



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:13 AM UTC

PDB ID : 9ESD / pdb_00009esd
Title : Holo TDO with a bound inhibitor
Authors : Wicki, M.; Mac Sweeney, A.
Deposited on : 2024-03-26
Resolution : 2.10 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

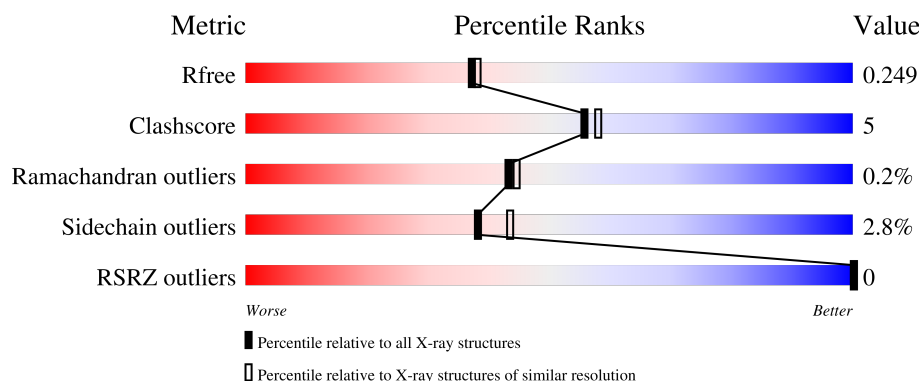
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	365	 80% 9% • 10%
1	B	365	 80% 8% • 11%
1	C	365	 81% 12% • 6%
1	D	365	 78% 11% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11368 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	1	0
			2735	1753	468	502	12			
1	B	326	Total	C	N	O	S	0	1	0
			2715	1740	469	494	12			
1	C	344	Total	C	N	O	S	0	1	0
			2849	1820	493	524	12			
1	D	331	Total	C	N	O	S	0	0	0
			2755	1763	475	505	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P20351
A	380	LEU	-	expression tag	UNP P20351
A	381	GLU	-	expression tag	UNP P20351
A	382	HIS	-	expression tag	UNP P20351
A	383	HIS	-	expression tag	UNP P20351
A	384	HIS	-	expression tag	UNP P20351
A	385	HIS	-	expression tag	UNP P20351
A	386	HIS	-	expression tag	UNP P20351
A	387	HIS	-	expression tag	UNP P20351
B	23	MET	-	initiating methionine	UNP P20351
B	380	LEU	-	expression tag	UNP P20351
B	381	GLU	-	expression tag	UNP P20351
B	382	HIS	-	expression tag	UNP P20351
B	383	HIS	-	expression tag	UNP P20351
B	384	HIS	-	expression tag	UNP P20351
B	385	HIS	-	expression tag	UNP P20351
B	386	HIS	-	expression tag	UNP P20351
B	387	HIS	-	expression tag	UNP P20351
C	23	MET	-	initiating methionine	UNP P20351
C	380	LEU	-	expression tag	UNP P20351
C	381	GLU	-	expression tag	UNP P20351

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Chain	Residue	Modelled	Actual	Comment	Reference
C	382	HIS	-	expression tag	UNP P20351
C	383	HIS	-	expression tag	UNP P20351
C	384	HIS	-	expression tag	UNP P20351
C	385	HIS	-	expression tag	UNP P20351
C	386	HIS	-	expression tag	UNP P20351
C	387	HIS	-	expression tag	UNP P20351
D	23	MET	-	initiating methionine	UNP P20351
D	380	LEU	-	expression tag	UNP P20351
D	381	GLU	-	expression tag	UNP P20351
D	382	HIS	-	expression tag	UNP P20351
D	383	HIS	-	expression tag	UNP P20351
D	384	HIS	-	expression tag	UNP P20351
D	385	HIS	-	expression tag	UNP P20351
D	386	HIS	-	expression tag	UNP P20351
D	387	HIS	-	expression tag	UNP P20351

