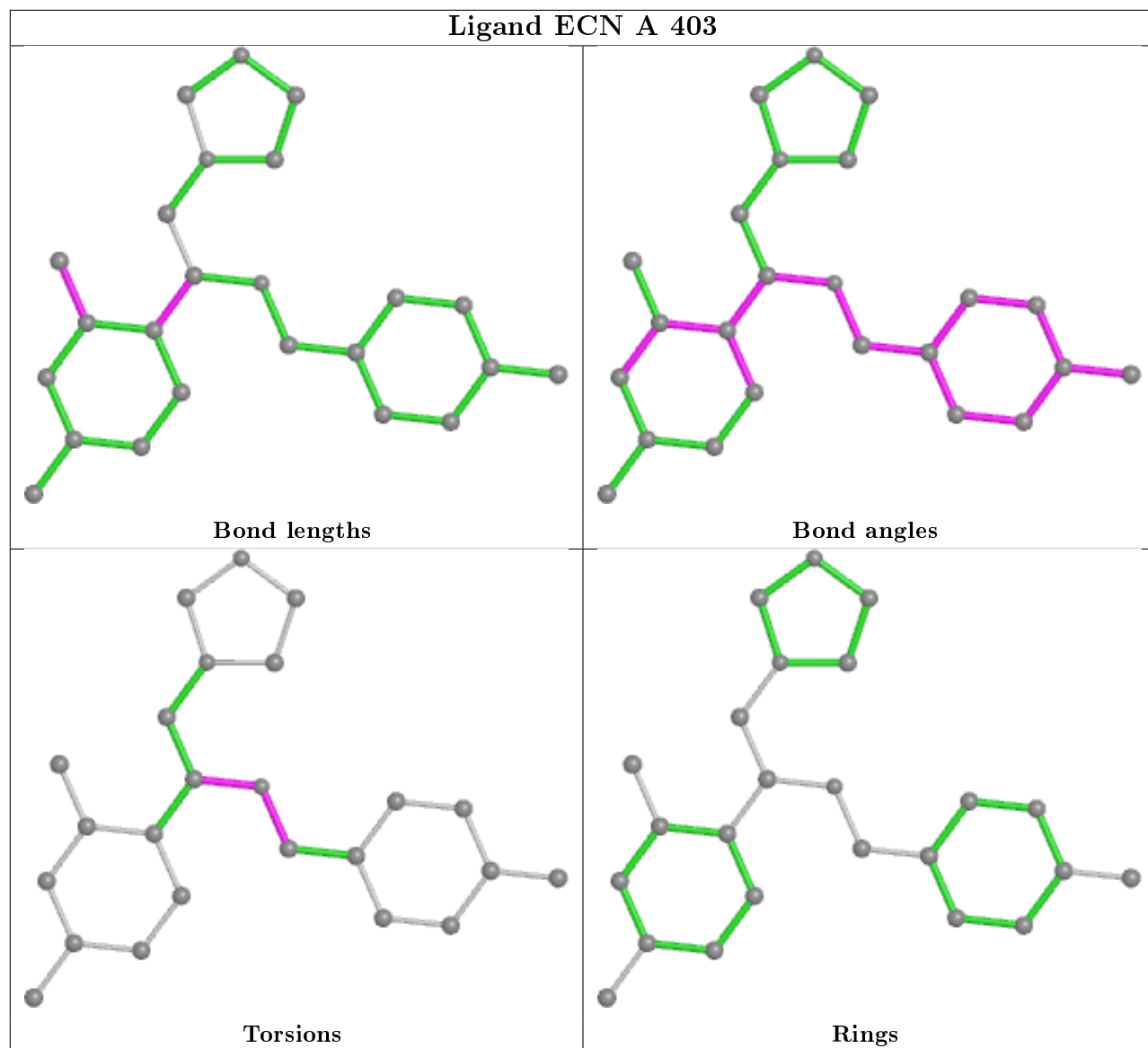


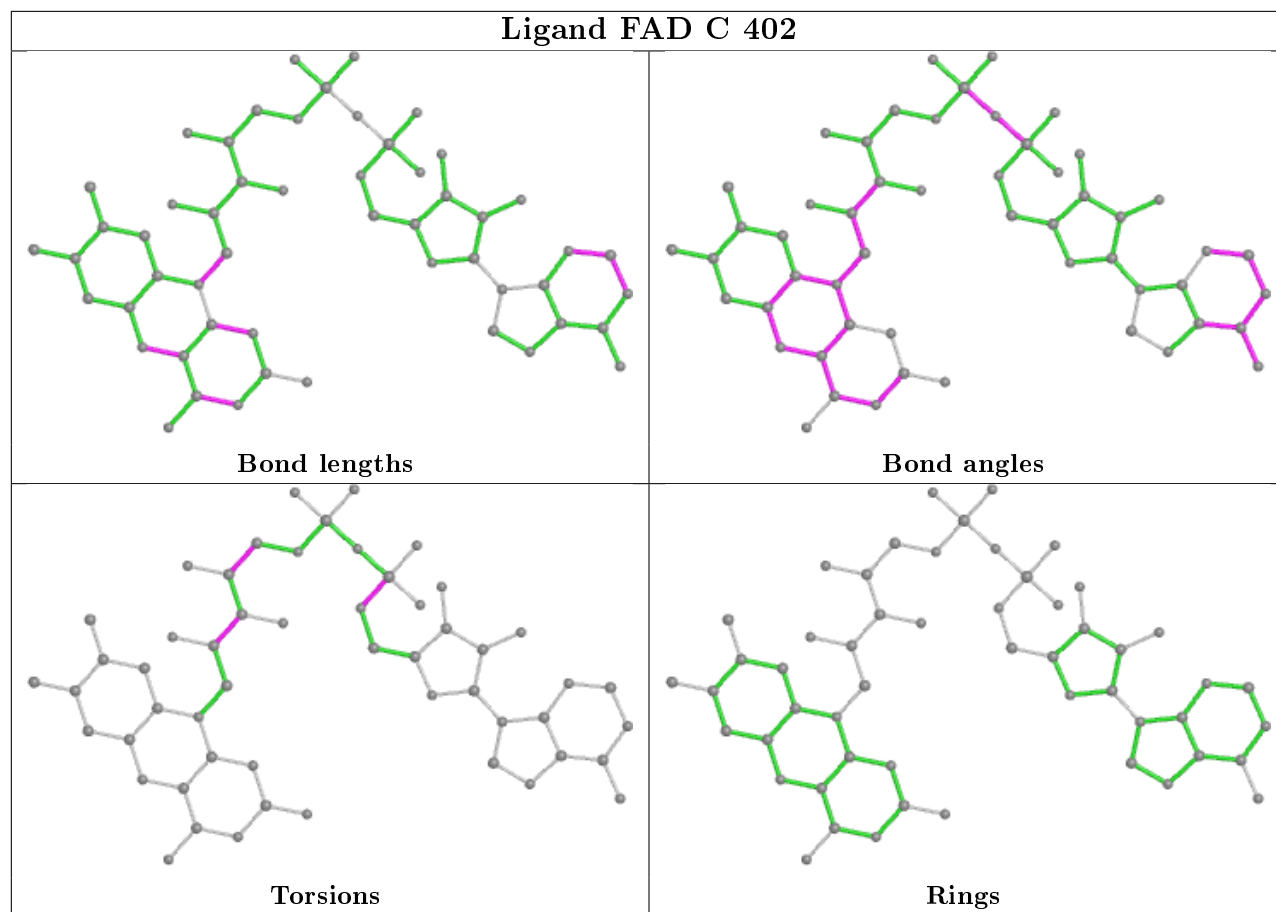
Rings

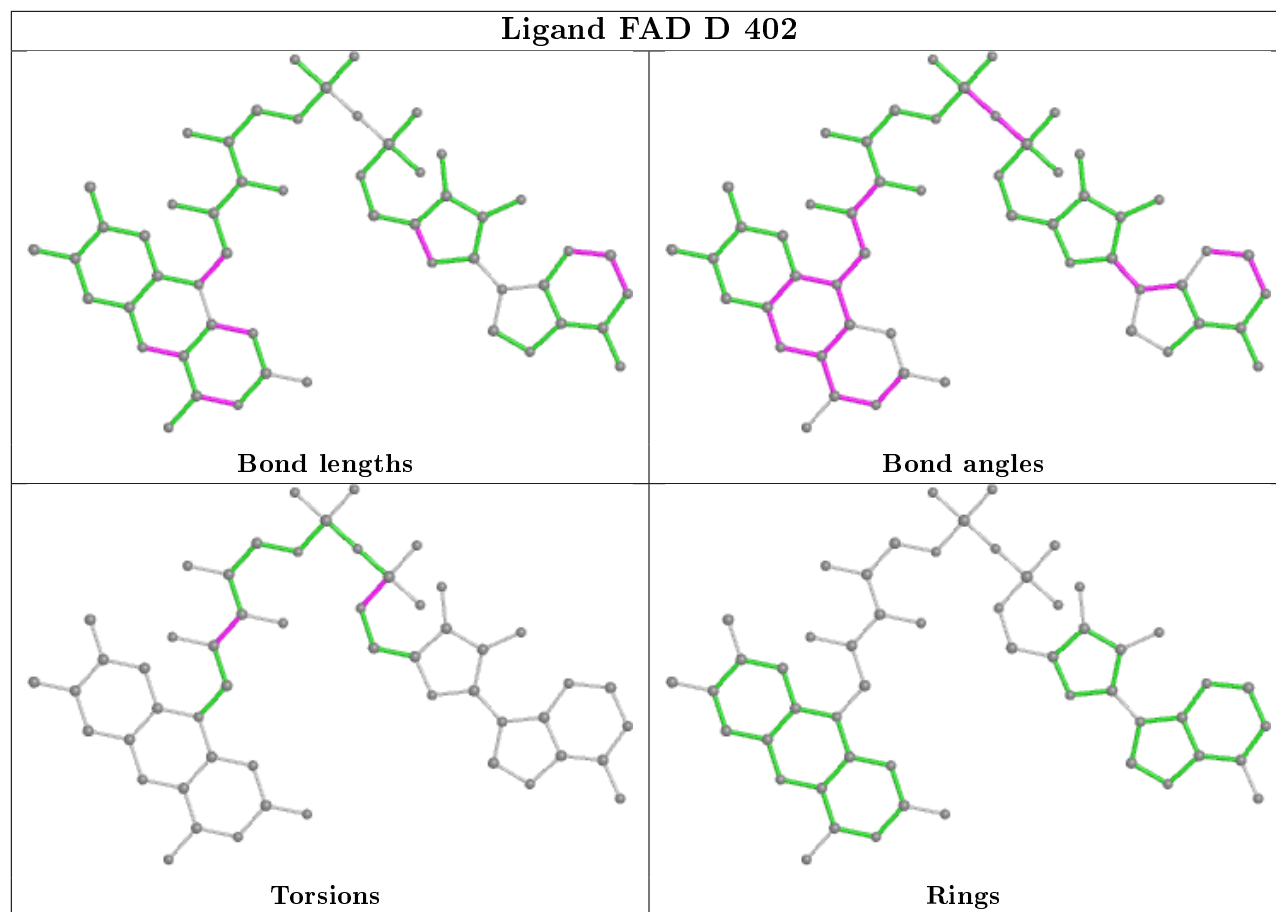


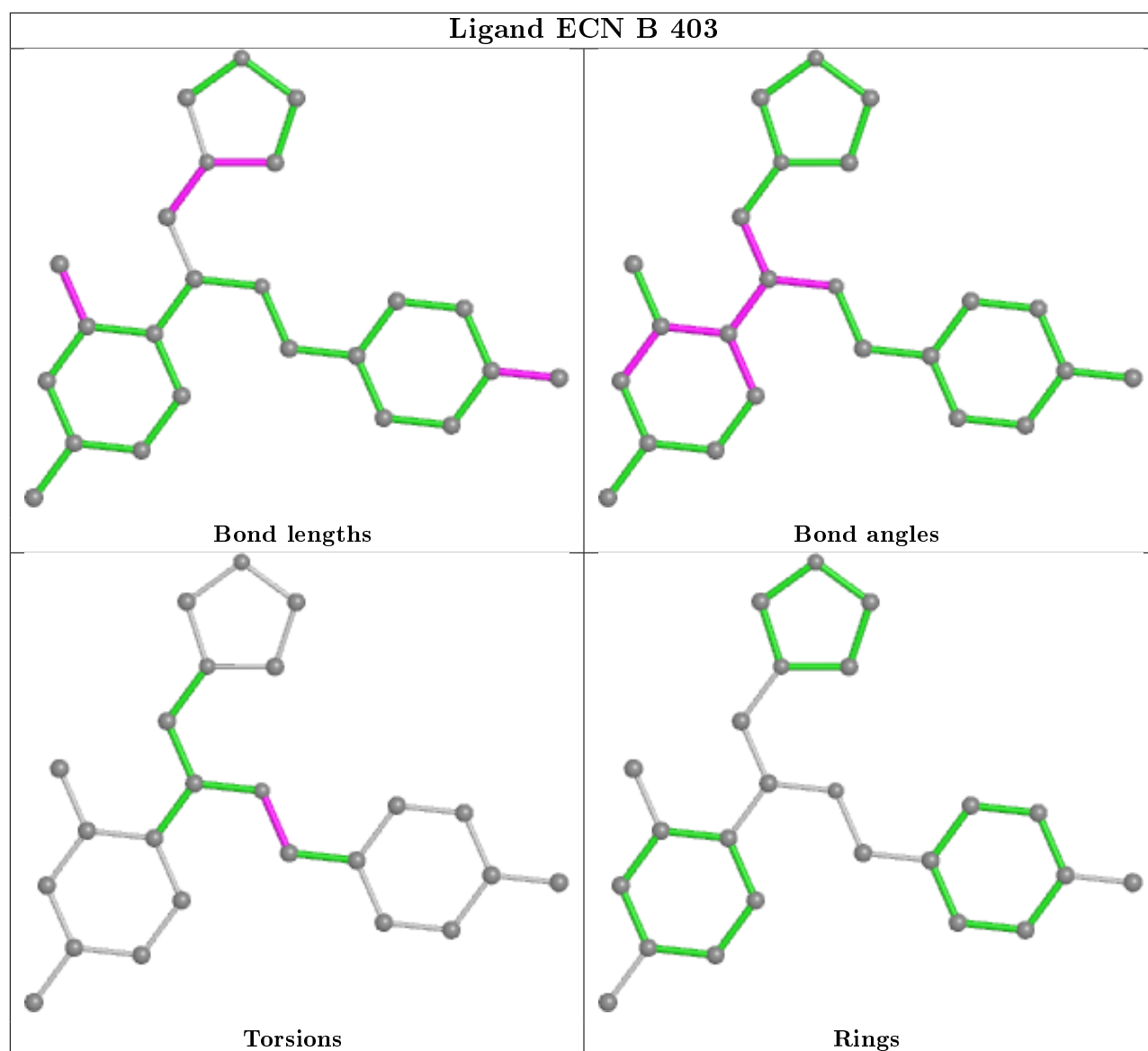


Ligand ECN A 403









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	398/399 (99%)	-0.29	11 (2%)	53 25	14, 40, 97, 240	0
1	B	398/399 (99%)	-0.09	16 (4%)	38 15	23, 50, 116, 198	0
1	C	398/399 (99%)	0.01	16 (4%)	38 15	29, 66, 102, 198	0
1	D	398/399 (99%)	0.14	17 (4%)	35 13	26, 74, 133, 190	0
All	All	1592/1596 (99%)	-0.06	60 (3%)	40 16	14, 57, 124, 240	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	GLN	8.2
