



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:13 AM UTC

PDB ID : 7ZSU / pdb_00007zsu
Title : Crystal structure of CYP125 from Mycobacterium tuberculosis in complex with an inhibitor
Authors : Snee, M.; Katariya, M.; Levy, C.; Leys, D.
Deposited on : 2022-05-09
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

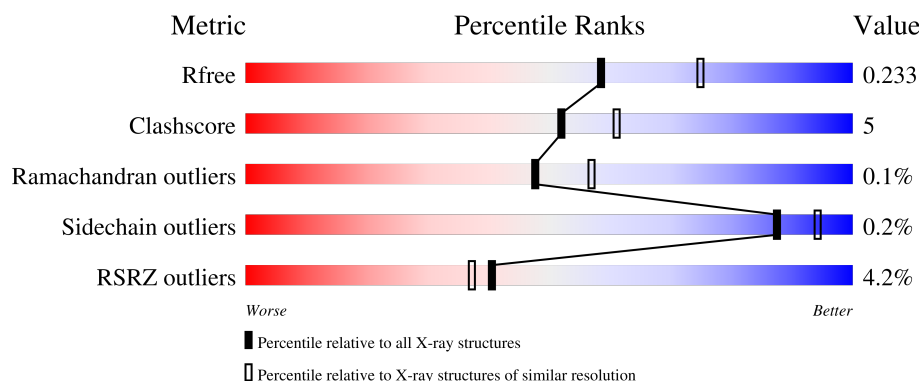
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	418	0% 90% 8% .
1	B	418	7% 86% 10% .
1	C	418	4% 87% 11% .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19395 atoms, of which 9322 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.

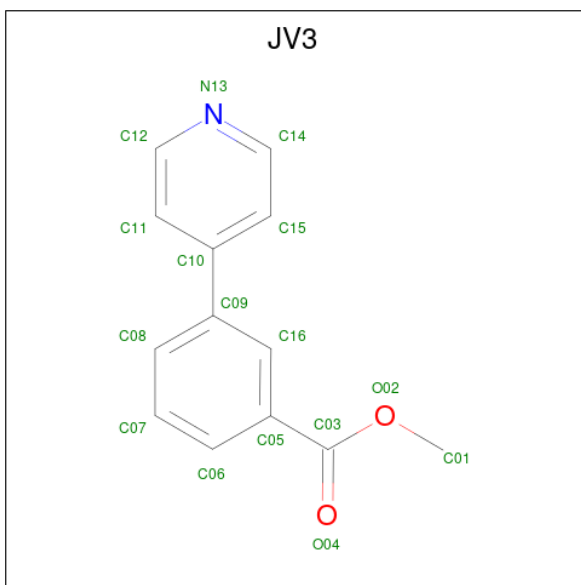
- Molecule 1 is a protein called Steroid C26-monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	H	N	O	S	0	0	0
			6338	2045	3105	569	606	13			
1	B	402	Total	C	H	N	O	S	0	0	0
			6168	1998	3013	554	590	13			
1	C	407	Total	C	H	N	O	S	0	0	0
			6270	2025	3070	560	602	13			

There are 6 discrepancies between the modelled and reference sequences:

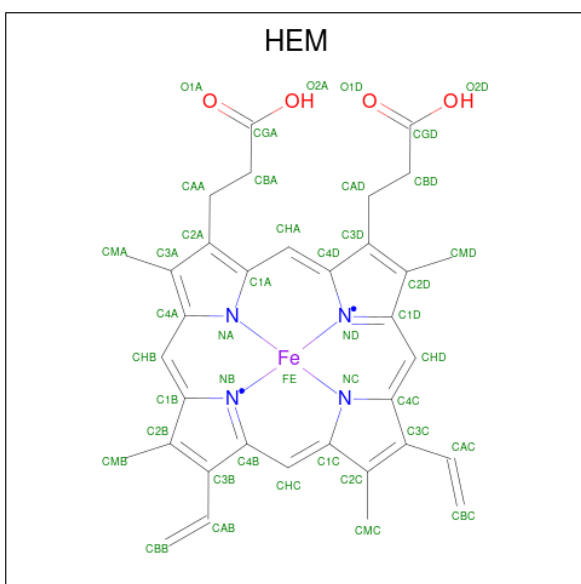
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	-	expression tag	UNP P9WPP1
A	17	GLY	-	expression tag	UNP P9WPP1
B	16	ASN	-	expression tag	UNP P9WPP1
B	17	GLY	-	expression tag	UNP P9WPP1
C	16	ASN	-	expression tag	UNP P9WPP1
C	17	GLY	-	expression tag	UNP P9WPP1

- Molecule 2 is methyl 3-pyridin-4-ylbenzoate (CCD ID: JV3) (formula: C₁₃H₁₁NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	13	11	1	2		
2	A	1	Total	C	H	N	O	0	0
			27	13	11	1	2		
2	B	1	Total	C	H	N	O	0	0
			27	13	11	1	2		
2	C	1	Total	C	H	N	O	0	0
			27	13	11	1	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

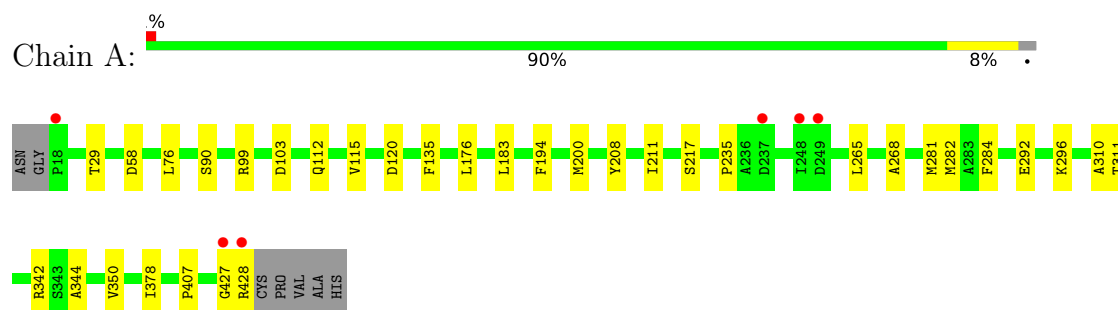
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total	O	0	0
			171	171		
5	B	66	Total	O	0	0
			66	66		
5	C	40	Total	O	0	0
			40	40		

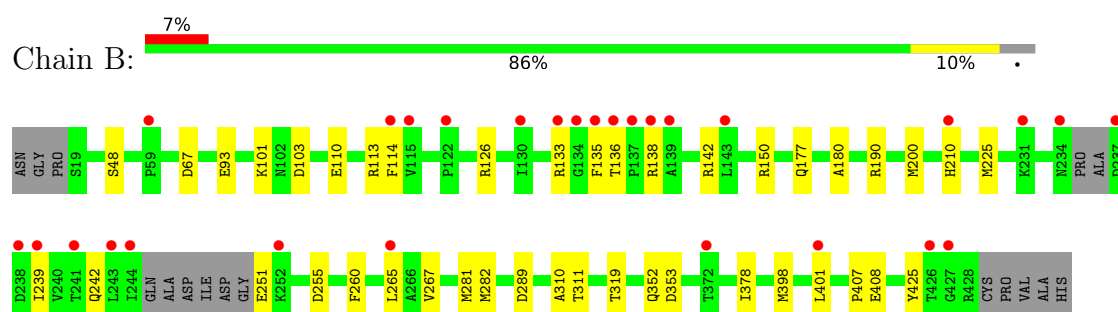
3 Residue-property plots [i](#)

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.

