Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 08:32 AM EDT

PDB ID	:	6CR2
Title	:	Crystal structure of sterol 14-alpha demethylase (CYP51B) from Aspergillus fumigatus in complex with the VNI derivative N-(1-(2,4-dichlorophenyl)-2-(1 H-imidazol-1-yl)ethyl)-4-(5-(2-fluoro-4-(2,2,2-trifluoroethoxy)phenyl)-1,3,4-ox adiazol-2-yl)benzamide
Authors	:	Friggeri, L.; Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on	:	2018-03-16
Resolution	:	2.38 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

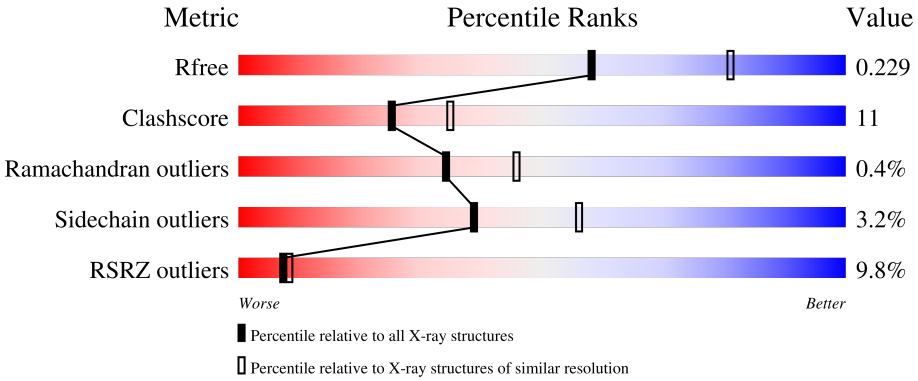
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	477	10% 80% 16%
1	B	477	9% 82% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7762 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.

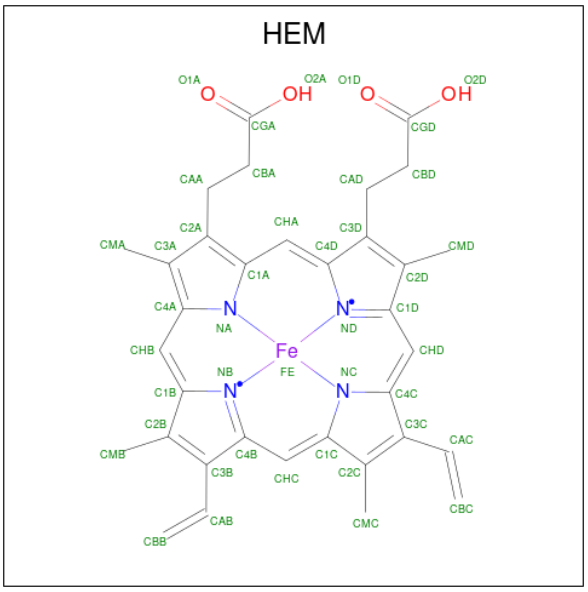
- Molecule 1 is a protein called 14-alpha sterol demethylase Cyp51B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3743	2405	637	684	17			
1	B	469	Total	C	N	O	S	0	0	0
			3743	2405	637	684	17			

There are 20 discrepancies between the modelled and reference sequences:

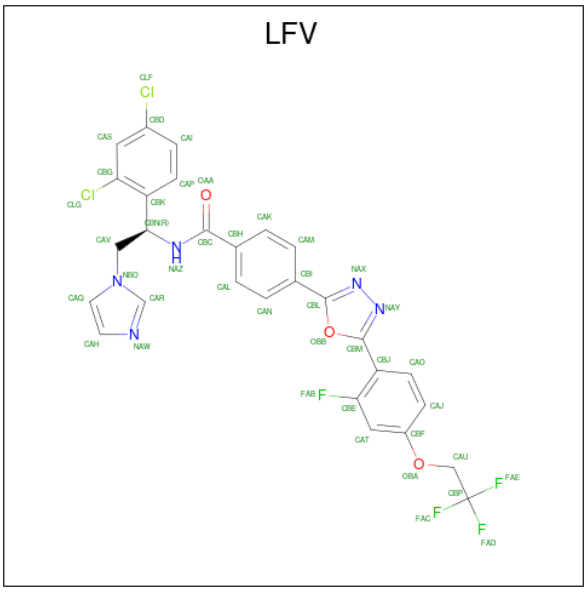
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MET	-	expression tag	UNP E9QY26
A	48	ALA	-	expression tag	UNP E9QY26
A	49	LYS	-	expression tag	UNP E9QY26
A	50	LYS	-	expression tag	UNP E9QY26
A	51	THR	GLU	engineered mutation	UNP E9QY26
A	519	HIS	-	expression tag	UNP E9QY26
A	520	HIS	-	expression tag	UNP E9QY26
A	521	HIS	-	expression tag	UNP E9QY26
A	522	HIS	-	expression tag	UNP E9QY26
A	523	HIS	-	expression tag	UNP E9QY26
B	47	MET	-	expression tag	UNP E9QY26
B	48	ALA	-	expression tag	UNP E9QY26
B	49	LYS	-	expression tag	UNP E9QY26
B	50	LYS	-	expression tag	UNP E9QY26
B	51	THR	GLU	engineered mutation	UNP E9QY26
B	519	HIS	-	expression tag	UNP E9QY26
B	520	HIS	-	expression tag	UNP E9QY26
B	521	HIS	-	expression tag	UNP E9QY26
B	522	HIS	-	expression tag	UNP E9QY26
B	523	HIS	-	expression tag	UNP E9QY26

- 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		

- Molecule 3 is N-[(1R)-1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-4-{5-[2-fluoro-4-(2,2,2-trifluoroethoxy)phenyl]-1,3,4-oxadiazol-2-yl}benzamide (three-letter code: LFV) (formula: $C_{28}H_{19}Cl_2F_4N_5O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			42	28	2	4	5	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			42	28	2	4	5	3		

- Molecule 4 is water.

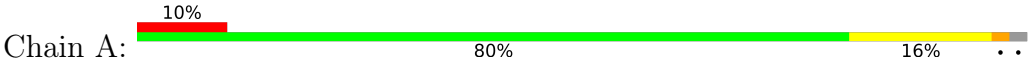
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	24	Total	O	0	0
			24	24		

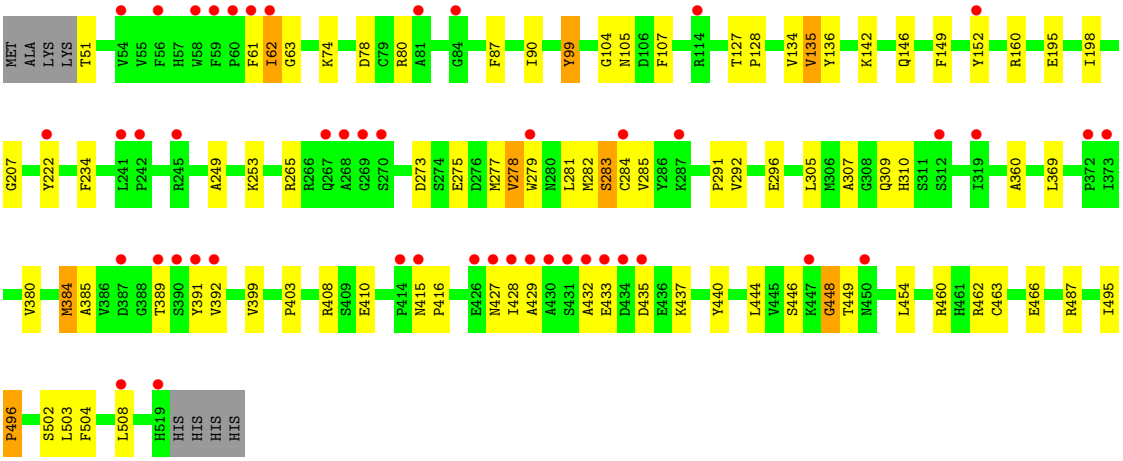
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 14-alpha sterol demethylase Cyp51B