1	D	230	ARG	7.3
1	D	52	ALA	7.1
1	B	231	GLU	7.0
1	D	398	GLN	6.7
1	D	51	GLY	6.6
1	C	54	PRO	6.5
1	A	56	ALA	5.4
1	B	53	GLN	5.2
1	B	230	ARG	5.1
1	B	50	VAL	5.0
1	C	396	THR	4.9
1	B	52	ALA	4.9
1	B	54	PRO	4.9
1	A	230	ARG	4.9
1	D	397	VAL	4.8
1	C	55	ASN	4.8
1	D	231	GLU	4.7
1	D	396	THR	4.5
1	C	53	GLN	4.3
1	A	52	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	51	GLY	4.3
1	D	70	ASP	4.3
1	A	398	GLN	4.1
1	C	231	GLU	4.1
1	D	69	ASP	4.0
1	C	340	THR	3.9
1	C	395	SER	3.7
1	D	112	ASP	3.6
1	C	62	LEU	3.6
1	A	231	GLU	3.5
1	C	397	VAL	3.3
1	C	230	ARG	3.3
1	C	52	ALA	3.3
1	C	398	GLN	3.1
1	A	53	GLN	2.8
1	B	396	THR	2.8
1	A	54	PRO	2.8
1	D	356	HIS	2.8
1	B	389	PRO	2.7
1	D	232	ASN	2.7
1	B	392	PRO	2.7
1	D	74	LEU	2.6
1	B	397	VAL	2.6
1	C	56	ALA	2.6
1	B	69	ASP	2.5
1	A	232	ASN	2.4
1	D	53	GLN	2.4
1	B	70	ASP	2.4
1	A	55	ASN	2.4
1	A	49	LYS	2.3
1	B	217	LYS	2.2
1	D	50	VAL	2.2
1	C	233	PHE	2.2
1	D	376	LYS	2.2
1	B	232	ASN	2.1
1	A	58	ALA	2.0
1	B	15	PRO	2.0
1	C	8	SER	2.0
1	D	75	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

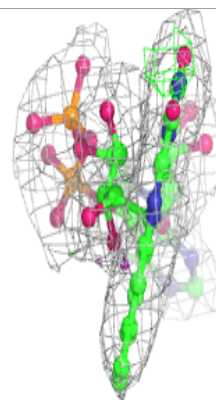
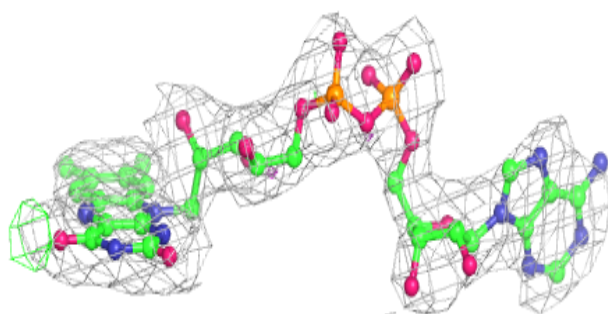
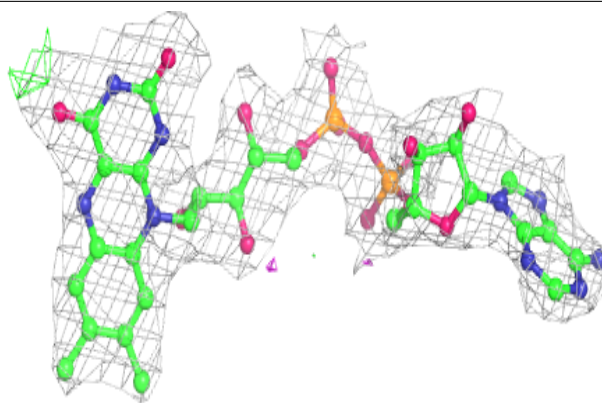
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	A	402	53/53	0.91	0.20	21,25,71,76	0
4	ECN	C	403	24/24	0.91	0.26	54,90,121,123	0
3	FAD	B	402	53/53	0.91	0.19	29,36,83,86	0
3	FAD	D	402	53/53	0.91	0.19	40,53,92,97	0
3	FAD	C	402	53/53	0.93	0.17	27,35,75,78	0
4	ECN	B	403	24/24	0.93	0.24	51,80,92,111	0
4	ECN	A	403	24/24	0.94	0.17	32,38,46,83	0
4	ECN	D	403	24/24	0.94	0.23	52,81,110,115	0
2	HEM	C	401	43/43	0.95	0.22	54,58,72,76	0
2	HEM	A	401	43/43	0.96	0.22	26,31,45,59	0
2	HEM	B	401	43/43	0.97	0.21	46,49,63,66	0
2	HEM	D	401	43/43	0.97	0.18	49,55,64,70	0