- # HEM

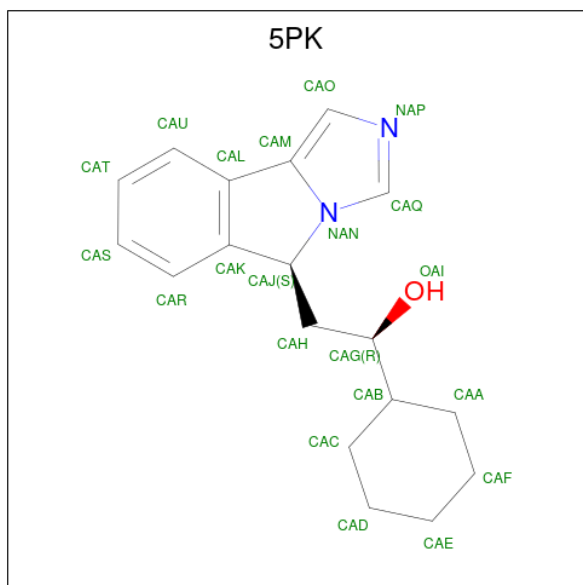
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



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

- Molecule 3 is (1 {R})-1-cyclohexyl-2-[(5 {S})-5 {H}-imidazo[1,5-b]isoindol-5-yl]ethanol (CCD ID: 5PK) (formula: C₁₈H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	18	2	1		
3	B	1	Total	C	N	O	0	0
			21	18	2	1		
3	C	1	Total	C	N	O	0	0
			21	18	2	1		
3	D	1	Total	C	N	O	0	0
			21	18	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	13	Total	O	0	0
			13	13		
4	C	17	Total	O	0	0
			17	17		
4	D	16	Total	O	0	0
			16	16		



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	143.74Å 143.74Å 141.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.05 – 2.10 47.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.05-2.10) 100.0 (47.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.233 , 0.255 0.223 , 0.249	Depositor DCC
R_{free} test set	4796 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.124 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11368	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: 5PK, 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	0.71	0/2793	1.03	1/3766 (0.0%)
1	B	0.70	0/2773	1.03	2/3738 (0.1%)
1	C	0.75	3/2910 (0.1%)	1.06	3/3927 (0.1%)
1	D	0.71	0/2811	1.01	1/3790 (0.0%)
All	All	0.72	3/11287 (0.0%)	1.03	7/15221 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	ARG	CA-C	7.63	1.60	1.52
1	C	118	THR	CA-C	5.30	1.60	1.52
1	C	154	GLU	CA-C	5.22	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	PRO	N-CA-C	6.81	122.99	113.53
1	B	133	PRO	N-CA-C	5.87	121.69	113.53
1	C	134	ALA	CA-C-N	5.59	128.22	120.29
1	C	134	ALA	C-N-CA	5.59	128.22	120.29
1	A	210	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	210	PHE	CA-CB-CG	5.15	118.95	113.80
1	D	210	PHE	CA-CB-CG	5.05	118.85	113.80