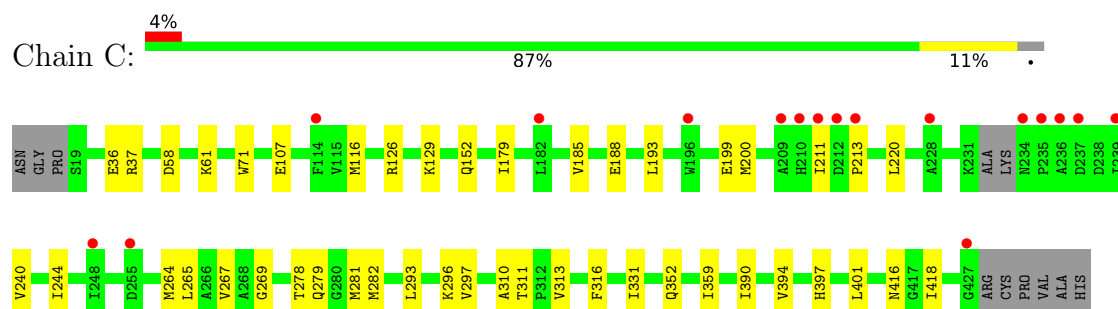
- Molecule 1: Steroid C26-monooxygenase



- Molecule 1: Steroid C26-monooxygenase



- Molecule 1: Steroid C26-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.19Å 68.90Å 144.10Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	60.20 – 2.20 60.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (60.20-2.20) 95.8 (60.20-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.233 0.209 , 0.233	Depositor DCC
R_{free} test set	3392 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19395	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JV3, SO4, 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	0.13	0/3317	0.34	0/4501
1	B	0.12	0/3235	0.28	0/4389
1	C	0.11	0/3281	0.29	0/4451
All	All	0.12	0/9833	0.30	0/13341

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3233	3105	3103	25	0
1	B	3155	3013	3011	28	0
1	C	3200	3070	3069	36	0
2	A	32	22	0	1	0
2	B	16	11	0	0	0
2	C	16	11	0	0	0
3	A	43	30	30	2	0
3	B	43	30	30	5	0
3	C	43	30	30	5	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	2	0
4	C	5	0	0	0	0
5	A	171	0	0	1	0
5	B	66	0	0	1	0
5	C	40	0	0	0	0
All	All	10073	9322	9273	97	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 5.

All (97) 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:B:281:MET:HE2	1:B:401:LEU:HD22	1.57	0.86
1:B:408:GLU:OE2	5:B:601:HOH:O	2.02	0.77
1:C:281:MET:HE2	1:C:401:LEU:HD22	1.76	0.67
1:C:278:THR:HG22	1:C:282:MET:HE2	1.76	0.67
3:B:502:HEM:HMC1	3:B:502:HEM:HBC2	1.77	0.66
1:C:185:VAL:HG21	1:C:193:LEU:HD22	1.77	0.64
3:C:502:HEM:HMC1	3:C:502:HEM:HBC2	1.78	0.63
1:B:136:THR:HG22	1:B:138:ARG:H	1.65	0.61
1:A:90:SER:OG	1:A:120:ASP:OD2	2.18	0.57
1:B:101:LYS:HE2	4:B:503:SO4:O1	2.05	0.56
1:B:210:HIS:H	1:B:210:HIS:CD2	2.23	0.56
3:C:502:HEM:HBC2	3:C:502:HEM:CMC	2.36	0.56
1:C:282:MET:HE1	1:C:418:ILE:CD1	2.36	0.55
1:C:264:MET:SD	3:C:502:HEM:HMD3	2.46	0.55
1:C:152:GLN:OE1	1:C:397:HIS:NE2	2.39	0.54
1:C:296:LYS:HG2	1:C:297:VAL:HG23	1.91	0.53
1:C:107:GLU:N	1:C:107:GLU:OE1	2.39	0.53
1:C:278:THR:HG22	1:C:282:MET:CE	2.40	0.52
1:A:428:ARG:HA	1:A:428:ARG:HE	1.75	0.52
1:C:279:GLN:HA	1:C:282:MET:HE3	1.92	0.52
3:A:602:HEM:HMC2	3:A:602:HEM:HBC2	1.90	0.52
1:A:112:GLN:O	1:A:115:VAL:HG22	2.10	0.51
3:B:502:HEM:HBC2	3:B:502:HEM:CMC	2.39	0.51
1:C:313:VAL:HG11	1:C:316:PHE:CE2	2.46	0.51
1:A:200:MET:HE2	1:A:217:SER:OG	2.11	0.51
1:C:126:ARG:O	1:C:129:LYS:HE3	2.10	0.50
1:C:116:MET:HG3	1:C:264:MET:HE1	1.93	0.50
1:C:282:MET:HE1	1:C:418:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ALA:HB1	1:B:190:ARG:NE	2.26	0.50
1:C:240:VAL:O	1:C:244:ILE:HG12	2.13	0.49
1:A:29:THR:O	1:A:99:ARG:HD3	2.12	0.49
1:A:427:GLY:O	1:A:428:ARG:HG2	2.13	0.49
1:B:93:GLU:HG2	1:B:319:THR:HG21	1.95	0.49
1:B:239:ILE:N	1:B:239:ILE:HD12	2.28	0.49
1:C:200:MET:HE3	1:C:267:VAL:CG2	2.43	0.49
1:C:265:LEU:CD1	3:C:502:HEM:HBC1	2.42	0.49
1:B:200:MET:HE2	1:B:267:VAL:HG21	1.95	0.48
1:A:76:LEU:HA	1:A:344:ALA:HB1	1.94	0.48
1:C:390:ILE:O	1:C:394:VAL:HG23	2.14	0.48
1:B:352:GLN:O	1:B:353:ASP:OD1	2.31	0.48
1:C:200:MET:HE2	1:C:220:LEU:CD1	2.44	0.48
1:A:292:GLU:O	1:A:296:LYS:HG2	2.13	0.47
1:B:110:GLU:OE1	1:B:113:ARG:NH1	2.47	0.47
1:A:176:LEU:HB3	1:A:194:PHE:CE2	2.48	0.47
1:A:427:GLY:O	1:A:428:ARG:CG	2.62	0.47
3:A:602:HEM:HBC2	3:A:602:HEM:CMC	2.45	0.47
1:C:179:ILE:HD11	1:C:269:GLY:C	2.40	0.46
1:B:310:ALA:O	1:B:311:THR:C	2.59	0.46
3:B:502:HEM:CMB	3:B:502:HEM:HBB2	2.46	0.46
1:A:208:TYR:O	1:A:211:ILE:HG12	2.16	0.46
3:B:502:HEM:HBB2	3:B:502:HEM:HMB2	1.98	0.45
1:B:67:ASP:OD1	1:B:67:ASP:N	2.49	0.45
1:A:183:LEU:HD21	1:A:265:LEU:HD12	1.99	0.45
1:B:133:ARG:HG2	1:B:242:GLN:HE21	1.81	0.44
1:B:398:MET:HE2	1:B:425:TYR:HB3	2.00	0.44
1:C:36:GLU:HG2	1:C:37:ARG:HD3	1.99	0.44
1:B:114:PHE:HD2	1:B:260:PHE:CZ	2.35	0.44
1:A:200:MET:CE	1:A:217:SER:HA	2.48	0.44
1:A:342:ARG:O	1:A:342:ARG:HD3	2.18	0.44
1:C:71:TRP:CD1	1:C:331:ILE:HD13	2.53	0.44
1:A:282:MET:HE3	1:A:407:PRO:HG2	1.99	0.44
1:B:101:LYS:HD3	4:B:503:SO4:O4	2.17	0.44
1:C:188:GLU:H	1:C:188:GLU:CD	2.25	0.43
1:A:76:LEU:HD13	1:A:350:VAL:HG11	2.00	0.43
1:A:135:PHE:CE1	1:A:378:ILE:HD12	2.53	0.43
1:B:225:MET:HE1	1:B:255:ASP:CG	2.42	0.43
1:B:282:MET:HE3	1:B:407:PRO:HG2	2.00	0.43
1:C:211:ILE:HG22	1:C:213:PRO:HD3	2.00	0.43
1:C:200:MET:HE3	1:C:267:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:OD1	5:A:701:HOH:O	2.21	0.43
1:B:103:ASP:OD1	1:B:103:ASP:C	2.61	0.43
1:C:281:MET:CE	1:C:401:LEU:HD22	2.44	0.43
1:A:268:ALA:HA	2:A:603:JV3:C15	2.49	0.43
1:C:401:LEU:C	1:C:401:LEU:HD23	2.44	0.43
1:C:282:MET:HE1	1:C:418:ILE:HD12	2.01	0.42
1:A:281:MET:HE3	1:A:284:PHE:HB2	2.01	0.42
1:C:310:ALA:O	1:C:416:ASN:ND2	2.52	0.42
1:A:310:ALA:O	1:A:311:THR:C	2.62	0.42
1:B:150:ARG:CD	1:B:177:GLN:HG3	2.49	0.42
1:B:150:ARG:HD3	1:B:177:GLN:HG3	2.02	0.42
1:C:199:GLU:HA	1:C:211:ILE:HD13	2.02	0.41
1:A:176:LEU:HB3	1:A:194:PHE:CD2	2.55	0.41
1:A:183:LEU:HD21	1:A:265:LEU:CD1	2.51	0.41
1:B:401:LEU:C	1:B:401:LEU:HD23	2.44	0.41
1:A:427:GLY:C	1:A:428:ARG:HD2	2.46	0.41
1:B:135:PHE:CZ	1:B:378:ILE:HD13	2.55	0.41
1:C:293:LEU:HD12	1:C:359:ILE:HD11	2.02	0.41
1:C:310:ALA:O	1:C:311:THR:C	2.64	0.41
1:A:428:ARG:HA	1:A:428:ARG:NE	2.36	0.41
1:B:265:LEU:CD1	3:B:502:HEM:HBC1	2.51	0.41
1:B:126:ARG:NH2	1:B:251:GLU:OE2	2.53	0.41
1:B:138:ARG:O	1:B:142:ARG:HG3	2.21	0.41
1:C:58:ASP:HB2	1:C:61:LYS:HG3	2.02	0.41
1:C:269:GLY:HA2	3:C:502:HEM:HMC3	2.03	0.40
1:B:289:ASP:OD1	1:B:289:ASP:N	2.54	0.40
1:C:352:GLN:HG2	1:C:352:GLN:O	2.21	0.40
1:C:282:MET:HE1	1:C:418:ILE:CG1	2.51	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	409/418 (98%)	398 (97%)	10 (2%)	1 (0%)	43	51
1	B	396/418 (95%)	384 (97%)	12 (3%)	0	100	100
1	C	403/418 (96%)	393 (98%)	10 (2%)	0	100	100
All	All	1208/1254 (96%)	1175 (97%)	32 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	PRO