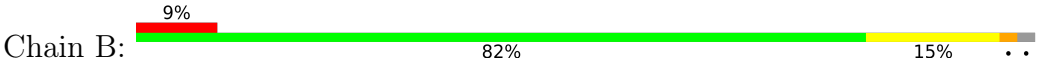
Chain A:

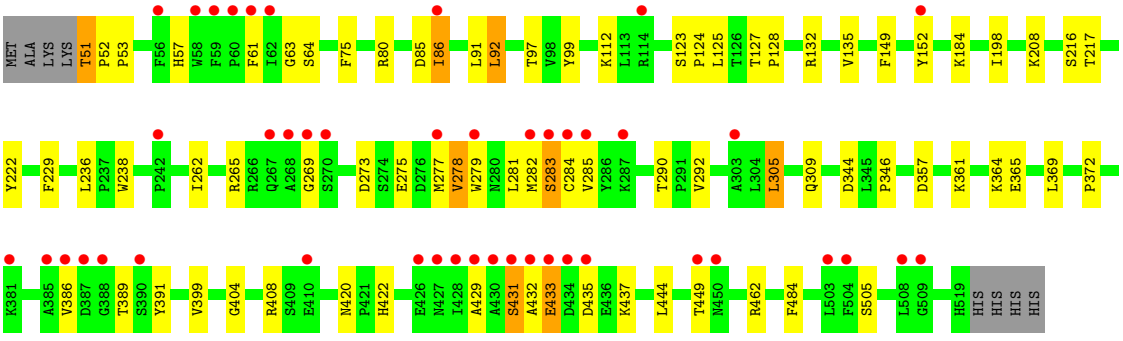




• Molecule 1: 14-alpha sterol demethylase Cyp51B

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	108.44Å 108.44Å 91.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.38 29.60 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.38) 97.0 (29.60-2.38)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.215 , 0.230 0.221 , 0.229	Depositor DCC
R_{free} test set	2251 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.027 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7762	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LFV, 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	0.43	0/3845	0.61	0/5218
1	B	0.41	0/3845	0.62	4/5218 (0.1%)
All	All	0.42	0/7690	0.62	4/10436 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	GLY	N-CA-C	5.56	127.01	113.10
1	B	431	SER	N-CA-C	-5.50	96.15	111.00
1	B	283	SER	N-CA-C	-5.31	96.66	111.00
1	B	484	PHE	N-CA-C	5.04	124.61	111.00

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	3743	0	3706	85	0
1	B	3743	0	3706	67	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
3	A	42	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	0	4	0
4	A	82	0	0	0	0
4	B	24	0	0	0	0
All	All	7762	0	7472	162	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 11.