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	2735	0	2734	28	0
1	B	2715	0	2718	25	0
1	C	2849	0	2838	37	0
1	D	2755	0	2761	38	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	21	0	22	2	0
3	B	21	0	22	2	0
3	C	21	0	22	5	0
3	D	21	0	22	2	0
4	A	12	0	0	0	0
4	B	13	0	0	0	0
4	C	17	0	0	0	0
4	D	16	0	0	0	0
All	All	11368	0	11259	107	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 (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:HIS:NE2	3:D:402:5PK:H22	1.87	0.89
1:B:101:ARG:HE	1:C:118:THR:CG2	1.87	0.88
1:A:101:ARG:HE	1:D:118:THR:CG2	1.88	0.87
1:A:118:THR:CG2	1:D:101:ARG:HE	1.89	0.86
1:B:118:THR:CG2	1:C:101:ARG:HE	1.90	0.84
1:A:132:ALA:HB2	1:D:25:LYS:HG3	1.64	0.79
1:C:61:HIS:NE2	3:C:402:5PK:H22	1.99	0.77
1:B:61:HIS:NE2	3:B:402:5PK:H22	2.01	0.75
1:D:152:LEU:CD2	1:D:267:ARG:HE	2.00	0.75
1:A:101:ARG:HE	1:D:118:THR:HG21	1.53	0.74
1:B:132:ALA:HB2	1:C:25:LYS:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:HEM:NA	3:C:402:5PK:H21	2.03	0.72
1:C:251:ILE:O	1:C:270:HIS:HE1	1.78	0.67
1:A:118:THR:HG22	1:D:101:ARG:HE	1.63	0.64
1:C:324:GLN:HE21	1:C:325:LEU:H	1.46	0.64
1:A:25:LYS:HG3	1:D:132:ALA:HB2	1.79	0.64
1:A:251:ILE:O	1:A:270:HIS:HE1	1.81	0.64
2:B:401:HEM:NA	3:B:402:5PK:H21	2.13	0.63
1:C:270:HIS:CD2	1:C:274:GLN:HE21	2.16	0.63
1:A:270:HIS:CD2	1:A:274:GLN:HE21	2.17	0.63
1:B:251:ILE:O	1:B:270:HIS:HE1	1.80	0.63
1:D:270:HIS:CD2	1:D:274:GLN:HE21	2.17	0.62
1:D:251:ILE:O	1:D:270:HIS:HE1	1.82	0.62
1:B:101:ARG:HE	1:C:118:THR:HG21	1.64	0.62
1:A:52:HIS:HE1	1:D:74:GLU:OE1	1.82	0.61
1:A:118:THR:HG21	1:D:101:ARG:HE	1.65	0.61
1:A:74:GLU:OE1	1:D:52:HIS:HE1	1.83	0.60
1:C:161:GLN:HG2	1:D:233:ALA:HA	1.84	0.60
1:B:270:HIS:CD2	1:B:274:GLN:HE21	2.19	0.59
1:B:74:GLU:OE1	1:C:52:HIS:HE1	1.87	0.58
1:D:49:ARG:NH1	1:D:130:TYR:OH	2.35	0.57
2:D:401:HEM:NA	3:D:402:5PK:H21	2.19	0.57
1:B:324:GLN:HE21	1:B:325:LEU:H	1.52	0.56
1:B:25:LYS:HD2	1:C:132:ALA:HB2	1.87	0.56
1:B:118:THR:HG21	1:C:101:ARG:HE	1.68	0.55
1:B:118:THR:HG22	1:C:101:ARG:HE	1.70	0.55
1:C:115:ILE:O	1:C:118:THR:HB	2.08	0.54
1:B:115:ILE:O	1:B:118:THR:HB	2.07	0.53
1:B:324:GLN:NE2	1:B:325:LEU:H	2.06	0.53
1:A:324:GLN:NE2	1:A:325:LEU:H	2.06	0.53
1:D:324:GLN:NE2	1:D:325:LEU:H	2.07	0.53
1:A:324:GLN:HE21	1:A:325:LEU:H	1.54	0.52
1:A:61:HIS:NE2	3:A:402:5PK:H22	2.24	0.52
1:C:128[A]:ARG:HB2	3:C:402:5PK:H4	1.91	0.52
1:C:324:GLN:NE2	1:C:325:LEU:H	2.06	0.52
1:C:125:MET:HA	1:C:128[A]:ARG:HG2	1.91	0.51
1:B:52:HIS:HE1	1:C:74:GLU:OE1	1.92	0.51
1:B:198:GLY:HA3	1:B:278:MET:HE1	1.93	0.50
1:D:153:THR:HA	1:D:156:ARG:HD2	1.93	0.50
1:D:115:ILE:O	1:D:118:THR:HB	2.13	0.49
1:A:115:ILE:O	1:A:118:THR:HB	2.12	0.49
1:B:333:TYR:CZ	1:B:337:ARG:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:TYR:CZ	1:A:337:ARG:HD2	2.47	0.48