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	334/341 (98%)	333 (100%)	1 (0%)	86	93
1	B	324/341 (95%)	323 (100%)	1 (0%)	86	93
1	C	331/341 (97%)	331 (100%)	0	100	100
All	All	989/1023 (97%)	987 (100%)	2 (0%)	87	94

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

Mol	Chain	Res	Type
1	A	103	ASP
1	B	48	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	242	GLN
1	B	123	HIS
1	B	203	ASN
1	B	210	HIS

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Mol	Chain	Res	Type
1	B	242	GLN
1	B	270	ASN
1	B	381	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	JV3	A	601	-	17,17,17	1.41	3 (17%)	22,22,22	1.38	1 (4%)
2	JV3	B	501	3	17,17,17	1.44	3 (17%)	22,22,22	1.38	1 (4%)
2	JV3	A	603	3	17,17,17	1.45	3 (17%)	22,22,22	1.28	1 (4%)
3	HEM	B	502	2,1	50,50,50	1.38	9 (18%)	67,82,82	1.17	6 (8%)
4	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.10	0
2	JV3	C	501	3	17,17,17	1.43	3 (17%)	22,22,22	1.33	1 (4%)
4	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	HEM	A	602	2,1	50,50,50	1.28	6 (12%)	67,82,82	1.18	6 (8%)
3	HEM	C	502	2,1	50,50,50	1.35	9 (18%)	67,82,82	1.11	5 (7%)

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	JV3	A	601	-	-	6/10/10/10	0/2/2/2
2	JV3	B	501	3	-	0/10/10/10	0/2/2/2
2	JV3	A	603	3	-	0/10/10/10	0/2/2/2
3	HEM	B	502	2,1	-	2/14/54/54	-
2	JV3	C	501	3	-	2/10/10/10	0/2/2/2
3	HEM	A	602	2,1	-	0/14/54/54	-
3	HEM	C	502	2,1	-	0/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	JV3	C10-C09	-4.11	1.39	1.49
2	B	501	JV3	C10-C09	-4.01	1.39	1.49
2	C	501	JV3	C10-C09	-3.89	1.39	1.49
2	A	601	JV3	C10-C09	-3.79	1.40	1.49
3	C	502	HEM	FE-NC	3.46	2.06	1.95
3	B	502	HEM	FE-ND	3.27	2.05	1.94
3	B	502	HEM	FE-NA	3.21	2.05	1.95
2	C	501	JV3	O02-C03	3.19	1.40	1.33
3	A	602	HEM	FE-NA	3.13	2.05	1.95
2	A	601	JV3	O02-C03	3.12	1.40	1.33
2	B	501	JV3	O02-C03	3.08	1.40	1.33
3	B	502	HEM	CAC-C3C	2.98	1.55	1.47
2	A	603	JV3	O02-C03	2.96	1.40	1.33
3	A	602	HEM	CAC-C3C	2.93	1.55	1.47
3	B	502	HEM	CAB-C3B	2.91	1.55	1.47
3	C	502	HEM	CAC-C3C	2.90	1.55	1.47
3	C	502	HEM	CAB-C3B	2.85	1.55	1.47
3	A	602	HEM	FE-NC	2.81	2.04	1.95
3	A	602	HEM	CAB-C3B	2.65	1.54	1.47
3	C	502	HEM	FE-NA	2.65	2.03	1.95
3	B	502	HEM	FE-NC	2.59	2.03	1.95
3	B	502	HEM	FE-NB	2.55	2.02	1.94
3	C	502	HEM	FE-ND	2.55	2.02	1.94
3	C	502	HEM	FE-NB	2.47	2.02	1.94
2	A	603	JV3	O02-C01	-2.30	1.40	1.45
3	B	502	HEM	CMC-C2C	2.21	1.55	1.50
2	B	501	JV3	O02-C01	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JV3	O02-C01	-2.20	1.40	1.45
3	C	502	HEM	CMC-C2C	2.17	1.55	1.50
2	C	501	JV3	O02-C01	-2.15	1.40	1.45
3	A	602	HEM	CMC-C2C	2.11	1.55	1.50
3	A	602	HEM	FE-ND	2.10	2.01	1.94
3	B	502	HEM	CMD-C2D	2.08	1.55	1.50
3	B	502	HEM	CMB-C2B	2.06	1.55	1.50
3	C	502	HEM	CMA-C3A	2.05	1.55	1.50
3	C	502	HEM	CMB-C2B	2.01	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JV3	O02-C03-C05	5.36	120.34	112.31
2	B	501	JV3	O02-C03-C05	5.13	120.00	112.31
2	C	501	JV3	O02-C03-C05	5.00	119.80	112.31
2	A	603	JV3	O02-C03-C05	4.27	118.70	112.31
3	B	502	HEM	C4D-ND-C1D	2.94	108.69	105.21
3	A	602	HEM	C4D-ND-C1D	2.71	108.41	105.21
3	C	502	HEM	C1B-NB-C4B	2.48	108.14	105.21
3	B	502	HEM	C3D-C4D-ND	-2.46	107.47	110.17
3	A	602	HEM	C3D-C4D-ND	-2.45	107.49	110.17
3	A	602	HEM	C1B-NB-C4B	2.36	108.00	105.21
3	B	502	HEM	C2D-C1D-ND	-2.30	107.24	109.90
3	C	502	HEM	C3B-C4B-NB	-2.27	107.84	109.47
3	B	502	HEM	C1B-NB-C4B	2.27	107.89	105.21
3	C	502	HEM	CAA-CBA-CGA	-2.26	107.66	113.67
3	C	502	HEM	C4D-ND-C1D	2.20	107.82	105.21
3	B	502	HEM	C2A-C1A-NA	-2.15	107.77	110.15
3	A	602	HEM	C2D-C1D-ND	-2.10	107.48	109.90
3	B	502	HEM	C3B-C2B-C1B	2.10	107.98	106.41
3	A	602	HEM	CHC-C4B-NB	2.08	126.66	124.42
3	C	502	HEM	C3B-C2B-C1B	2.06	107.96	106.41
3	A	602	HEM	C3B-C4B-NB	-2.05	108.00	109.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	HEM	C1A-C2A-CAA-CBA
2	A	601	JV3	C05-C03-O02-C01
2	A	601	JV3	O02-C03-C05-C06

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Mol	Chain	Res	Type	Atoms
2	A	601	JV3	O02-C03-C05-C16
2	C	501	JV3	C05-C03-O02-C01
2	A	601	JV3	O04-C03-C05-C16
2	A	601	JV3	O04-C03-C05-C06
2	A	601	JV3	O04-C03-O02-C01
2	C	501	JV3	O04-C03-O02-C01
3	B	502	HEM	C3A-C2A-CAA-CBA