All (162) 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:152:TYR:HB3	1:A:279:TRP:CZ2	1.53	1.40
3:A:602:LFV:FAB	3:A:602:LFV:CBE	1.57	1.40
1:A:152:TYR:CB	1:A:279:TRP:CZ2	2.40	1.03
1:A:152:TYR:CB	1:A:279:TRP:HZ2	1.73	1.00
1:A:435:ASP:OD2	1:A:448:GLY:HA2	1.60	0.99
1:A:207:GLY:HA3	1:A:275:GLU:OE1	1.60	0.98
1:B:125:LEU:HB2	3:B:602:LFV:CAO	1.97	0.94
1:A:135:VAL:HG12	1:A:136:TYR:N	1.84	0.92
1:B:429:ALA:HB1	1:B:431:SER:O	1.74	0.86
1:A:284:CYS:SG	1:A:291:PRO:HB3	2.17	0.84
1:B:344:ASP:OD1	1:B:346:PRO:HD3	1.75	0.84
1:B:222:TYR:CZ	1:B:305:LEU:HG	2.13	0.84
1:A:222:TYR:CE1	1:A:305:LEU:HD22	2.13	0.84
1:B:279:TRP:CZ2	1:B:283:SER:HB2	2.13	0.83
1:B:279:TRP:CE2	1:B:283:SER:HB2	2.14	0.82
1:A:222:TYR:CZ	1:A:305:LEU:HD22	2.15	0.82
1:A:284:CYS:HB2	1:A:292:VAL:H	1.45	0.81
1:A:152:TYR:HB3	1:A:279:TRP:HZ2	1.04	0.81
1:A:284:CYS:HB2	1:A:292:VAL:N	1.97	0.78
1:A:234:PHE:CE2	3:A:602:LFV:CAJ	2.66	0.78
1:B:386:VAL:HG23	1:B:389:THR:OG1	1.84	0.78
1:A:234:PHE:CE1	3:A:602:LFV:CAO	2.68	0.77
1:A:249:ALA:O	1:A:253:LYS:HG3	1.85	0.76
1:B:222:TYR:CE1	1:B:305:LEU:HD12	2.21	0.75
1:B:278:VAL:O	1:B:282:MET:SD	2.44	0.75
1:B:273:ASP:OD1	1:B:275:GLU:HG3	1.86	0.75
1:A:135:VAL:HG12	1:A:136:TYR:H	1.49	0.75
1:B:284:CYS:O	1:B:292:VAL:HG23	1.86	0.74
1:A:234:PHE:CZ	3:A:602:LFV:CAO	2.70	0.74
1:A:135:VAL:HG12	1:A:136:TYR:CG	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:HG23	1:B:52:PRO:HD2	1.71	0.73
1:B:152:TYR:HB3	1:B:279:TRP:CZ2	2.23	0.73
1:A:435:ASP:OD2	1:A:448:GLY:CA	2.36	0.72
1:A:433:GLU:HB2	1:A:446:SER:OG	1.90	0.71
1:B:61:PHE:O	1:B:61:PHE:CD2	2.46	0.69
1:B:284:CYS:O	1:B:292:VAL:N	2.24	0.69
1:A:234:PHE:CZ	1:A:502:SER:HA	2.28	0.68
1:A:273:ASP:OD1	1:A:275:GLU:HG2	1.93	0.67
1:A:105:ASN:HB2	1:A:449:THR:HG21	1.77	0.66
1:A:495:ILE:HD12	1:A:496:PRO:O	1.96	0.66
1:A:107:PHE:CZ	1:A:384:MET:HE2	2.31	0.66
1:B:279:TRP:CE2	1:B:283:SER:CB	2.79	0.66
1:B:222:TYR:OH	1:B:305:LEU:HG	1.96	0.65
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.77	0.65
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.81	0.63
1:B:51:THR:HG23	1:B:52:PRO:CD	2.29	0.62
1:A:135:VAL:CG1	1:A:136:TYR:N	2.54	0.61
1:A:105:ASN:HB2	1:A:449:THR:CG2	2.29	0.61
1:A:403:PRO:HB3	1:A:454:LEU:HB2	1.82	0.61
1:A:234:PHE:CD2	3:A:602:LFV:CAJ	2.84	0.60
1:B:435:ASP:CG	1:B:449:THR:O	2.40	0.60
1:B:437:LYS:HB3	1:B:444:LEU:HG	1.82	0.60
1:A:279:TRP:O	1:A:283:SER:HB3	2.02	0.60
1:A:429:ALA:HB3	1:A:432:ALA:HB2	1.83	0.59
1:B:309:GLN:HA	1:B:309:GLN:OE1	2.03	0.59
1:A:107:PHE:CE2	1:A:384:MET:HE2	2.38	0.59
1:A:265:ARG:NH1	1:A:278:VAL:HG13	2.18	0.58
1:A:61:PHE:CG	1:A:61:PHE:O	2.56	0.58
1:B:279:TRP:CZ2	1:B:283:SER:CB	2.86	0.58
1:B:61:PHE:O	1:B:61:PHE:CG	2.56	0.58
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.87	0.57
1:A:142:LYS:NZ	1:A:296:GLU:OE2	2.34	0.57
1:B:265:ARG:NH1	1:B:278:VAL:HG13	2.20	0.57
1:A:195:GLU:O	1:A:198:ILE:HG22	2.05	0.56
1:B:282:MET:SD	1:B:282:MET:N	2.78	0.56
1:B:229:PHE:HE1	3:B:602:LFV:CAL	2.19	0.56
1:A:503:LEU:HG	3:A:602:LFV:CAO	2.36	0.56
1:B:222:TYR:CE1	1:B:305:LEU:CD1	2.88	0.56
1:B:357:ASP:OD2	1:B:361:LYS:NZ	2.25	0.56
1:B:273:ASP:OD1	1:B:275:GLU:CG	2.53	0.56
1:B:281:LEU:HB2	1:B:282:MET:SD	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.89	0.55
1:A:265:ARG:NH2	1:A:275:GLU:OE2	2.32	0.54
1:A:433:GLU:HG2	1:A:433:GLU:O	2.07	0.54
1:B:432:ALA:O	1:B:433:GLU:HB2	2.08	0.54
1:B:435:ASP:OD1	1:B:449:THR:O	2.25	0.54
1:B:216:SER:OG	1:B:217:THR:N	2.38	0.54
1:A:134:VAL:HA	1:A:146:GLN:HE22	1.72	0.54
1:A:437:LYS:HB3	1:A:444:LEU:HG	1.89	0.54
1:A:234:PHE:CZ	3:A:602:LFV:CAJ	2.91	0.54
1:A:61:PHE:O	1:A:61:PHE:CD2	2.62	0.53
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.38	0.53
1:B:57:HIS:CD2	1:B:63:GLY:HA2	2.44	0.53
1:A:463:CYS:HA	2:A:601:HEM:C4D	2.44	0.53
1:A:283:SER:O	1:A:283:SER:OG	2.09	0.53
1:A:284:CYS:O	1:A:292:VAL:N	2.40	0.53
1:A:360:ALA:HB3	1:A:428:ILE:HD11	1.91	0.53
1:B:364:LYS:HZ1	1:B:429:ALA:C	2.12	0.53
1:B:435:ASP:OD2	1:B:449:THR:O	2.26	0.52
1:B:404:GLY:O	1:B:408:ARG:HG2	2.08	0.52
1:A:207:GLY:CA	1:A:275:GLU:OE1	2.45	0.52
1:A:135:VAL:CG1	1:A:136:TYR:H	2.10	0.52
1:A:74:LYS:NZ	1:A:78:ASP:OD2	2.43	0.51
1:A:152:TYR:CG	1:A:279:TRP:HZ2	2.27	0.51
1:B:279:TRP:CH2	1:B:283:SER:HB2	2.44	0.51