1:C:333:TYR:CZ	1:C:337:ARG:HD2	2.50	0.47
1:B:101:ARG:HE	1:C:118:THR:HG22	1.74	0.47
1:D:333:TYR:CZ	1:D:337:ARG:HD2	2.49	0.47
1:A:288:PHE:C	1:A:291:PRO:HD2	2.40	0.46
1:D:288:PHE:C	1:D:291:PRO:HD2	2.40	0.46
1:A:132:ALA:CB	1:D:25:LYS:HG3	2.40	0.46
1:C:161:GLN:HG2	1:D:233:ALA:CA	2.45	0.46
2:C:401:HEM:C4A	3:C:402:5PK:H21	2.50	0.46
1:D:324:GLN:HE21	1:D:325:LEU:H	1.62	0.46
1:C:33:LEU:HB3	1:C:37:LEU:HD22	1.99	0.45
1:A:198:GLY:HA3	1:A:278:MET:HE1	1.99	0.45
1:A:316:VAL:HG22	2:A:401:HEM:C1B	2.52	0.45
1:D:33:LEU:HB3	1:D:37:LEU:HD22	1.97	0.45
1:D:207:TRP:O	1:D:211:GLN:HG3	2.17	0.45
1:B:299:MET:HE3	1:B:351:PHE:CD1	2.51	0.45
1:D:81:MET:HG2	1:D:91:LYS:NZ	2.32	0.44
1:D:44:SER:HB2	1:D:49:ARG:O	2.18	0.44
1:D:81:MET:HG2	1:D:91:LYS:HZ1	1.82	0.44
1:A:299:MET:HE3	1:A:351:PHE:CD1	2.53	0.44
1:B:288:PHE:C	1:B:291:PRO:HD2	2.42	0.44
1:C:44:SER:HB2	1:C:49:ARG:O	2.17	0.44
1:C:288:PHE:C	1:C:291:PRO:HD2	2.42	0.44
1:C:128[A]:ARG:HA	1:C:131:LEU:HD22	2.00	0.43
1:C:316:VAL:HG22	2:C:401:HEM:C1B	2.53	0.43
1:D:198:GLY:HA3	1:D:278:MET:HE1	1.98	0.43
1:B:316:VAL:HG22	2:B:401:HEM:C1B	2.53	0.43
1:A:44:SER:HB2	1:A:49:ARG:O	2.18	0.43
1:D:155:GLN:HB3	1:D:343:ARG:HB3	2.00	0.43
1:A:128:ARG:HA	1:A:131:LEU:HD22	2.01	0.42
3:A:402:5PK:OAI	3:A:402:5PK:H21	2.19	0.42
1:C:198:GLY:HA3	1:C:278:MET:HE1	2.00	0.42
1:C:364:PRO:HA	1:C:365:PRO:HD3	1.93	0.42
1:D:316:VAL:HG22	2:D:401:HEM:C1B	2.54	0.42
1:A:101:ARG:HE	1:D:118:THR:HG22	1.78	0.42
1:C:167:PHE:CE2	1:C:173:ARG:HG3	2.55	0.42
1:C:177:ARG:O	1:C:181:LYS:HG2	2.20	0.42
1:A:33:LEU:HB3	1:A:37:LEU:HD22	2.02	0.42
1:C:161:GLN:HG2	1:D:233:ALA:CB	2.50	0.42
1:C:207:TRP:O	1:C:211:GLN:HG3	2.20	0.42
1:D:299:MET:HE3	1:D:351:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:HIS:CD2	1:D:274:GLN:NE2	2.86	0.41
1:B:207:TRP:O	1:B:211:GLN:HG3	2.20	0.41
1:C:270:HIS:CD2	1:C:274:GLN:NE2	2.84	0.41
1:B:44:SER:HB2	1:B:49:ARG:O	2.20	0.41
1:B:128:ARG:HA	1:B:131:LEU:HD22	2.02	0.41
1:A:35:LYS:HG3	1:D:35:LYS:HG3	2.02	0.41
1:C:251:ILE:O	1:C:270:HIS:CE1	2.66	0.41
1:D:128:ARG:HA	1:D:131:LEU:HD22	2.03	0.41
1:A:207:TRP:O	1:A:211:GLN:HG3	2.20	0.41
1:C:128[B]:ARG:HB2	3:C:402:5PK:H4	2.03	0.41
1:B:270:HIS:CD2	1:B:274:GLN:NE2	2.87	0.40
1:A:251:ILE:O	1:A:270:HIS:CE1	2.68	0.40
1:C:128[B]:ARG:HA	1:C:131:LEU:HD22	2.03	0.40
1:C:318:ARG:NH2	1:D:300:ASP:OD1	2.54	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	323/365 (88%)	318 (98%)	5 (2%)	0	100	100
1	B	321/365 (88%)	316 (98%)	5 (2%)	0	100	100
1	C	343/365 (94%)	333 (97%)	7 (2%)	3 (1%)	14	10
1	D	327/365 (90%)	322 (98%)	5 (2%)	0	100	100
All	All	1314/1460 (90%)	1289 (98%)	22 (2%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	ALA