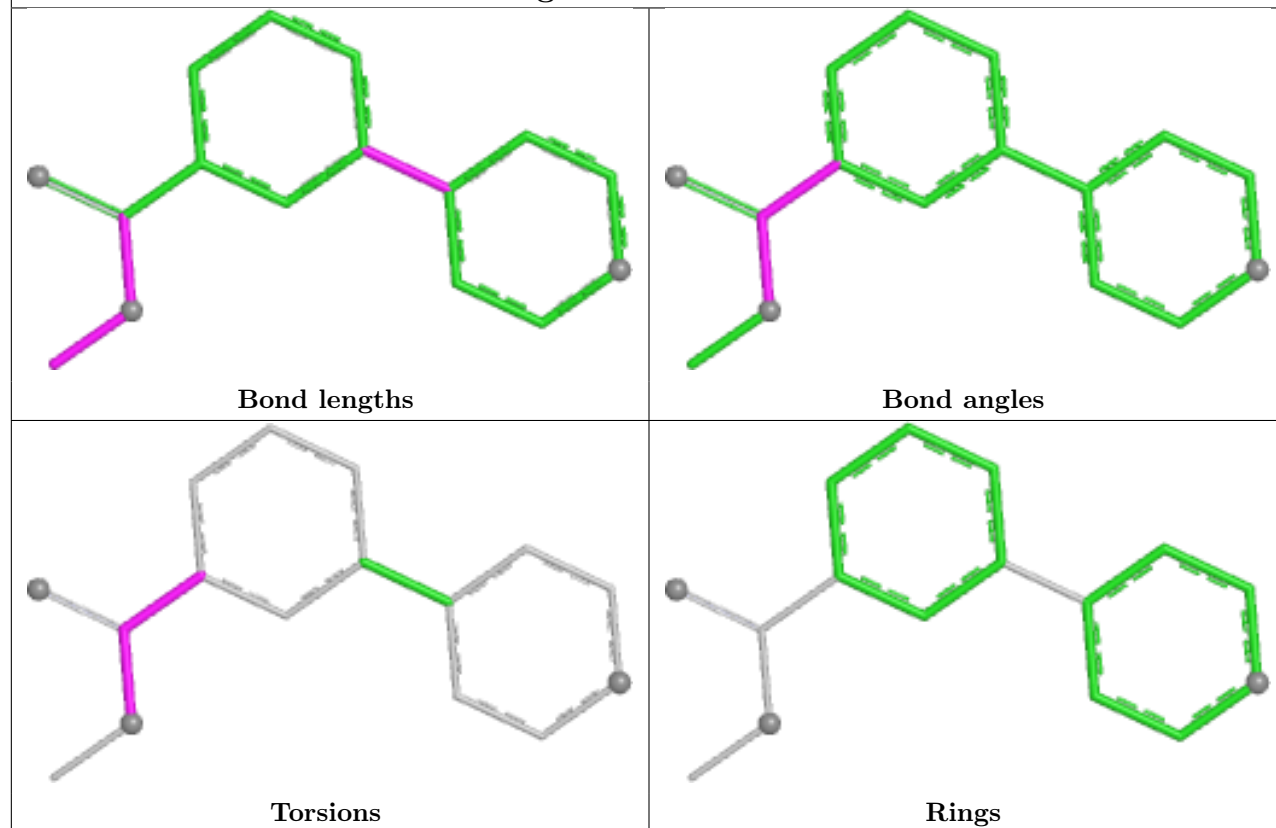
There are no ring outliers.

5 monomers are involved in 15 short contacts:

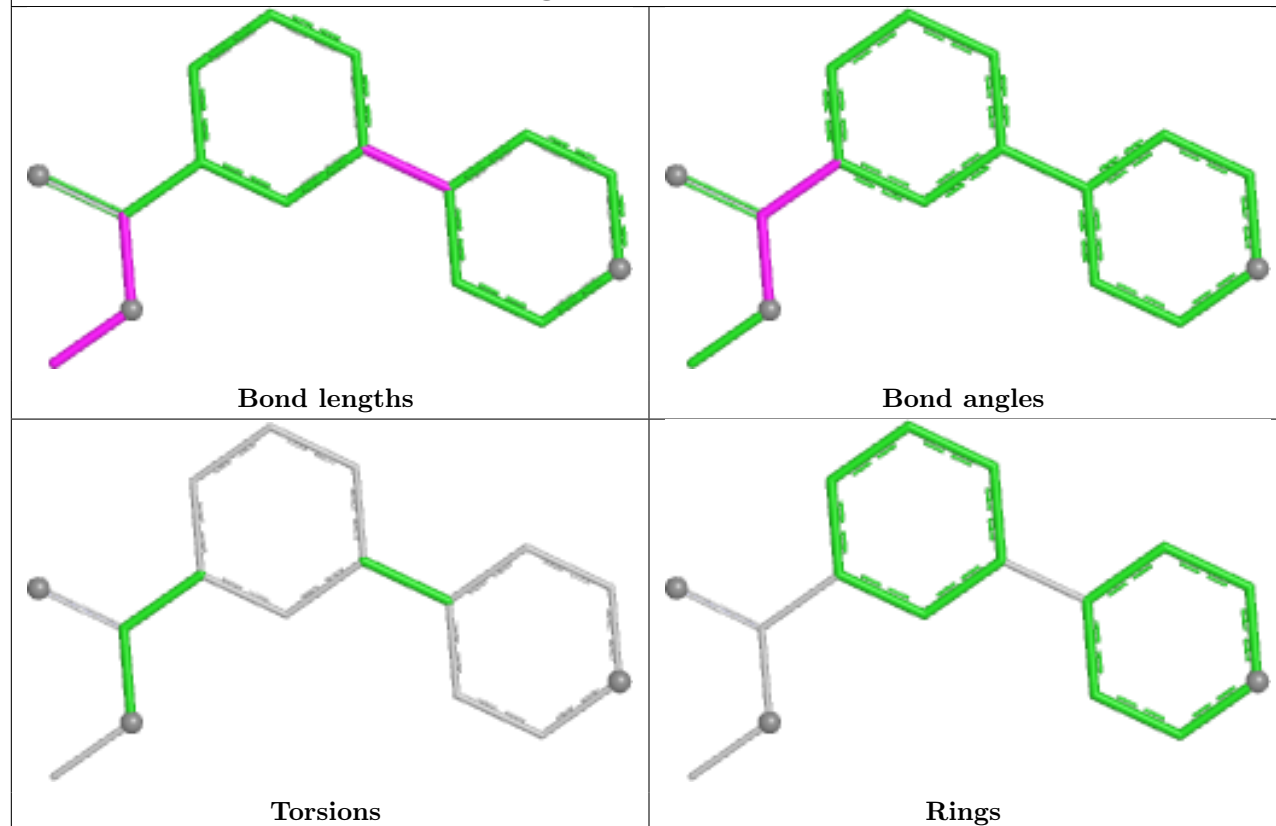
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	JV3	1	0
3	B	502	HEM	5	0
4	B	503	SO4	2	0
3	A	602	HEM	2	0
3	C	502	HEM	5	0

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 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.