1:B:125:LEU:HD22	3:B:602:LFV:CAN	2.40	0.51
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.41	0.50
1:A:284:CYS:CB	1:A:292:VAL:H	2.20	0.50
1:B:372:PRO:HA	1:B:505:SER:HB2	1.93	0.50
1:B:262:ILE:HG12	1:B:281:LEU:HD21	1.94	0.50
1:A:234:PHE:CE2	1:A:502:SER:HA	2.47	0.49
1:B:127:THR:HB	1:B:128:PRO:HD3	1.93	0.49
1:A:310:HIS:ND1	1:A:504:PHE:CE2	2.78	0.49
1:B:262:ILE:HG23	1:B:281:LEU:HD21	1.94	0.49
1:B:112:LYS:H	1:B:112:LYS:HD2	1.78	0.49
1:B:285:VAL:HA	1:B:290:THR:O	2.13	0.49
1:B:149:PHE:O	1:B:279:TRP:NE1	2.43	0.48
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.42	0.48
1:A:198:ILE:HD11	1:A:305:LEU:HD11	1.96	0.48
1:A:275:GLU:HG2	1:A:278:VAL:HG22	1.95	0.48
1:B:198:ILE:HD11	1:B:305:LEU:HD11	1.95	0.48
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HB	1:A:128:PRO:HD3	1.96	0.48
1:B:365:GLU:HA	1:B:365:GLU:OE1	2.14	0.48
1:A:135:VAL:HG12	1:A:136:TYR:CD2	2.48	0.47
1:A:107:PHE:CE2	1:A:384:MET:CE	2.97	0.47
1:B:51:THR:HG23	1:B:52:PRO:N	2.30	0.47
1:A:90:ILE:N	1:A:90:ILE:HD12	2.29	0.47
1:A:234:PHE:HZ	1:A:502:SER:HA	1.76	0.47
1:B:236:LEU:HD23	1:B:238:TRP:CH2	2.50	0.47
1:A:149:PHE:O	1:A:152:TYR:HB2	2.16	0.46
1:B:97:THR:HG23	1:B:399:VAL:HG12	1.97	0.46
1:B:125:LEU:CB	3:B:602:LFV:CAO	2.83	0.46
1:B:80:ARG:NH1	1:B:85:ASP:OD1	2.48	0.46
1:B:279:TRP:CD2	1:B:283:SER:HB2	2.51	0.46
3:A:602:LFV:FAB	3:A:602:LFV:NAY	2.39	0.45
1:B:51:THR:HA	1:B:52:PRO:HD3	1.53	0.45
1:A:62:ILE:HD13	1:A:62:ILE:HA	1.78	0.45
1:A:385:ALA:HB2	1:A:392:VAL:HG22	1.99	0.45
1:B:236:LEU:CD2	1:B:238:TRP:CH2	3.00	0.45
1:B:262:ILE:HG23	1:B:281:LEU:CD2	2.47	0.45
1:A:265:ARG:HH12	1:A:278:VAL:HG13	1.81	0.45
1:B:64:SER:HB3	1:B:75:PHE:CE1	2.52	0.45
1:A:275:GLU:CG	1:A:278:VAL:HG22	2.46	0.44
1:A:449:THR:O	1:A:449:THR:HG22	2.17	0.44
1:B:91:LEU:O	1:B:92:LEU:HB2	2.17	0.44
1:A:462:ARG:NH2	1:A:466:GLU:OE1	2.49	0.44
1:B:277:MET:O	1:B:281:LEU:HG	2.17	0.44
1:A:135:VAL:CG1	1:A:136:TYR:CD2	3.00	0.44
1:A:99:TYR:CG	1:A:104:GLY:HA2	2.52	0.44
1:A:415:ASN:N	1:A:416:PRO:HD3	2.33	0.44
1:A:309:GLN:HA	1:A:309:GLN:OE1	2.18	0.43
1:A:277:MET:C	1:A:279:TRP:N	2.69	0.43
1:A:369:LEU:O	1:A:408:ARG:NH2	2.51	0.43
1:A:440:TYR:CD2	1:A:460:ARG:HA	2.54	0.43
1:A:380:VAL:CG2	1:A:399:VAL:HG13	2.48	0.43
1:A:504:PHE:CZ	3:A:602:LFV:OAA	2.72	0.43
1:B:86:ILE:HD12	1:B:86:ILE:N	2.34	0.43
1:A:63:GLY:HA3	1:A:90:ILE:HB	2.01	0.42
1:A:152:TYR:CB	1:A:279:TRP:CE2	3.00	0.42
1:B:420:ASN:OD1	1:B:422:HIS:HB2	2.19	0.42
1:A:504:PHE:HZ	3:A:602:LFV:OAA	2.02	0.42
1:B:369:LEU:O	1:B:408:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:HG1	1:A:391:TYR:HD2	1.61	0.42
1:B:123:SER:N	1:B:124:PRO:HD2	2.36	0.41
1:A:307:ALA:HB2	3:A:602:LFV:CAS	2.51	0.41
1:B:53:PRO:HD3	1:B:391:TYR:CE1	2.56	0.41
1:A:284:CYS:HG	1:A:291:PRO:HB3	1.81	0.41
1:B:152:TYR:CB	1:B:279:TRP:CZ2	3.01	0.41
1:B:432:ALA:O	1:B:433:GLU:CB	2.69	0.41
1:A:277:MET:O	1:A:281:LEU:HD13	2.20	0.40
1:A:234:PHE:CD2	3:A:602:LFV:CBF	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/477 (98%)	457 (98%)	8 (2%)	2 (0%)	34	46
1	B	467/477 (98%)	457 (98%)	8 (2%)	2 (0%)	34	46
All	All	934/954 (98%)	914 (98%)	16 (2%)	4 (0%)	34	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLY
1	B	433	GLU
1	A	135	VAL
1	B	135	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	410/417 (98%)	394 (96%)	16 (4%)	32 48
1	B	410/417 (98%)	400 (98%)	10 (2%)	49 66
All	All	820/834 (98%)	794 (97%)	26 (3%)	39 56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	62	ILE
1	A	80	ARG
1	A	87	PHE
1	A	99	TYR
1	A	160	ARG
1	A	278	VAL
1	A	282	MET
1	A	283	SER
1	A	285	VAL
1	A	384	MET
1	A	410	GLU
1	A	427	ASN
1	A	487	ARG
1	A	496	PRO
1	A	508	LEU
1	B	51	THR
1	B	86	ILE
1	B	92	LEU
1	B	99	TYR
1	B	132	ARG
1	B	184	LYS
1	B	208	LYS
1	B	278	VAL
1	B	305	LEU
1	B	462	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LFV	A	602	2	38,46,46	2.87	10 (26%)	57,66,66	2.17	20 (35%)
2	HEM	B	601	3,1	41,50,50	1.40	7 (17%)	45,82,82	2.10	15 (33%)
3	LFV	B	602	2	38,46,46	1.99	6 (15%)	57,66,66	1.64	12 (21%)
2	HEM	A	601	3,1	41,50,50	1.40	7 (17%)	45,82,82	2.02	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFV	A	602	2	-	1/25/30/30	0/5/5/5
2	HEM	B	601	3,1	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFV	B	602	2	-	2/25/30/30	0/5/5/5