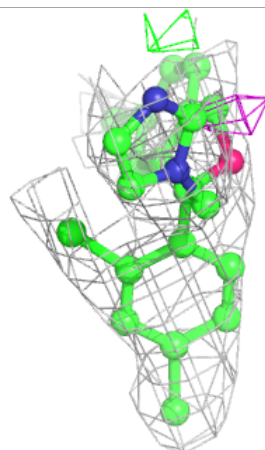
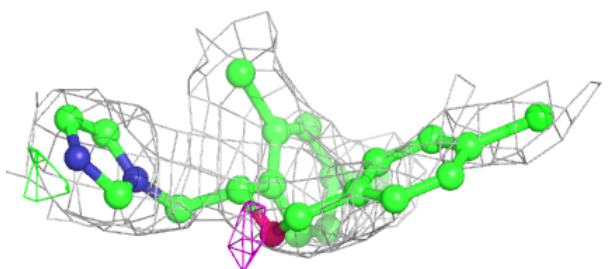
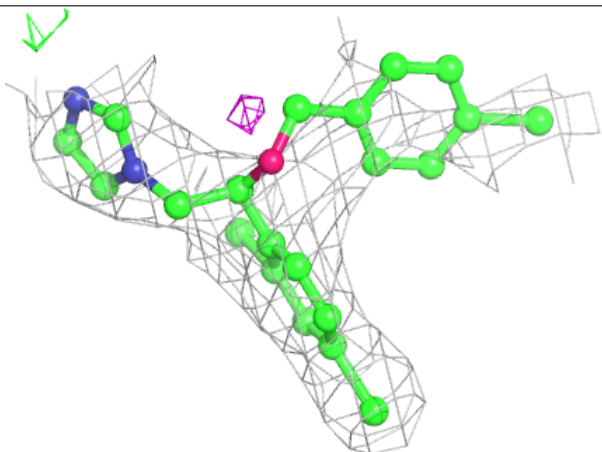
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 402:

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

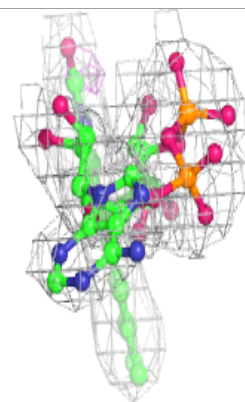
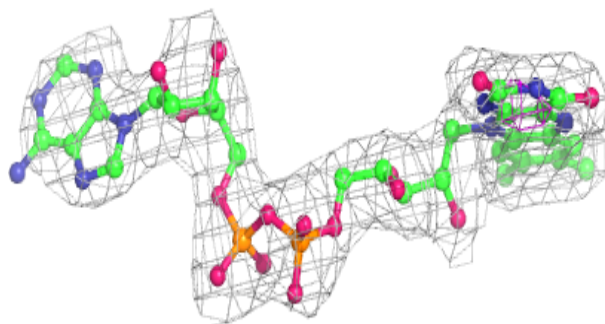
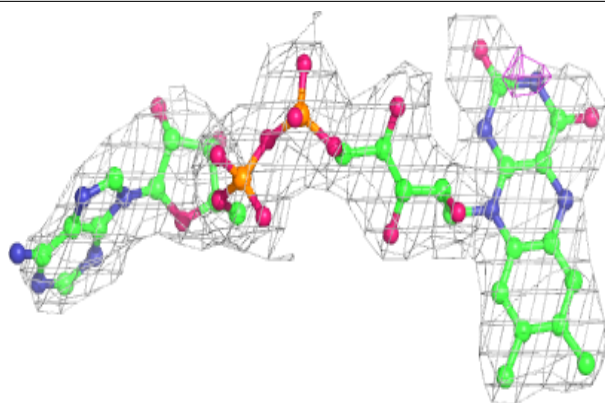
**Electron density around ECN C 403:**

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

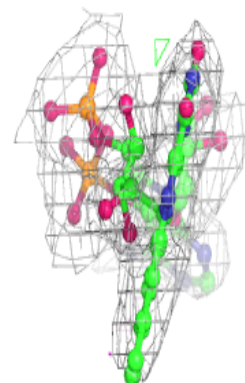
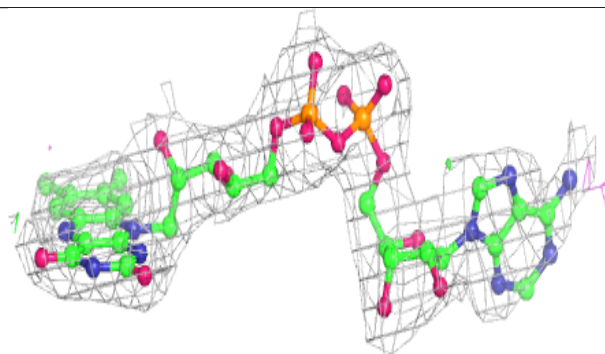
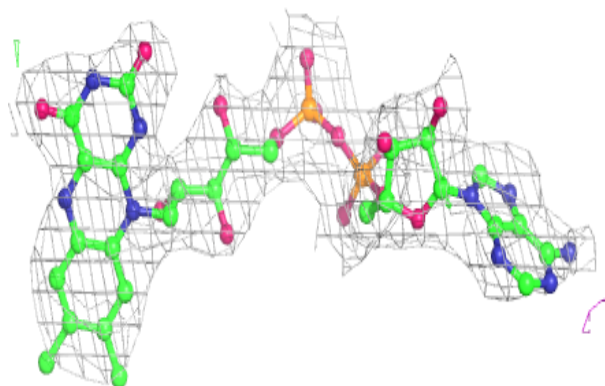


Electron density around FAD B 402:

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

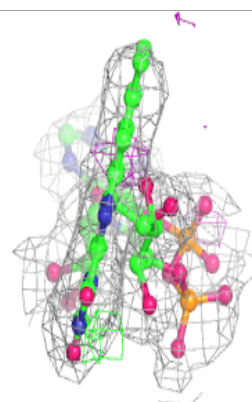
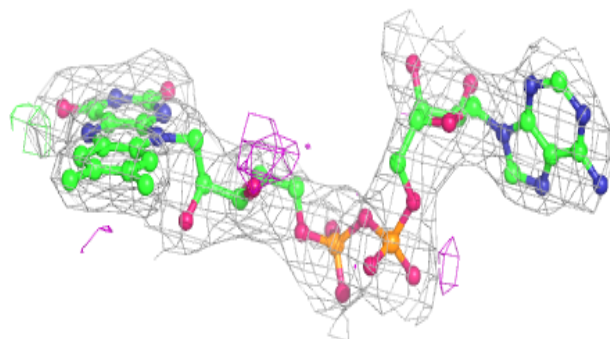
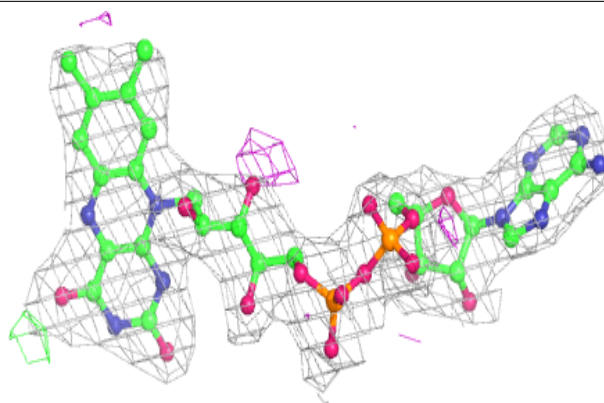
**Electron density around FAD D 402:**

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

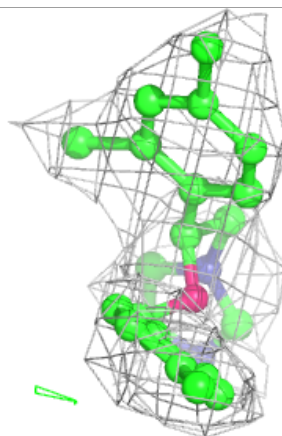
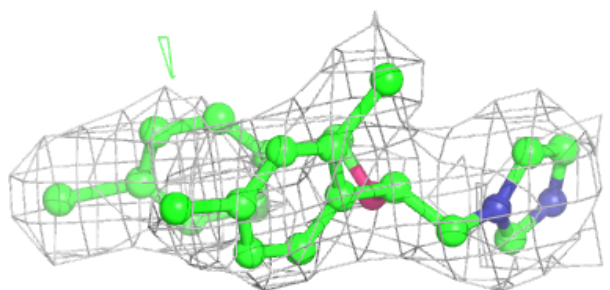
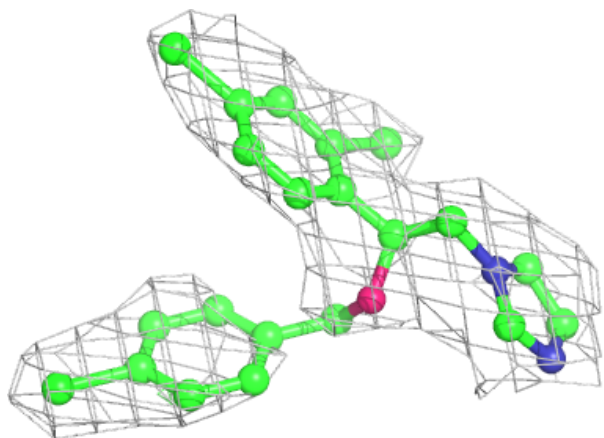


Electron density around FAD C 402:

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

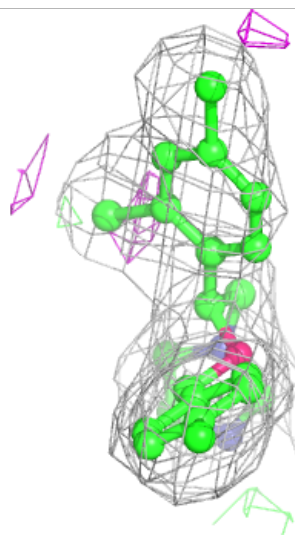
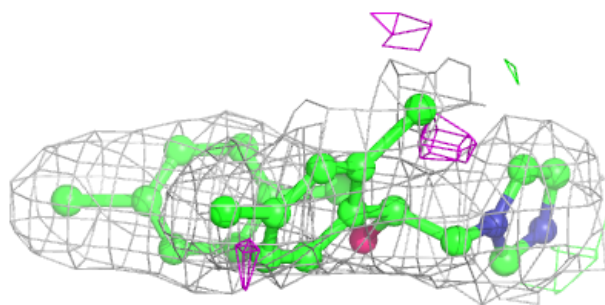
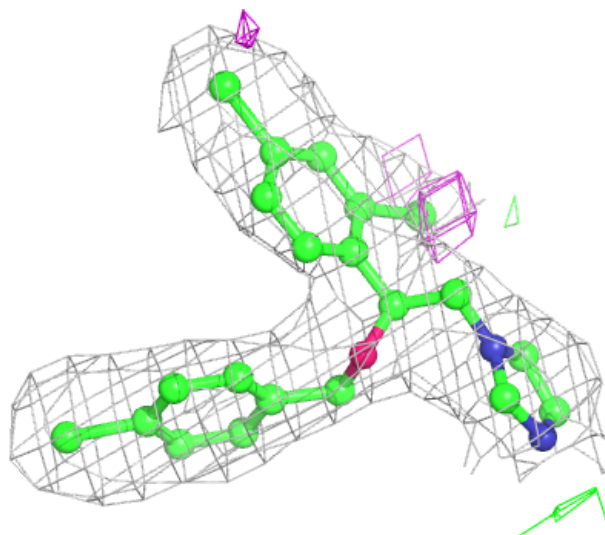
**Electron density around ECN B 403:**