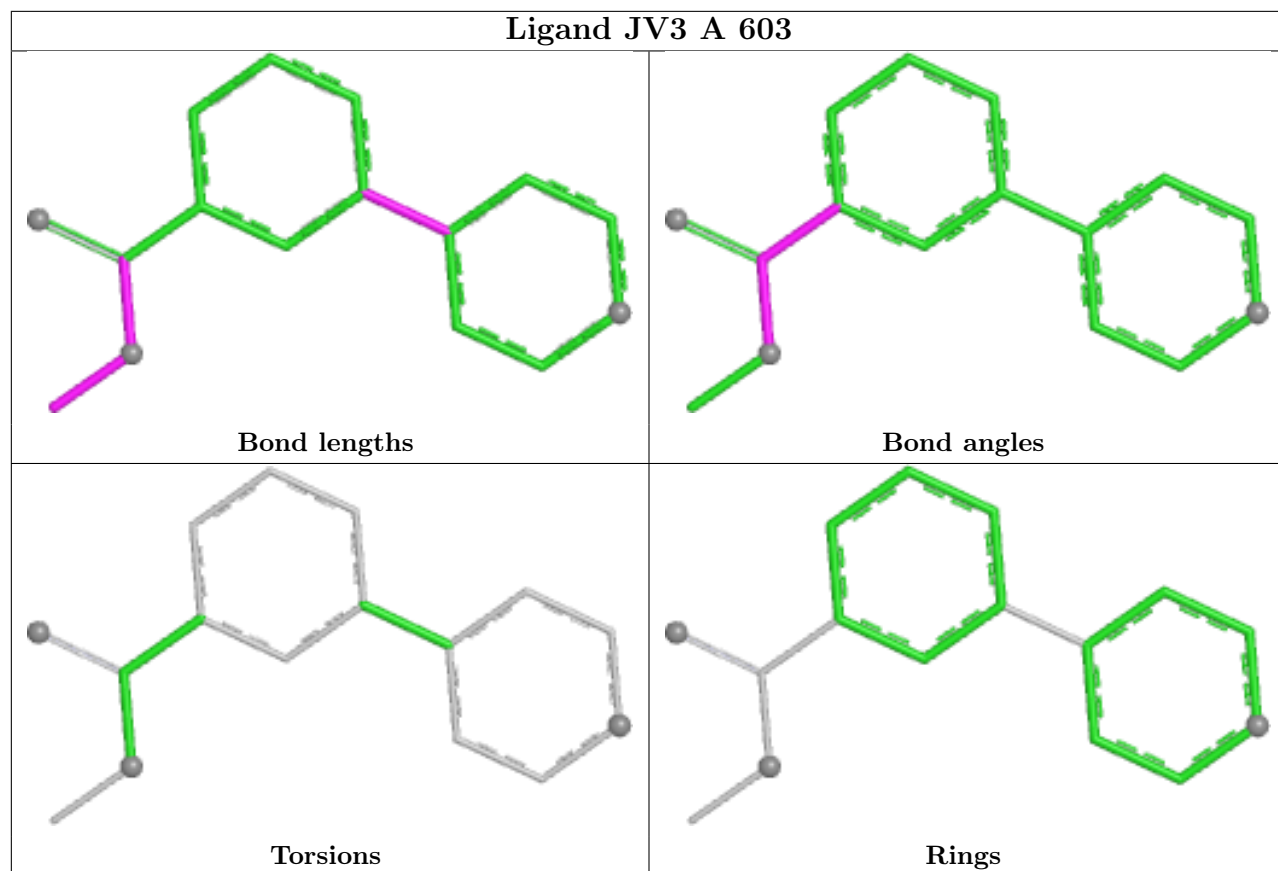
Ligand JV3 A 601

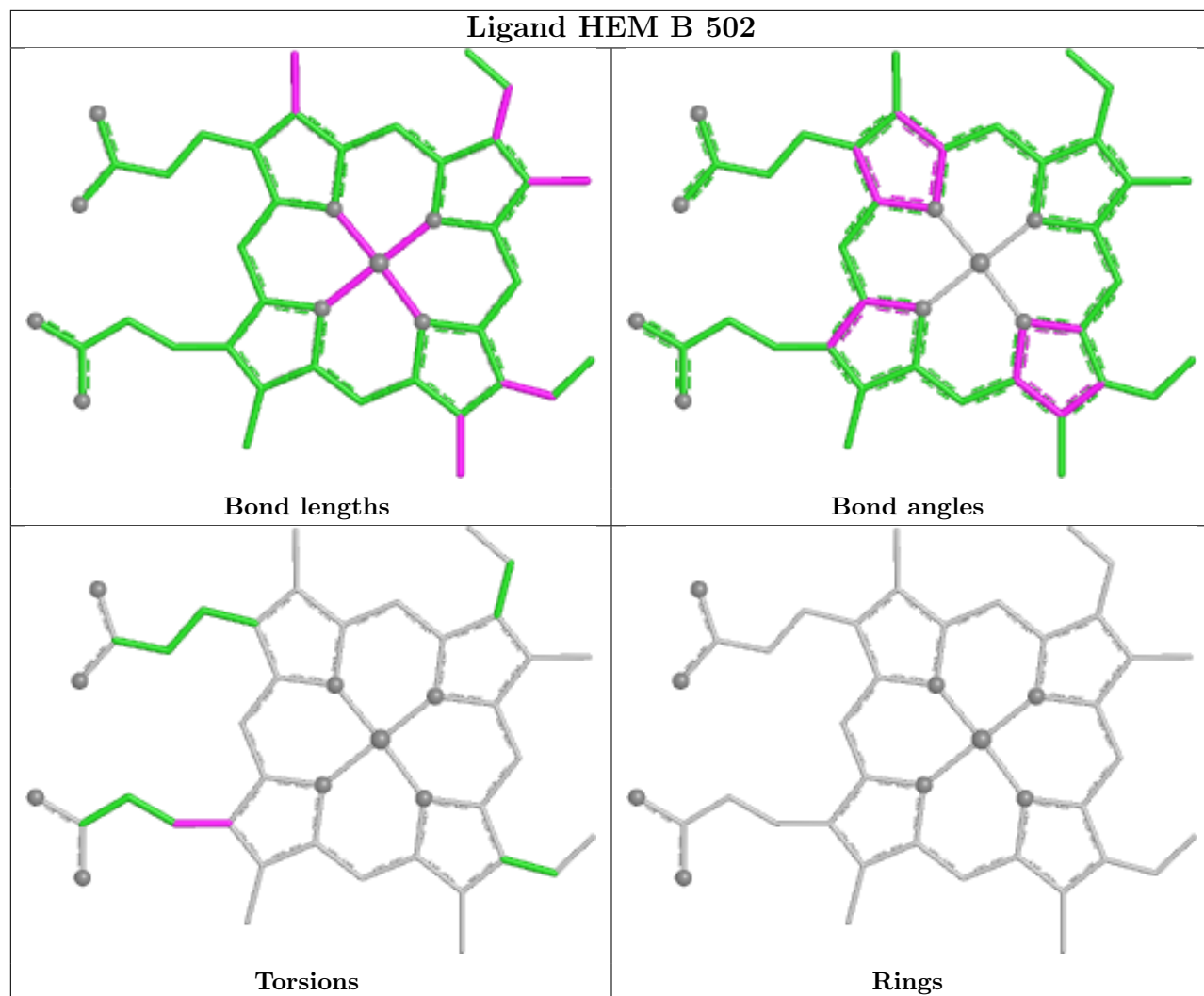


Ligand JV3 B 501

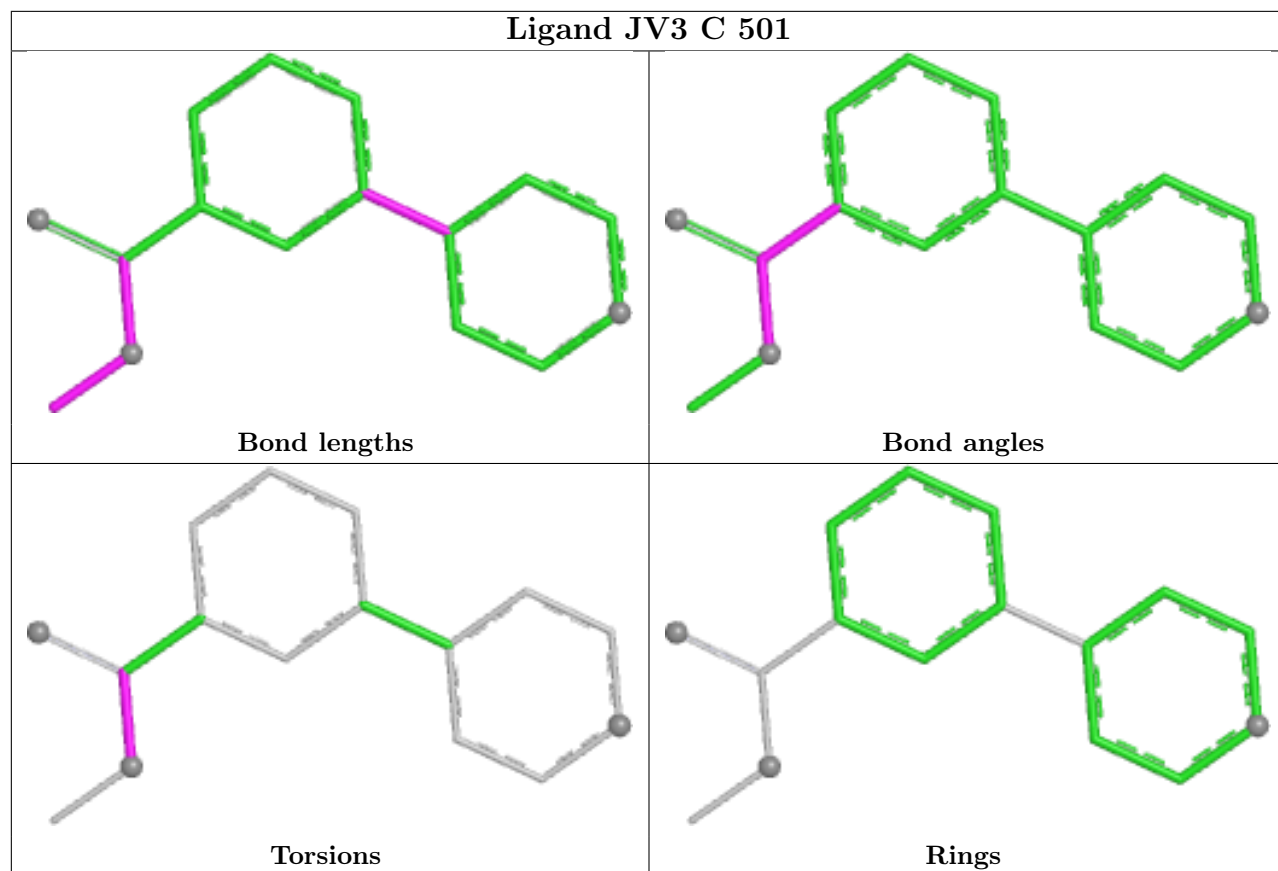


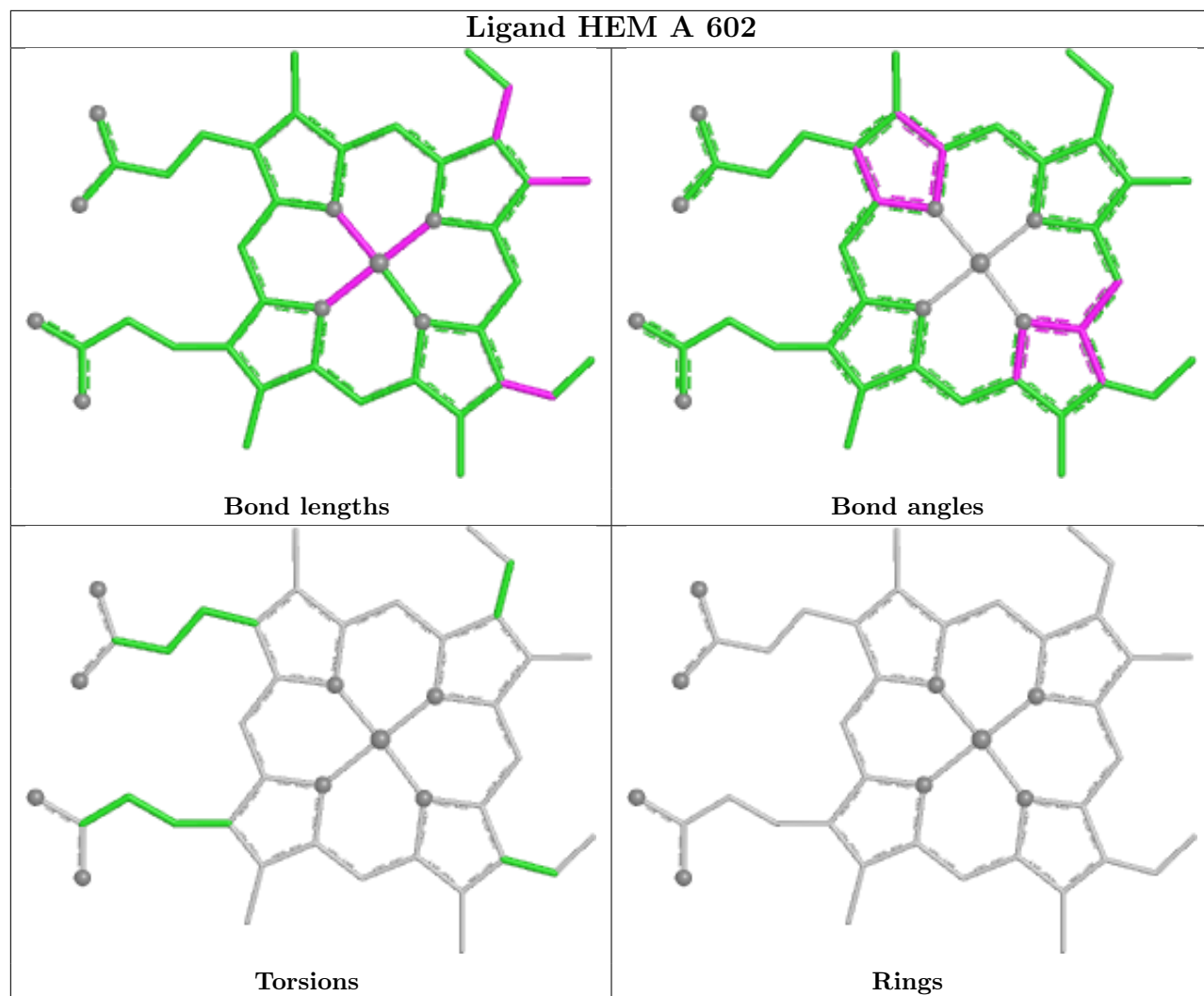
Ligand JV3 A 603

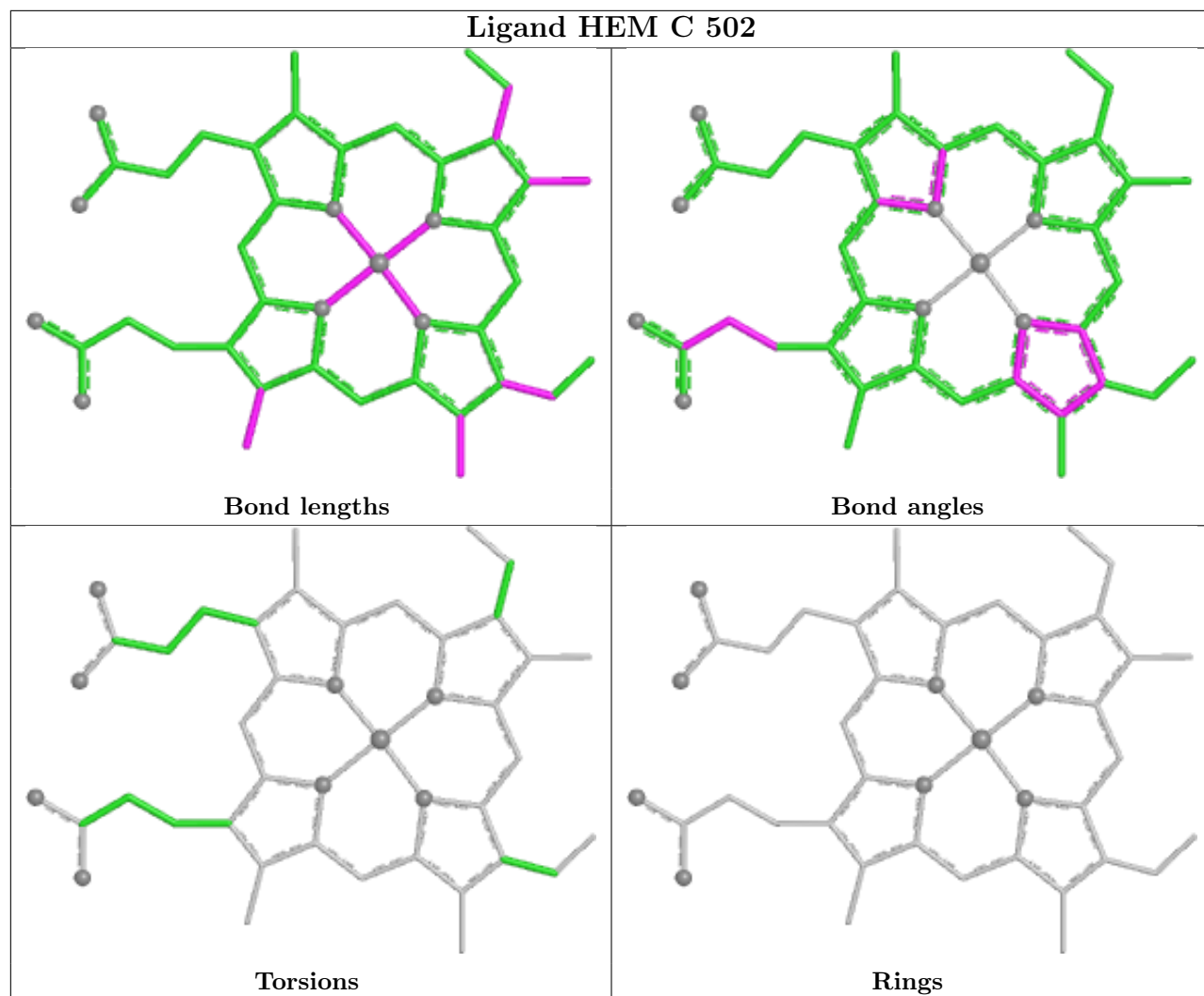




Ligand JV3 C 501







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	411/418 (98%)	-0.08	6 (1%) 72 69	23, 37, 66, 115	0
1	B	402/418 (96%)	0.50	28 (6%) 22 19	36, 59, 102, 128	0
1	C	407/418 (97%)	0.52	17 (4%) 40 37	44, 60, 92, 115	0
All	All	1220/1254 (97%)	0.31	51 (4%) 40 37	23, 53, 92, 128	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	5.0
1	B	238	ASP	4.5
1	B	244	ILE	4.3
1	B	137	PRO	4.2
1	C	210	HIS	4.0
1	C	239	ILE	3.9
1	C	236	ALA	3.7
1	B	135	PHE	3.5
1	C	248	ILE	3.5
1	C	237	ASP	3.3
1	B	252	LYS	3.1
1	B	136	THR	3.1
1	B	239	ILE	3.0
1	B	138	ARG	2.9
1	B	427	GLY	2.9
1	B	139	ALA	2.8
1	B	241	THR	2.8
1	C	211	ILE	2.8