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Mol	Chain	Res	Type
1	C	154	GLU
1	C	157	VAL

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	302/337 (90%)	293 (97%)	9 (3%)	36	41
1	B	298/337 (88%)	292 (98%)	6 (2%)	48	56
1	C	313/337 (93%)	302 (96%)	11 (4%)	32	35
1	D	304/337 (90%)	296 (97%)	8 (3%)	40	46
All	All	1217/1348 (90%)	1183 (97%)	34 (3%)	38	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	85	GLU
1	A	91	LYS
1	A	118	THR
1	A	131	LEU
1	A	143	ARG
1	A	200	GLU
1	A	263	ARG
1	A	324	GLN
1	B	37	LEU
1	B	85	GLU
1	B	118	THR
1	B	131	LEU
1	B	200	GLU
1	B	324	GLN
1	C	37	LEU
1	C	85	GLU
1	C	91	LYS
1	C	118	THR

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Mol	Chain	Res	Type
1	C	131	LEU
1	C	135	SER
1	C	143	ARG
1	C	171	GLU
1	C	200	GLU
1	C	263	ARG
1	C	324	GLN
1	D	37	LEU
1	D	118	THR
1	D	131	LEU
1	D	152	LEU
1	D	155	GLN
1	D	170	GLU
1	D	200	GLU
1	D	324	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	112	GLN
1	A	190	GLN
1	A	221	GLN
1	A	223	GLN
1	A	270	HIS
1	A	274	GLN
1	A	323	GLN
1	A	324	GLN
1	B	52	HIS
1	B	112	GLN
1	B	141	GLN
1	B	190	GLN
1	B	221	GLN
1	B	270	HIS
1	B	274	GLN
1	B	323	GLN
1	B	324	GLN
1	C	52	HIS
1	C	112	GLN
1	C	190	GLN
1	C	270	HIS
1	C	274	GLN

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Mol	Chain	Res	Type
1	C	323	GLN
1	C	324	GLN
1	D	52	HIS
1	D	112	GLN
1	D	141	GLN
1	D	190	GLN
1	D	221	GLN
1	D	270	HIS
1	D	274	GLN
1	D	292	HIS
1	D	323	GLN
1	D	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	401	1,3	50,50,50	1.26	7 (14%)	67,82,82	0.71	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	401	1,3	50,50,50	1.22	7 (14%)	67,82,82	0.59	0
2	HEM	B	401	1,3	50,50,50	1.26	6 (12%)	67,82,82	0.67	2 (2%)
2	HEM	D	401	1,3	50,50,50	1.23	5 (10%)	67,82,82	0.71	1 (1%)
3	5PK	D	402	2	24,24,24	3.18	8 (33%)	27,34,34	3.12	7 (25%)
3	5PK	B	402	2	24,24,24	3.29	9 (37%)	27,34,34	2.87	6 (22%)
3	5PK	C	402	2	24,24,24	3.07	8 (33%)	27,34,34	2.54	8 (29%)
3	5PK	A	402	2	24,24,24	3.42	8 (33%)	27,34,34	3.73	6 (22%)