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



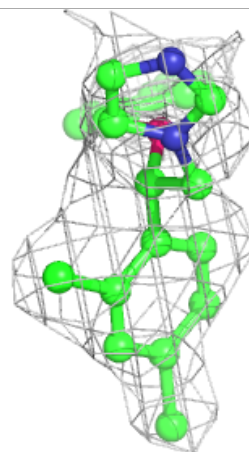
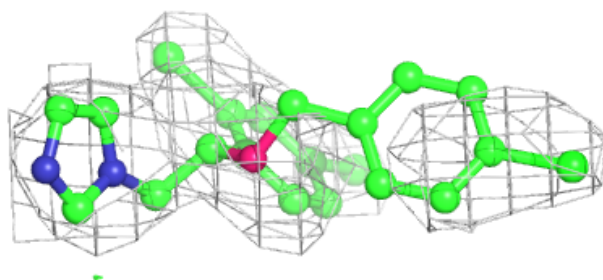
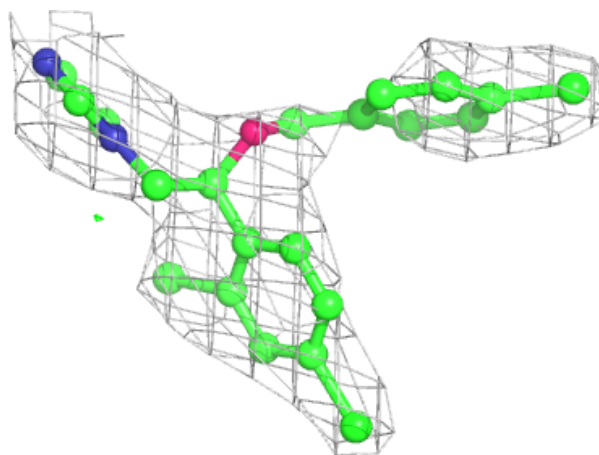
Electron density around ECN A 403:

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



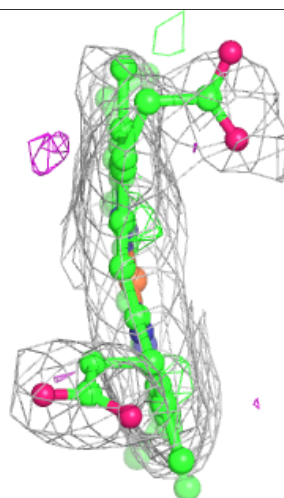
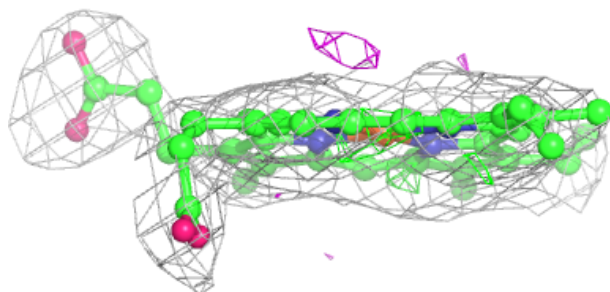
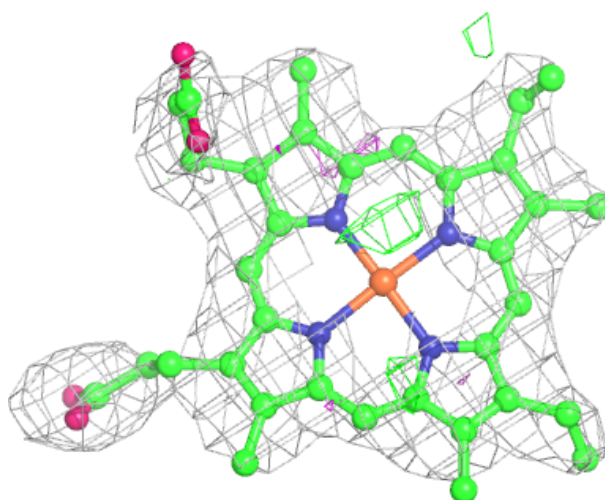
Electron density around ECN D 403:

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



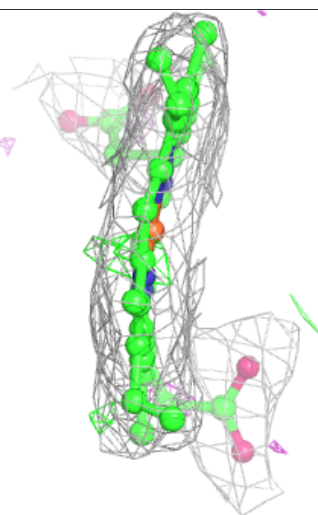
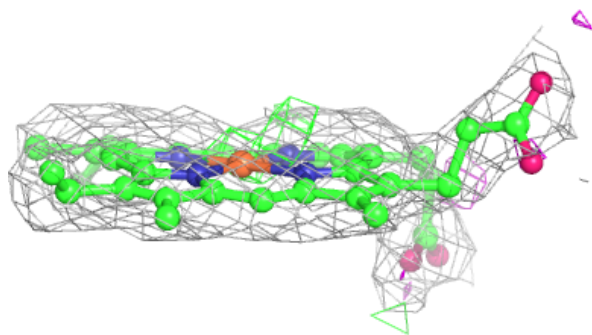
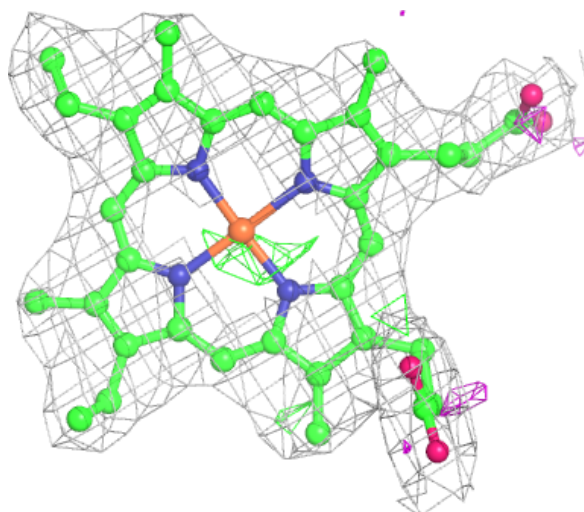
Electron density around HEM C 401:

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



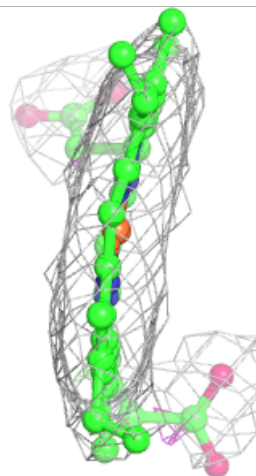
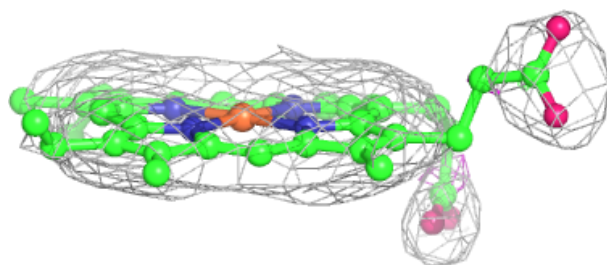
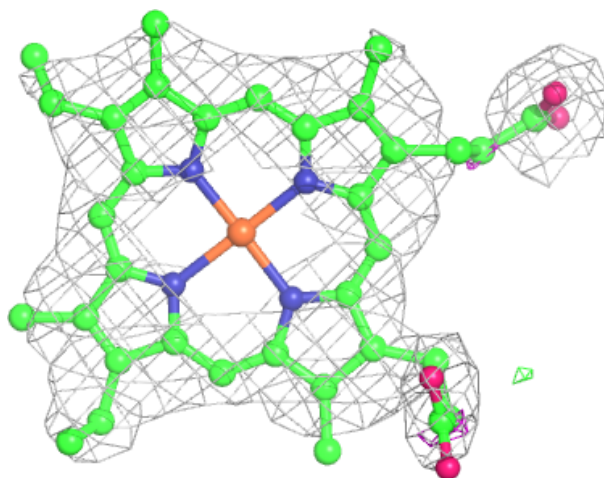
Electron density around HEM A 401:

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



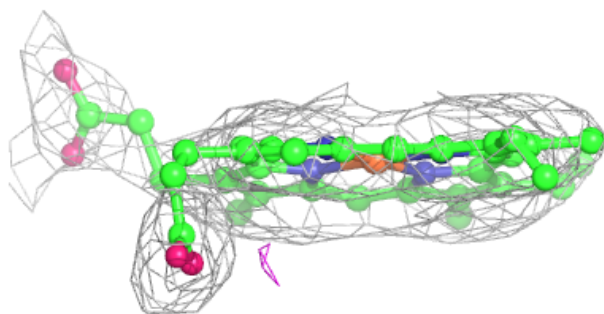
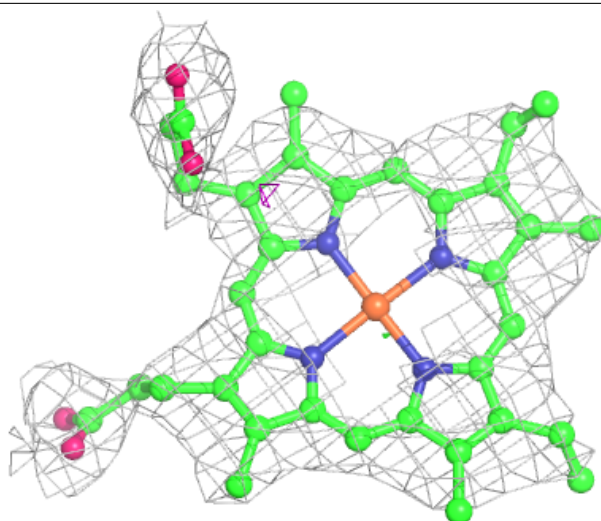
Electron density around HEM B 401:

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



Electron density around HEM D 401:

$2mF_o-DF_c$ (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.