1	B	134	GLY	2.7
1	C	427	GLY	2.7
1	B	243	LEU	2.7
1	B	237	ASP	2.7
1	A	428	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	231	LYS	2.6
1	C	235	PRO	2.6
1	B	265	LEU	2.5
1	B	122	PRO	2.5
1	C	234	ASN	2.5
1	A	237	ASP	2.5
1	C	255	ASP	2.5
1	C	182	LEU	2.4
1	B	59	PRO	2.4
1	B	210	HIS	2.3
1	C	212	ASP	2.3
1	A	427	GLY	2.3
1	C	228	ALA	2.3
1	A	18	PRO	2.2
1	B	143	LEU	2.2
1	C	213	PRO	2.2
1	B	372	THR	2.2
1	B	234	ASN	2.2
1	B	426	THR	2.2
1	B	401	LEU	2.1
1	B	115	VAL	2.1
1	B	133	ARG	2.1
1	C	196	TRP	2.1
1	A	249	ASP	2.0
1	A	248	ILE	2.0
1	B	114	PHE	2.0
1	C	114	PHE	2.0
1	B	130	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

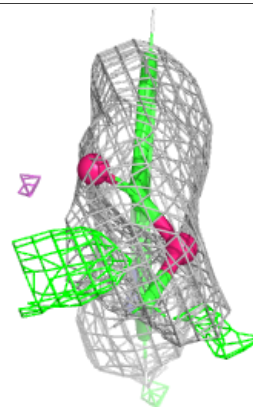
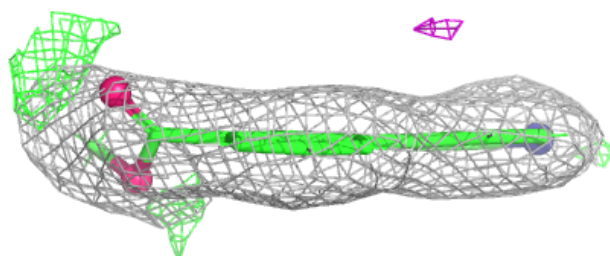
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	503	5/5	0.76	0.11	80,81,89,91	0
4	SO4	A	604	5/5	0.78	0.12	64,68,78,84	0
2	JV3	A	601	16/16	0.84	0.17	52,63,80,80	0
2	JV3	B	501	16/16	0.85	0.15	50,62,84,84	0