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	A	401	1,3	-	3/14/54/54	-
2	HEM	C	401	1,3	-	2/14/54/54	-
2	HEM	B	401	1,3	-	3/14/54/54	-
2	HEM	D	401	1,3	-	3/14/54/54	-
3	5PK	D	402	2	-	0/8/28/28	0/4/4/4
3	5PK	B	402	2	-	1/8/28/28	0/4/4/4
3	5PK	C	402	2	-	1/8/28/28	0/4/4/4
3	5PK	A	402	2	-	0/8/28/28	0/4/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	5PK	CAK-CAJ	-10.73	1.39	1.51
3	B	402	5PK	CAK-CAJ	-9.20	1.41	1.51
3	D	402	5PK	CAL-CAM	-9.14	1.33	1.46
3	C	402	5PK	CAL-CAM	-9.11	1.33	1.46
3	B	402	5PK	CAL-CAM	-8.88	1.34	1.46
3	A	402	5PK	CAL-CAM	-8.67	1.34	1.46
3	D	402	5PK	CAK-CAJ	-8.19	1.42	1.51
3	C	402	5PK	CAK-CAJ	-7.07	1.43	1.51
3	B	402	5PK	CAR-CAK	-4.64	1.34	1.39
3	D	402	5PK	CAR-CAK	-4.51	1.34	1.39
3	B	402	5PK	CAO-CAM	-4.45	1.33	1.37
3	D	402	5PK	CAO-CAM	-4.36	1.33	1.37
3	A	402	5PK	CAR-CAK	-4.35	1.34	1.39
3	C	402	5PK	CAR-CAK	-4.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	5PK	CAO-CAM	-4.16	1.33	1.37
3	D	402	5PK	CAU-CAL	-4.06	1.33	1.39
3	A	402	5PK	CAO-CAM	-4.03	1.33	1.37
3	A	402	5PK	CAU-CAL	-3.98	1.33	1.39
3	C	402	5PK	CAU-CAL	-3.76	1.34	1.39
3	B	402	5PK	CAM-NAN	-3.61	1.32	1.39
2	D	401	HEM	FE-NB	3.60	2.06	1.94
3	B	402	5PK	CAU-CAL	-3.57	1.34	1.39
2	A	401	HEM	FE-NB	3.53	2.05	1.94
3	D	402	5PK	CAM-NAN	-3.50	1.32	1.39
2	C	401	HEM	FE-NB	3.46	2.05	1.94
2	B	401	HEM	FE-NB	3.42	2.05	1.94
2	D	401	HEM	FE-NC	3.40	2.06	1.95
2	B	401	HEM	FE-NC	3.36	2.06	1.95
2	D	401	HEM	FE-NA	3.35	2.06	1.95
2	C	401	HEM	FE-NC	3.33	2.06	1.95
3	C	402	5PK	CAM-NAN	-3.33	1.33	1.39
2	A	401	HEM	FE-NC	3.30	2.06	1.95
2	B	401	HEM	FE-ND	3.28	2.05	1.94
2	A	401	HEM	FE-NA	3.28	2.06	1.95
2	C	401	HEM	FE-ND	3.26	2.04	1.94
2	B	401	HEM	FE-NA	3.23	2.05	1.95
3	A	402	5PK	CAM-NAN	-3.20	1.33	1.39
2	A	401	HEM	FE-ND	3.17	2.04	1.94
2	D	401	HEM	FE-ND	3.12	2.04	1.94
2	C	401	HEM	FE-NA	3.05	2.05	1.95
3	A	402	5PK	CAL-CAK	-2.93	1.35	1.39
3	A	402	5PK	CAO-NAP	-2.80	1.32	1.37
3	D	402	5PK	CAL-CAK	-2.73	1.35	1.39
3	B	402	5PK	CAL-CAK	-2.66	1.35	1.39
3	C	402	5PK	CAO-NAP	-2.43	1.33	1.37