2	HEM	A	601	3,1	-	0/12/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	LFV	FAB-CBE	8.36	1.57	1.35
3	A	602	LFV	CBK-CBN	-8.22	1.39	1.52
3	B	602	LFV	CBK-CBN	-8.14	1.39	1.52
3	A	602	LFV	CBH-CBC	-6.49	1.36	1.50
3	A	602	LFV	FAD-CBP	-5.50	1.11	1.33
3	A	602	LFV	FAE-CBP	-5.29	1.12	1.33
3	B	602	LFV	CBH-CBC	-5.09	1.39	1.50
3	B	602	LFV	FAD-CBP	-5.04	1.13	1.33
3	A	602	LFV	CAQ-NBO	-4.43	1.29	1.37
2	B	601	HEM	C1B-NB	-3.66	1.34	1.40
2	A	601	HEM	C1B-NB	-3.61	1.34	1.40
2	B	601	HEM	C4D-ND	-3.61	1.34	1.40
2	A	601	HEM	C4D-ND	-3.59	1.34	1.40
3	A	602	LFV	NAX-NAY	-3.29	1.31	1.37
3	A	602	LFV	CBD-CLF	-3.26	1.67	1.74
3	A	602	LFV	FAC-CBP	-2.79	1.22	1.33
2	A	601	HEM	FE-NB	2.64	2.09	1.96
2	B	601	HEM	FE-NB	2.62	2.09	1.96
3	B	602	LFV	FAE-CBP	-2.49	1.23	1.33
2	B	601	HEM	C1D-ND	-2.37	1.33	1.38
2	A	601	HEM	C1D-ND	-2.35	1.34	1.38
2	A	601	HEM	C4B-NB	-2.32	1.34	1.38
2	B	601	HEM	C4B-NB	-2.32	1.34	1.38
2	A	601	HEM	FE-ND	-2.31	1.85	1.96
2	B	601	HEM	FE-ND	-2.30	1.85	1.96
3	B	602	LFV	CAQ-NBO	-2.23	1.33	1.37
3	B	602	LFV	FAC-CBP	-2.20	1.24	1.33
2	B	601	HEM	CHB-C1B	2.15	1.40	1.35
2	A	601	HEM	CHB-C1B	2.13	1.40	1.35
3	A	602	LFV	CAK-CBH	-2.08	1.35	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CHC-C4B-NB	6.07	131.03	124.43
2	A	601	HEM	CHC-C4B-NB	5.98	130.93	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	LFV	CBN-CAV-NBO	5.64	119.55	112.25
3	A	602	LFV	OBA-CAU-CBP	5.60	120.90	108.15
3	A	602	LFV	CBI-CBL-NAX	4.83	132.29	124.12
2	B	601	HEM	CHD-C1D-ND	4.76	129.60	124.43
3	A	602	LFV	CAP-CAI-CBD	4.67	124.17	119.24
3	A	602	LFV	CBN-CAV-NBO	4.39	117.93	112.25
2	A	601	HEM	CHD-C1D-ND	4.19	128.98	124.43
2	B	601	HEM	CHD-C1D-C2D	-3.95	118.80	124.98
3	A	602	LFV	CAI-CBD-CAS	-3.88	116.38	121.53
3	B	602	LFV	CAP-CBK-CBG	3.84	120.63	116.81
2	A	601	HEM	CHA-C4D-ND	3.80	129.07	124.38
2	B	601	HEM	C1B-NB-C4B	3.68	108.87	105.07
3	A	602	LFV	CAV-CBN-NAZ	-3.66	104.07	110.45
3	A	602	LFV	CAP-CBK-CBG	3.65	120.44	116.81
3	B	602	LFV	CAS-CBD-CLF	3.58	123.62	119.15
2	A	601	HEM	CHA-C4D-C3D	-3.53	118.70	125.33
3	A	602	LFV	CAM-CBI-CBL	3.47	125.74	120.44
3	A	602	LFV	CAS-CBD-CLF	3.46	123.48	119.15
2	B	601	HEM	CHA-C4D-C3D	-3.38	118.98	125.33
2	A	601	HEM	CHD-C1D-C2D	-3.37	119.71	124.98
2	B	601	HEM	CHA-C4D-ND	3.33	128.50	124.38
2	B	601	HEM	CHB-C1B-NB	3.18	128.31	124.38
2	A	601	HEM	C1B-NB-C4B	3.12	108.29	105.07
3	A	602	LFV	CAJ-CBF-CAT	-3.06	116.32	120.53
3	A	602	LFV	CAT-CBE-CBJ	-3.02	118.89	123.64
2	A	601	HEM	CHB-C1B-NB	2.99	128.08	124.38
3	B	602	LFV	CAV-CBN-NAZ	-2.98	105.25	110.45
2	B	601	HEM	CAD-C3D-C4D	2.93	129.78	124.66
2	A	601	HEM	CHC-C4B-C3B	-2.87	120.17	124.57
3	A	602	LFV	CAO-CBJ-CBE	2.86	120.22	116.10
3	B	602	LFV	CAV-NBO-CAQ	2.84	131.78	125.92
3	A	602	LFV	CAU-OBA-CBF	-2.81	108.99	117.81
3	B	602	LFV	CAS-CBG-CBK	-2.68	119.20	122.41
2	B	601	HEM	CHC-C4B-C3B	-2.58	120.62	124.57
2	A	601	HEM	C4B-C3B-C2B	-2.48	105.14	107.11
3	B	602	LFV	CBI-CBL-NAX	2.45	128.27	124.12
2	B	601	HEM	O2D-CGD-CBD	2.39	121.70	114.03
2	B	601	HEM	CBA-CAA-C2A	-2.38	108.56	112.62
3	A	602	LFV	FAB-CBE-CAT	2.35	123.28	118.61
3	B	602	LFV	CAV-NBO-CAR	-2.33	121.17	125.76
3	A	602	LFV	CAI-CAP-CBK	-2.30	117.24	121.13
3	B	602	LFV	CAS-CBG-CLG	2.29	122.19	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	LFV	CBM-NAY-NAX	-2.29	100.57	105.29
2	A	601	HEM	CAD-C3D-C4D	2.24	128.58	124.66
3	A	602	LFV	CBG-CAS-CBD	2.22	121.20	118.71
3	B	602	LFV	CBJ-CBM-NAY	2.19	127.55	123.86
2	B	601	HEM	O2A-CGA-CBA	2.18	121.03	114.03
2	A	601	HEM	O2D-CGD-CBD	2.15	120.94	114.03
3	B	602	LFV	CAI-CBD-CLF	-2.14	116.01	119.35
3	A	602	LFV	FAD-CBP-FAE	2.13	114.25	106.43
2	A	601	HEM	O2A-CGA-CBA	2.13	120.86	114.03
2	B	601	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
3	B	602	LFV	CAT-CBE-CBJ	-2.11	120.31	123.64
2	B	601	HEM	C3D-C4D-ND	2.10	112.51	110.17
2	A	601	HEM	CHB-C1B-C2B	-2.03	121.11	126.72
2	B	601	HEM	CMD-C2D-C1D	2.02	128.12	125.04
3	A	602	LFV	CAO-CAJ-CBF	2.02	122.20	119.73
3	A	602	LFV	CAQ-NBO-CAR	-2.02	106.22	108.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	LFV	CAM-CBI-CBL-NAX
3	B	602	LFV	CAN-CBI-CBL-NAX
2	B	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O1D
3	A	602	LFV	CAO-CBJ-CBM-NAY