4	SO4	B	503	5/5	0.86	0.10	83,87,92,95	0
2	JV3	C	501	16/16	0.88	0.12	53,64,79,79	0
2	JV3	A	603	16/16	0.95	0.08	25,32,54,54	0
3	HEM	C	502	43/43	0.96	0.09	42,52,66,70	0
3	HEM	B	502	43/43	0.96	0.10	38,50,64,67	0
3	HEM	A	602	43/43	0.97	0.07	19,26,34,41	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.

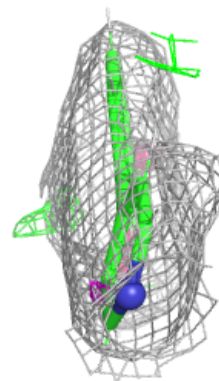
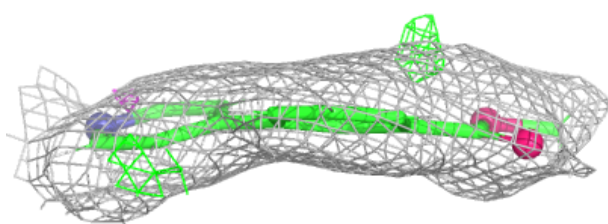
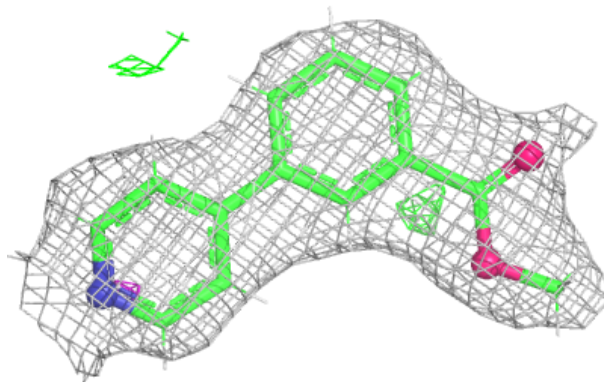
Electron density around JV3 A 601:

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

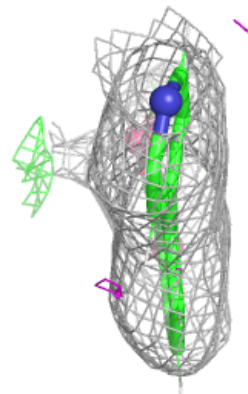
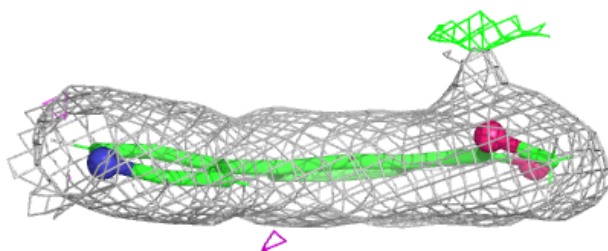
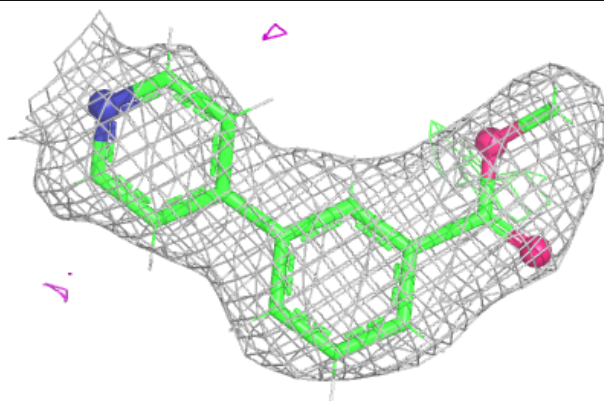


Electron density around JV3 B 501:

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

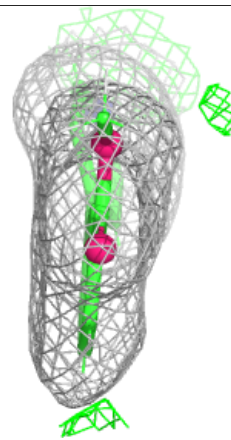
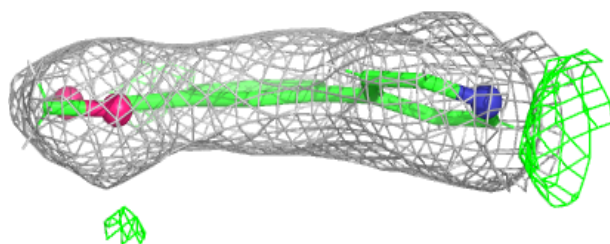
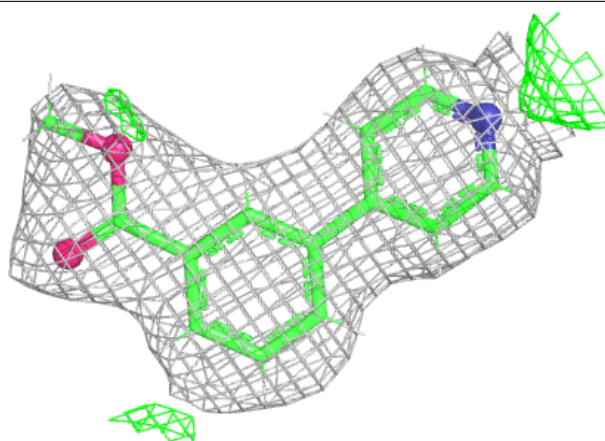
**Electron density around JV3 C 501:**