3	D	402	5PK	CAO-NAP	-2.40	1.33	1.37
3	C	402	5PK	CAL-CAK	-2.37	1.36	1.39
2	B	401	HEM	C1B-NB	-2.34	1.36	1.40
3	B	402	5PK	CAO-NAP	-2.31	1.33	1.37
2	B	401	HEM	CHB-C1B	2.29	1.43	1.38
2	A	401	HEM	C1B-NB	-2.28	1.36	1.40
2	C	401	HEM	CHB-C1B	2.18	1.42	1.38
2	A	401	HEM	CHB-C1B	2.18	1.42	1.38
2	C	401	HEM	CHC-C1C	2.11	1.42	1.38
2	A	401	HEM	CHC-C1C	2.10	1.42	1.38
2	C	401	HEM	C1B-NB	-2.08	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	5PK	CAQ-NAN	-2.02	1.33	1.37
2	D	401	HEM	C1B-NB	-2.02	1.36	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	5PK	CAJ-NAN-CAM	-14.77	106.67	113.77
3	D	402	5PK	CAJ-NAN-CAM	-10.41	108.77	113.77
3	B	402	5PK	CAJ-NAN-CAM	-9.26	109.32	113.77
3	A	402	5PK	CAL-CAM-NAN	7.84	110.15	107.44
3	C	402	5PK	CAJ-NAN-CAM	-7.25	110.29	113.77
3	D	402	5PK	CAL-CAM-NAN	6.47	109.68	107.44
3	B	402	5PK	CAH-CAJ-NAN	-6.21	102.85	113.40
3	A	402	5PK	CAL-CAM-CAO	-5.97	142.38	146.18
3	D	402	5PK	CAH-CAJ-NAN	-5.79	103.57	113.40
3	C	402	5PK	CAL-CAM-NAN	5.47	109.33	107.44
3	B	402	5PK	CAL-CAM-NAN	4.97	109.16	107.44
3	D	402	5PK	CAL-CAM-CAO	-4.50	143.32	146.18
3	A	402	5PK	CAK-CAL-CAM	4.40	110.35	107.78
3	B	402	5PK	CAL-CAM-CAO	-4.39	143.39	146.18
3	C	402	5PK	CAL-CAM-CAO	-4.37	143.40	146.18
3	C	402	5PK	NAN-CAQ-NAP	-4.28	107.63	111.68
3	D	402	5PK	NAN-CAQ-NAP	-4.24	107.67	111.68
3	B	402	5PK	NAN-CAQ-NAP	-4.16	107.75	111.68
3	D	402	5PK	CAK-CAL-CAM	3.95	110.09	107.78
3	C	402	5PK	CAK-CAL-CAM	3.49	109.82	107.78
3	B	402	5PK	CAK-CAL-CAM	3.48	109.81	107.78
3	C	402	5PK	CAH-CAJ-NAN	-3.33	107.74	113.40
3	A	402	5PK	NAN-CAQ-NAP	-3.23	108.63	111.68
3	A	402	5PK	OAI-CAG-CAH	3.09	115.33	109.15
2	A	401	HEM	CAD-C3D-C4D	2.25	128.62	124.70
2	B	401	HEM	C3C-C2C-C1C	-2.23	104.94	107.05
3	C	402	5PK	CAO-NAP-CAQ	2.21	108.14	105.24
2	A	401	HEM	C3C-C2C-C1C	-2.13	105.03	107.05
3	D	402	5PK	CAS-CAT-CAU	-2.11	117.63	120.24
2	D	401	HEM	CAD-C3D-C4D	2.08	128.33	124.70
2	B	401	HEM	CAD-C3D-C4D	2.07	128.31	124.70
3	C	402	5PK	CAR-CAK-CAL	-2.02	118.67	120.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