There are no ring outliers.

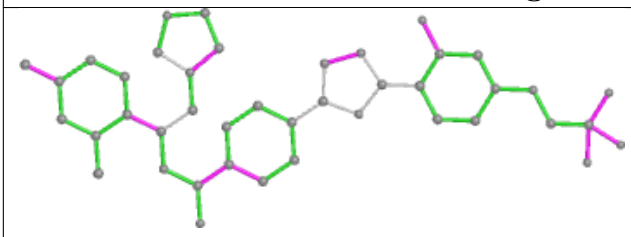
4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	LFV	12	0
2	B	601	HEM	4	0
3	B	602	LFV	4	0
2	A	601	HEM	5	0

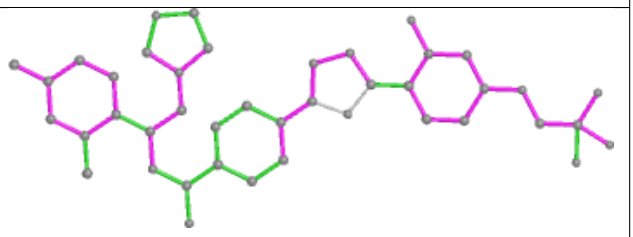
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

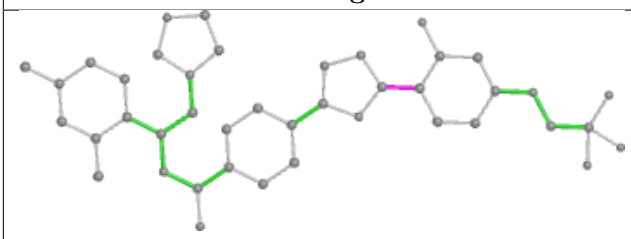
Ligand LFV A 602



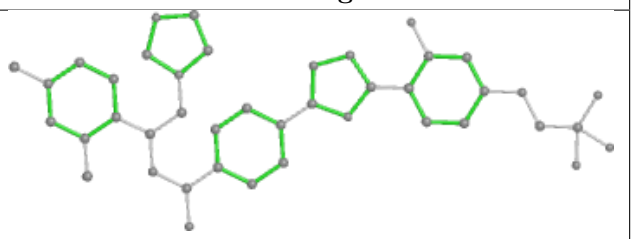
Bond lengths



Bond angles

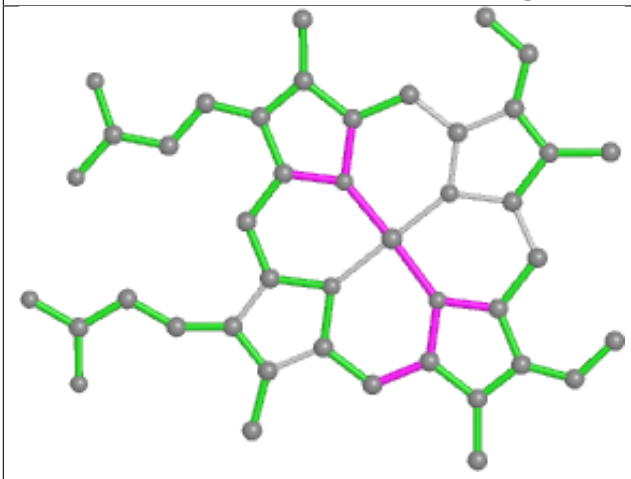


Torsions

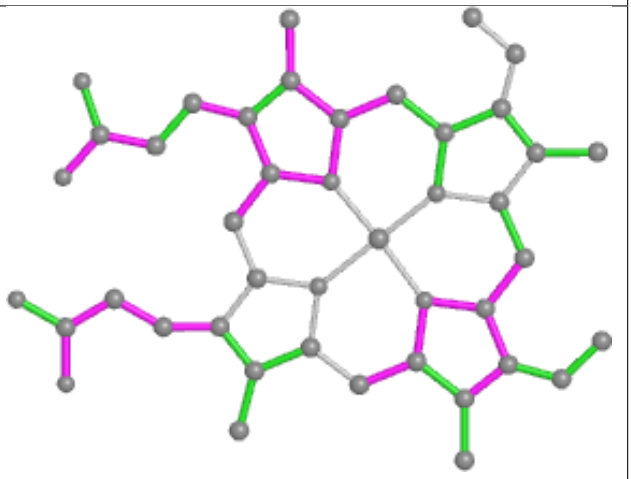


Rings

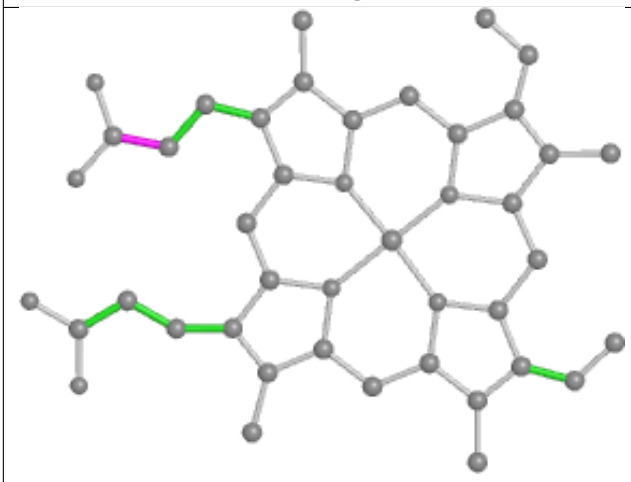
Ligand HEM B 601



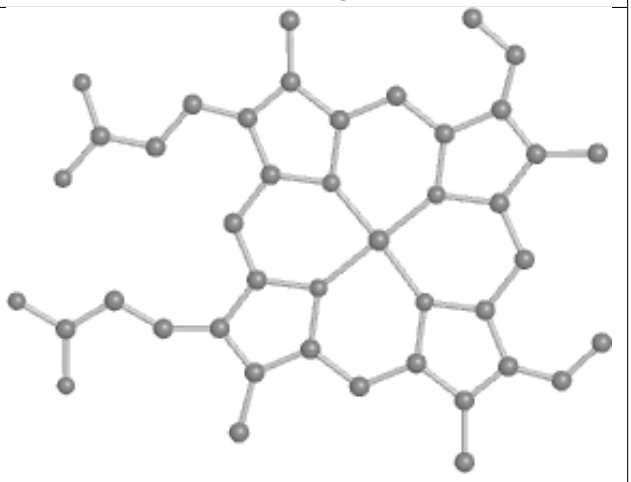
Bond lengths



Bond angles

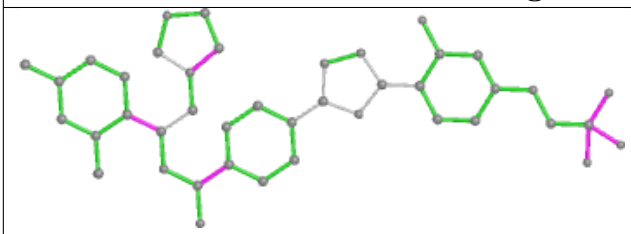


Torsions

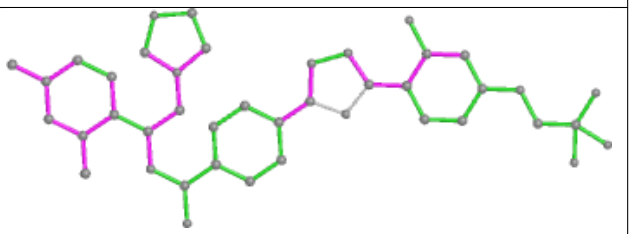


Rings

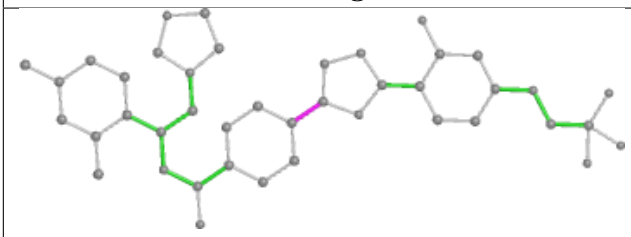
Ligand LFV B 602



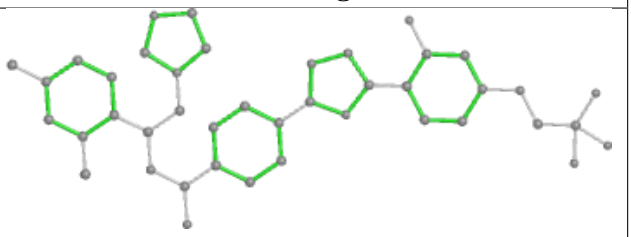
Bond lengths



Bond angles

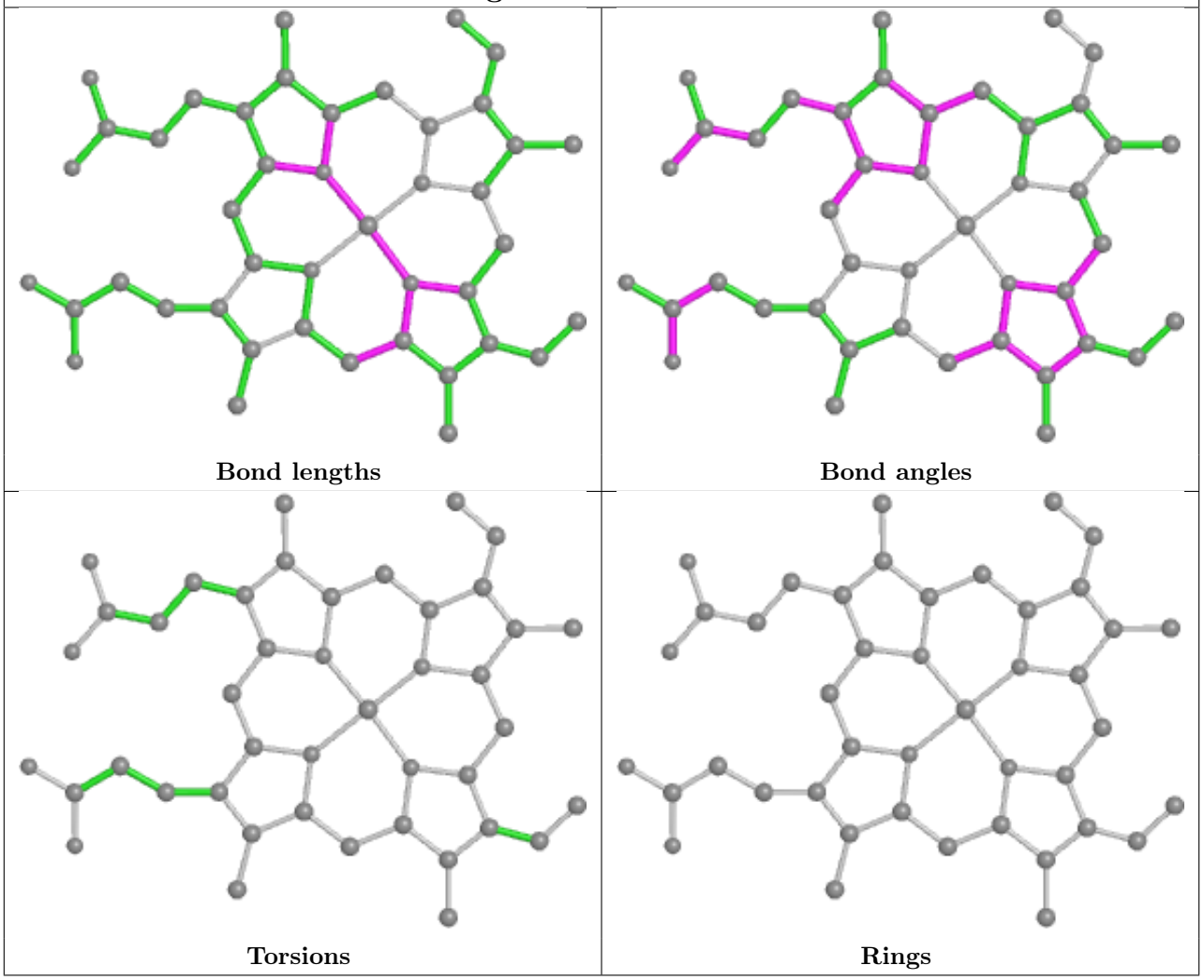


Torsions



Rings

Ligand HEM A 601



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, 95^{th} 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	469/477 (98%)	0.70	47 (10%)	7	8	15, 38, 77, 163	0
1	B	469/477 (98%)	0.62	45 (9%)	8	9	13, 34, 73, 181	0
All	All	938/954 (98%)	0.66	92 (9%)	7	8	13, 36, 76, 181	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	ALA	19.3
1	B	432	ALA	15.8
1	B	431	SER	15.3
1	A	430	ALA	13.9
1	A	427	ASN	13.4
1	A	432	ALA	11.8
1	B	433	GLU	11.4
1	A	431	SER	10.3
1	A	428	ILE	10.0
1	B	429	ALA	9.8
1	B	427	ASN	8.9
1	A	284	CYS	8.6
1	B	428	ILE	7.9
1	A	433	GLU	6.9
1	A	269	GLY	6.7
1	B	430	ALA	6.7
1	A	434	ASP	6.4
1	A	270	SER	6.3
1	B	283	SER	6.3
1	A	426	GLU	5.8
1	B	284	CYS	5.7
1	B	434	ASP	5.6