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



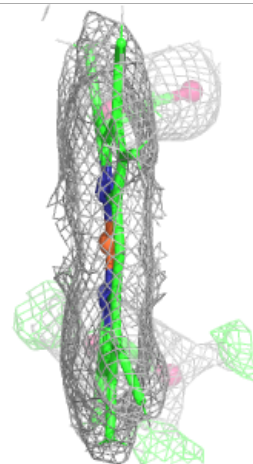
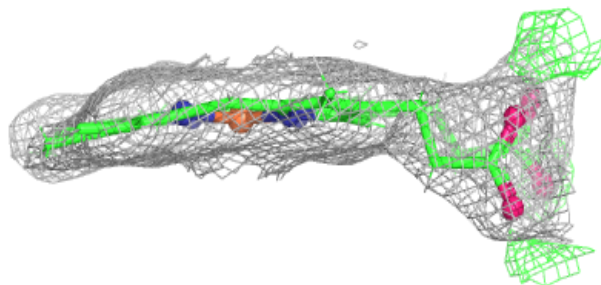
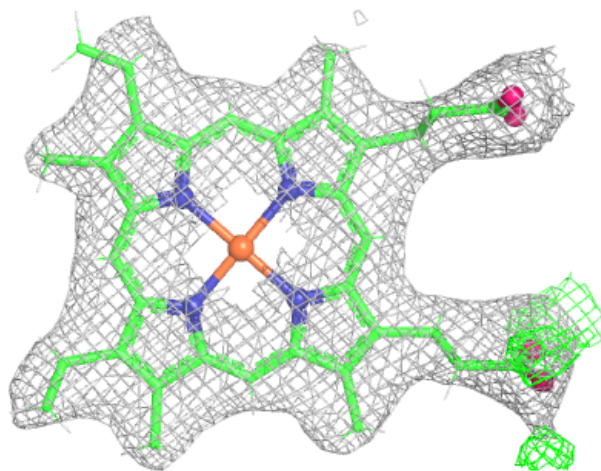
Electron density around JV3 A 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



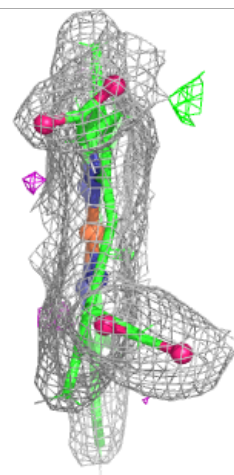
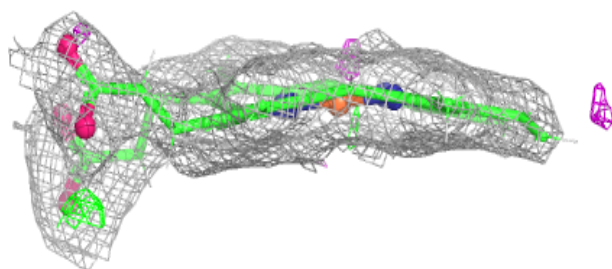
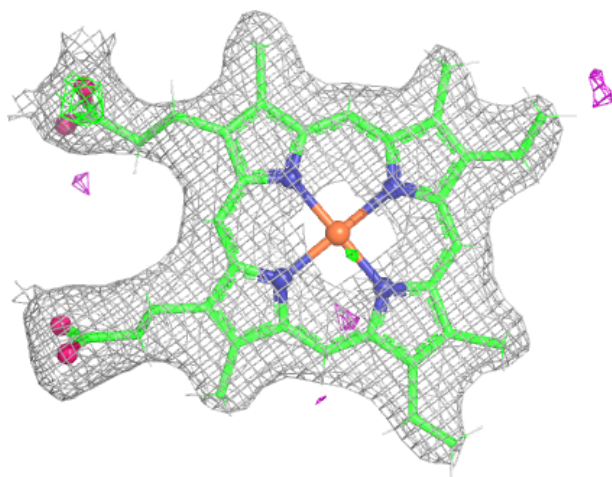
Electron density around HEM C 502:

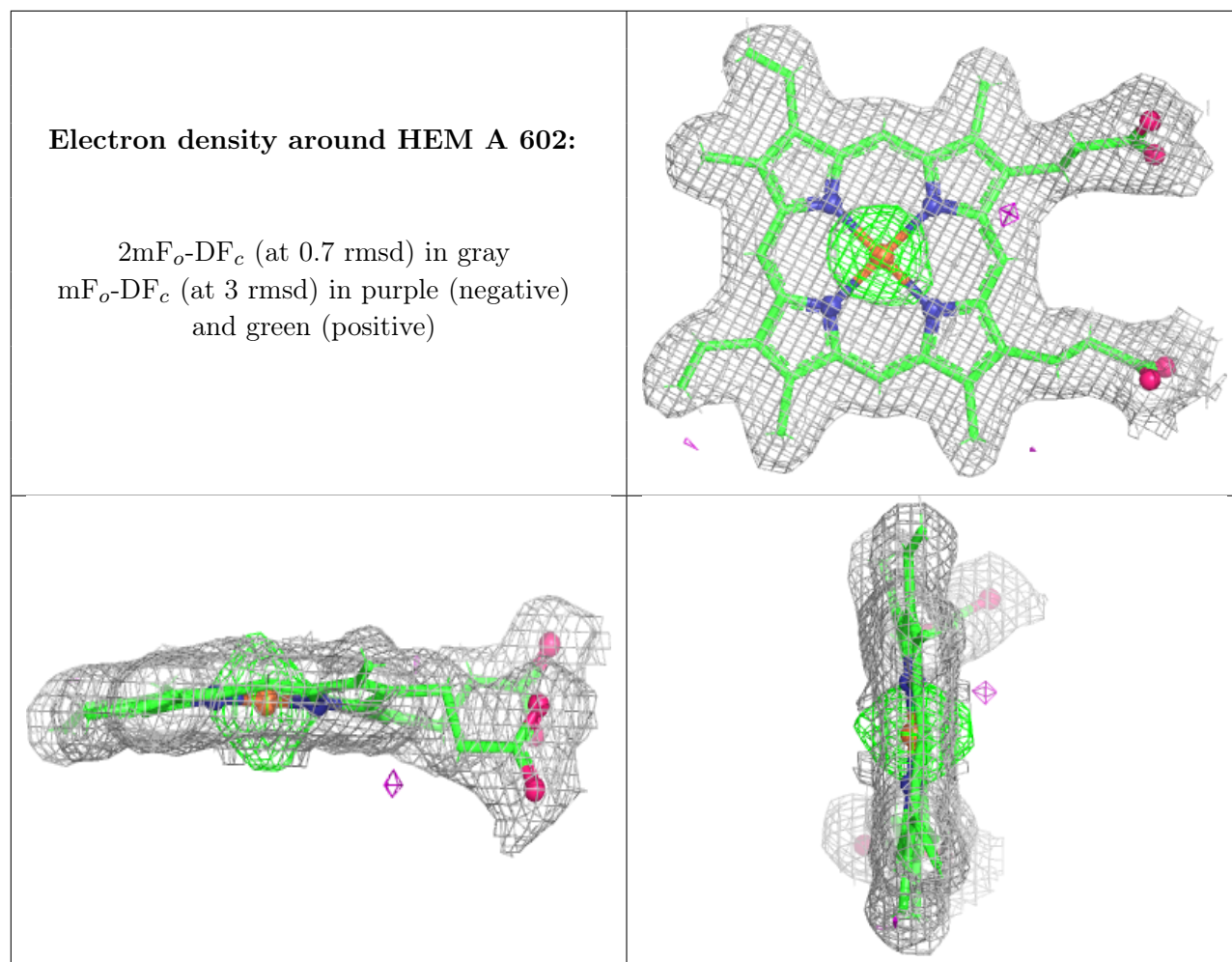
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.