1	B	268	ALA	5.6
1	B	270	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	58	TRP	4.7
1	B	269	GLY	4.6
1	B	390	SER	4.4
1	A	56	PHE	4.4
1	A	61	PHE	4.3
1	A	387	ASP	4.3
1	B	60	PRO	4.2
1	B	59	PHE	4.2
1	B	386	VAL	4.2
1	B	387	ASP	4.0
1	B	58	TRP	4.0
1	B	61	PHE	3.8
1	B	435	ASP	3.8
1	B	56	PHE	3.8
1	A	59	PHE	3.6
1	B	152	TYR	3.6
1	A	241	LEU	3.4
1	B	287	LYS	3.3
1	B	449	THR	3.3
1	A	60	PRO	3.3
1	B	114	ARG	3.2
1	B	282	MET	3.2
1	A	392	VAL	3.1
1	A	245	ARG	3.1
1	B	242	PRO	3.0
1	B	279	TRP	3.0
1	B	62	ILE	3.0
1	A	519	HIS	2.9
1	A	267	GLN	2.9
1	A	268	ALA	2.9
1	A	450	ASN	2.9
1	B	410	GLU	2.9
1	B	426	GLU	2.9
1	B	508	LEU	2.9
1	A	391	TYR	2.9
1	A	114	ARG	2.8
1	A	435	ASP	2.8
1	A	415	ASN	2.7
1	A	319	ILE	2.7
1	A	279	TRP	2.7
1	B	504	PHE	2.7
1	B	450	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	285	VAL	2.6
1	A	389	THR	2.6
1	A	373	ILE	2.5
1	B	267	GLN	2.5
1	A	372	PRO	2.5
1	B	277	MET	2.4
1	B	388	GLY	2.4
1	B	503	LEU	2.4
1	A	390	SER	2.4
1	A	287	LYS	2.3
1	B	385	ALA	2.3
1	A	222	TYR	2.2
1	A	152	TYR	2.2
1	A	447	LYS	2.2
1	A	242	PRO	2.2
1	A	414	PRO	2.2
1	A	54	VAL	2.2
1	B	509	GLY	2.2
1	A	312	SER	2.2
1	B	303	ALA	2.1
1	B	381	LYS	2.1
1	A	81	ALA	2.1
1	A	62	ILE	2.1
1	A	84	GLY	2.1
1	B	86	ILE	2.1
1	A	508	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

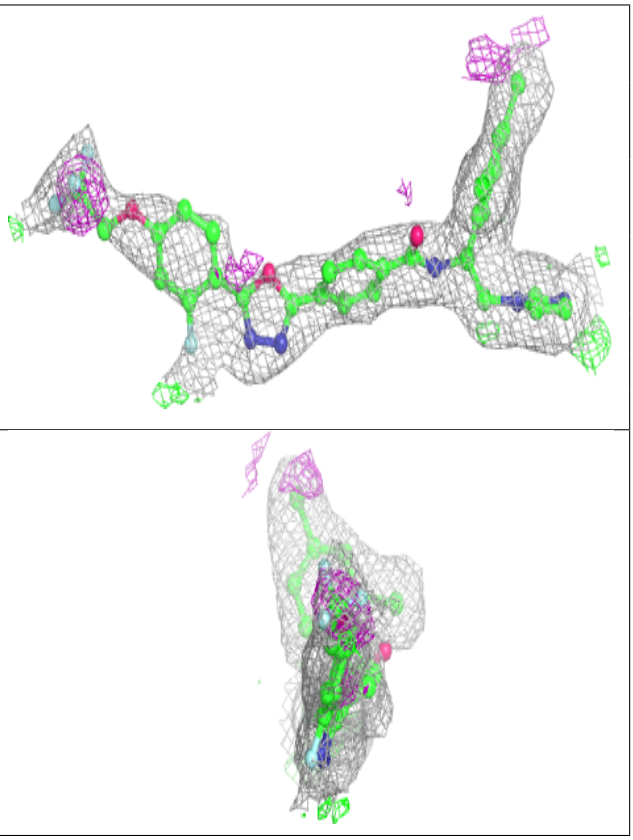
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFV	B	602	42/42	0.80	0.24	27,55,72,83	0
3	LFV	A	602	42/42	0.94	0.18	23,71,124,138	0
2	HEM	A	601	43/43	0.96	0.17	19,23,28,29	0
2	HEM	B	601	43/43	0.97	0.17	14,17,26,31	0

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

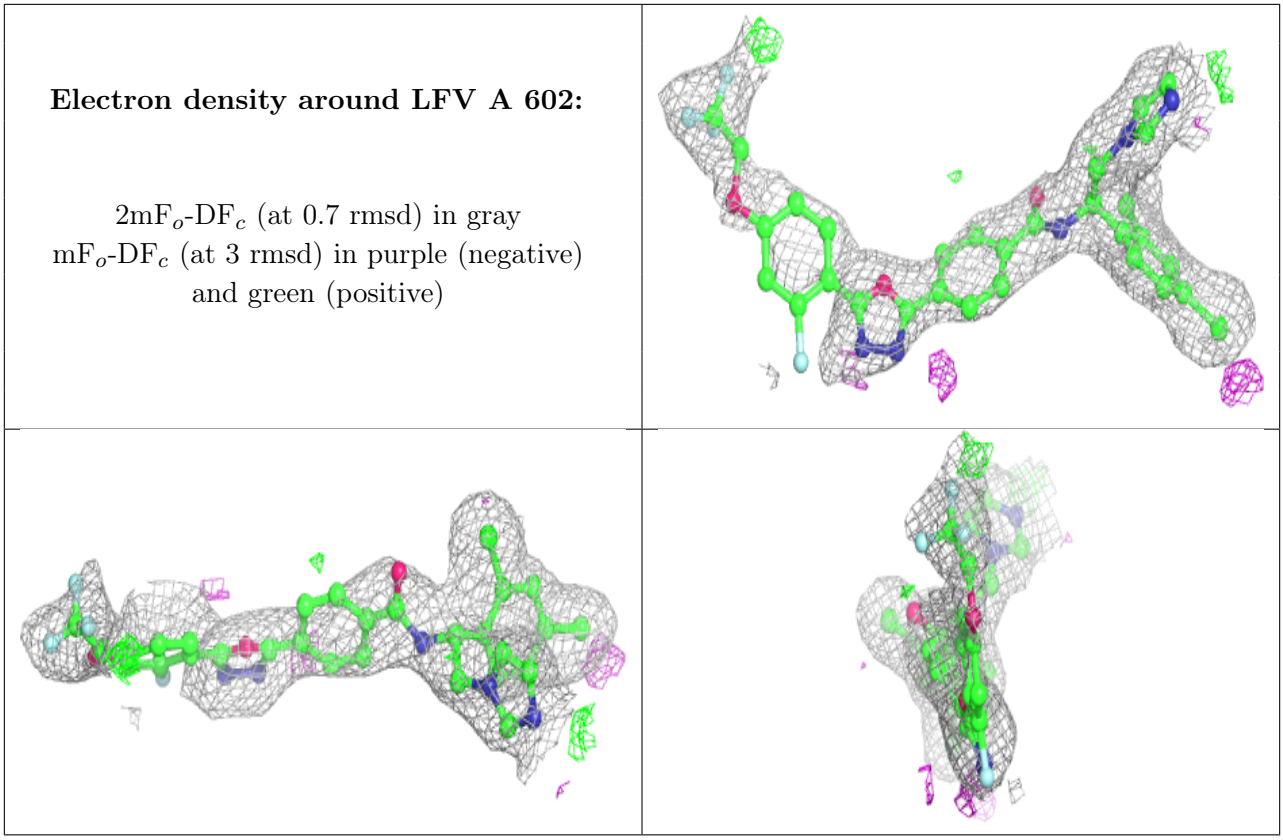
Electron density around LFV B 602:

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



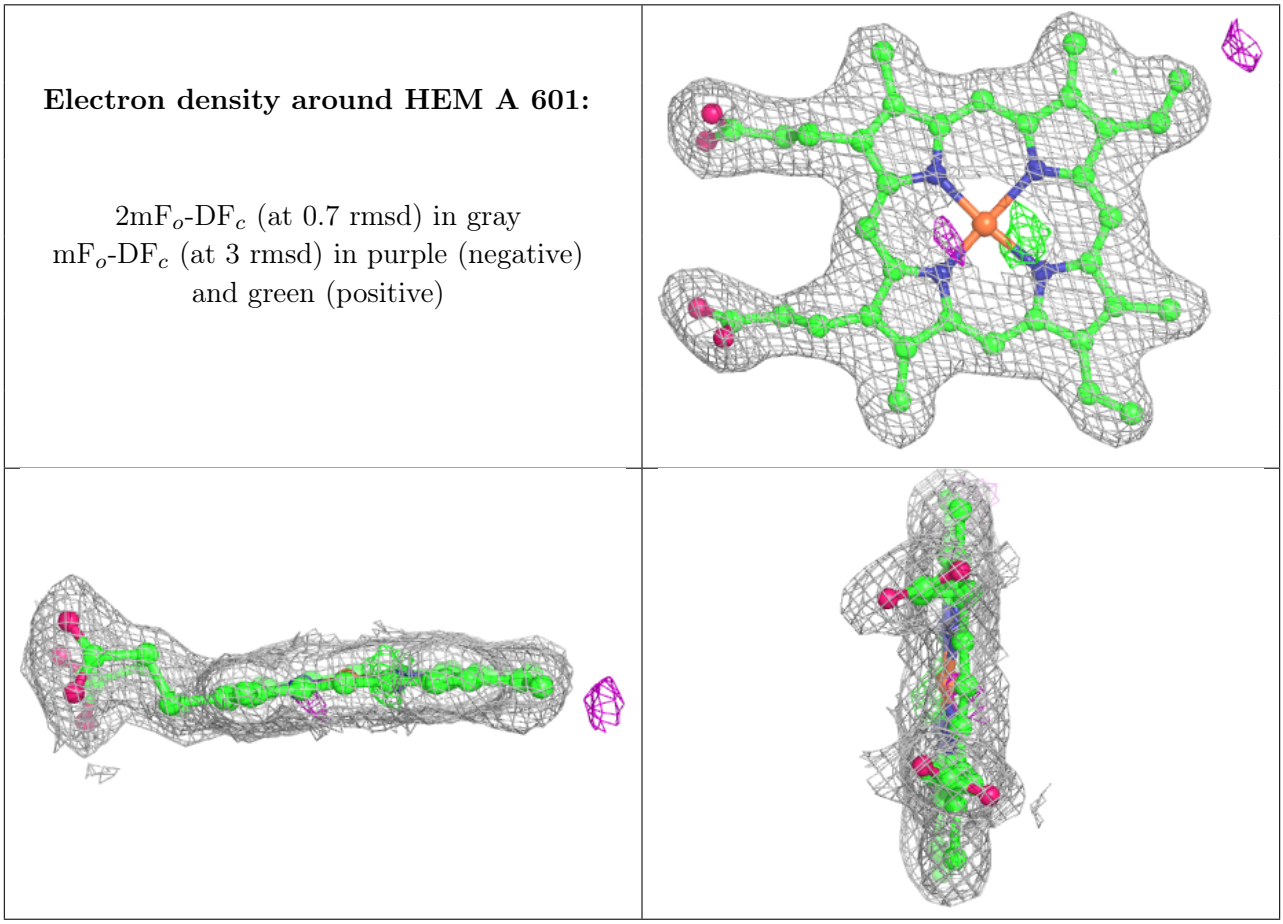
Electron density around LFV A 602:

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



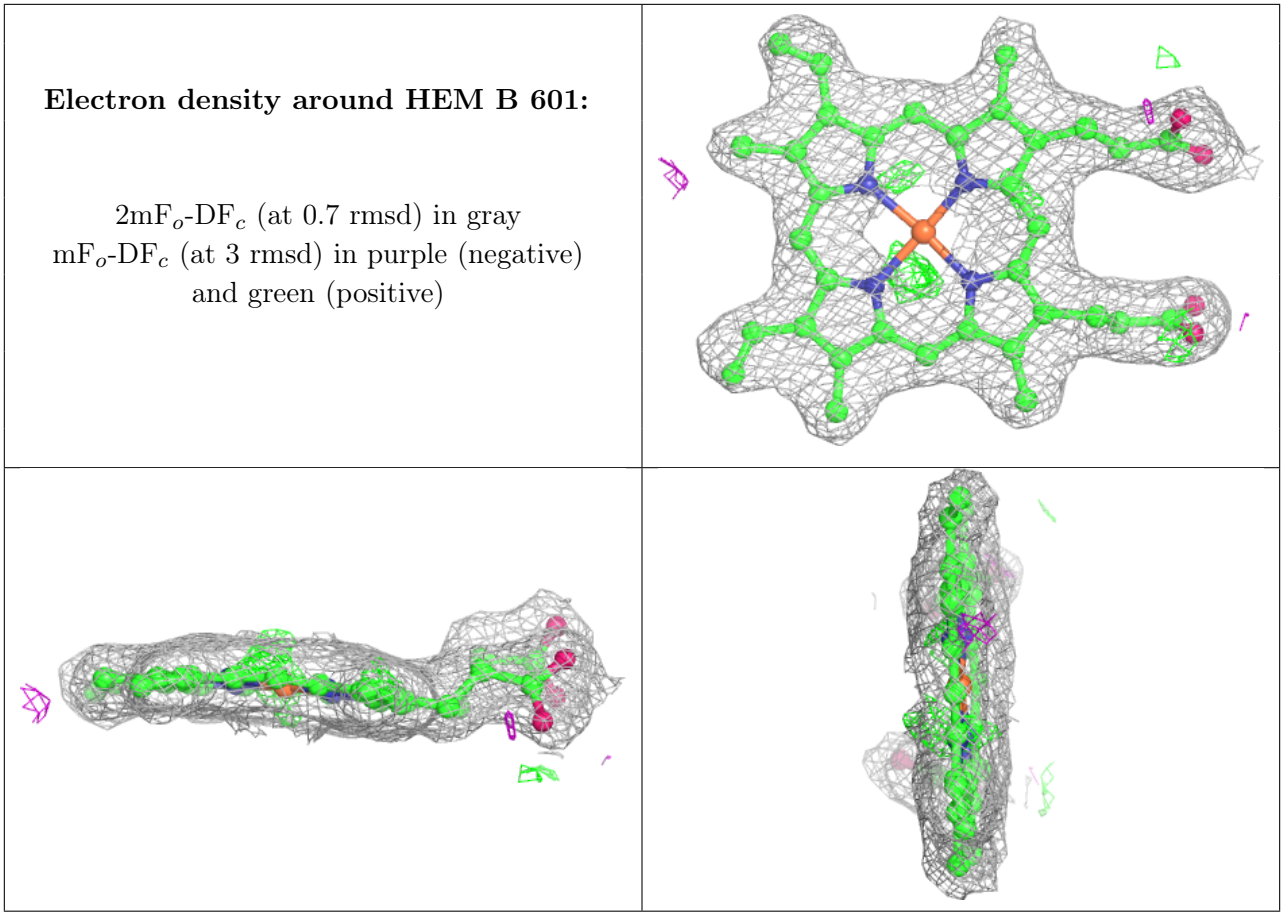
Electron density around HEM A 601:

$2mF_o$-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 601:

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



6.5 Other polymers

There are no such residues in this entry.