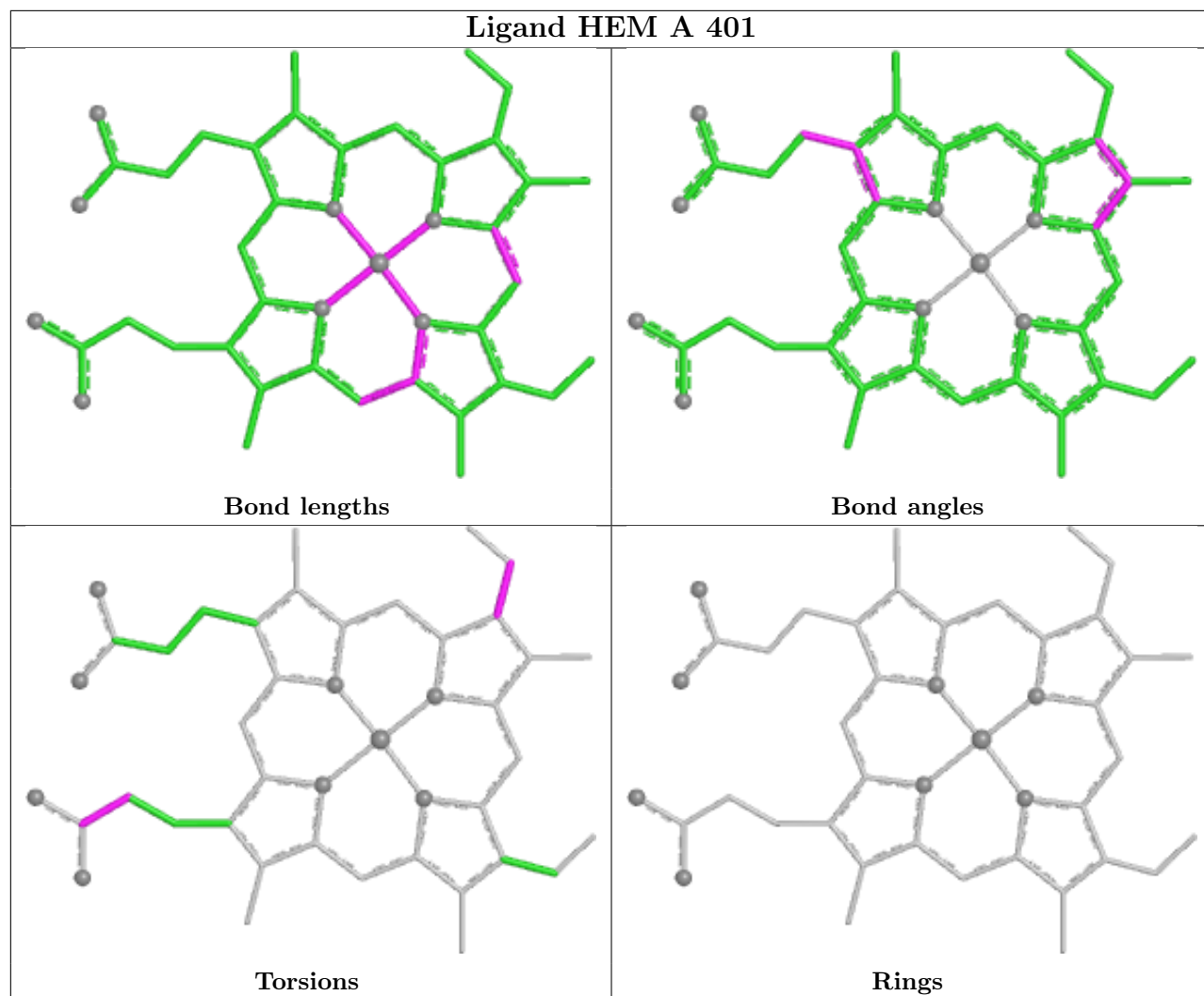
Mol	Chain	Res	Type	Atoms
3	C	402	5PK	CAG-CAH-CAJ-CAK
2	A	401	HEM	C2C-C3C-CAC-CBC
2	A	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	C2C-C3C-CAC-CBC
3	B	402	5PK	CAG-CAH-CAJ-CAK
2	D	401	HEM	CAD-CBD-CGD-O2D

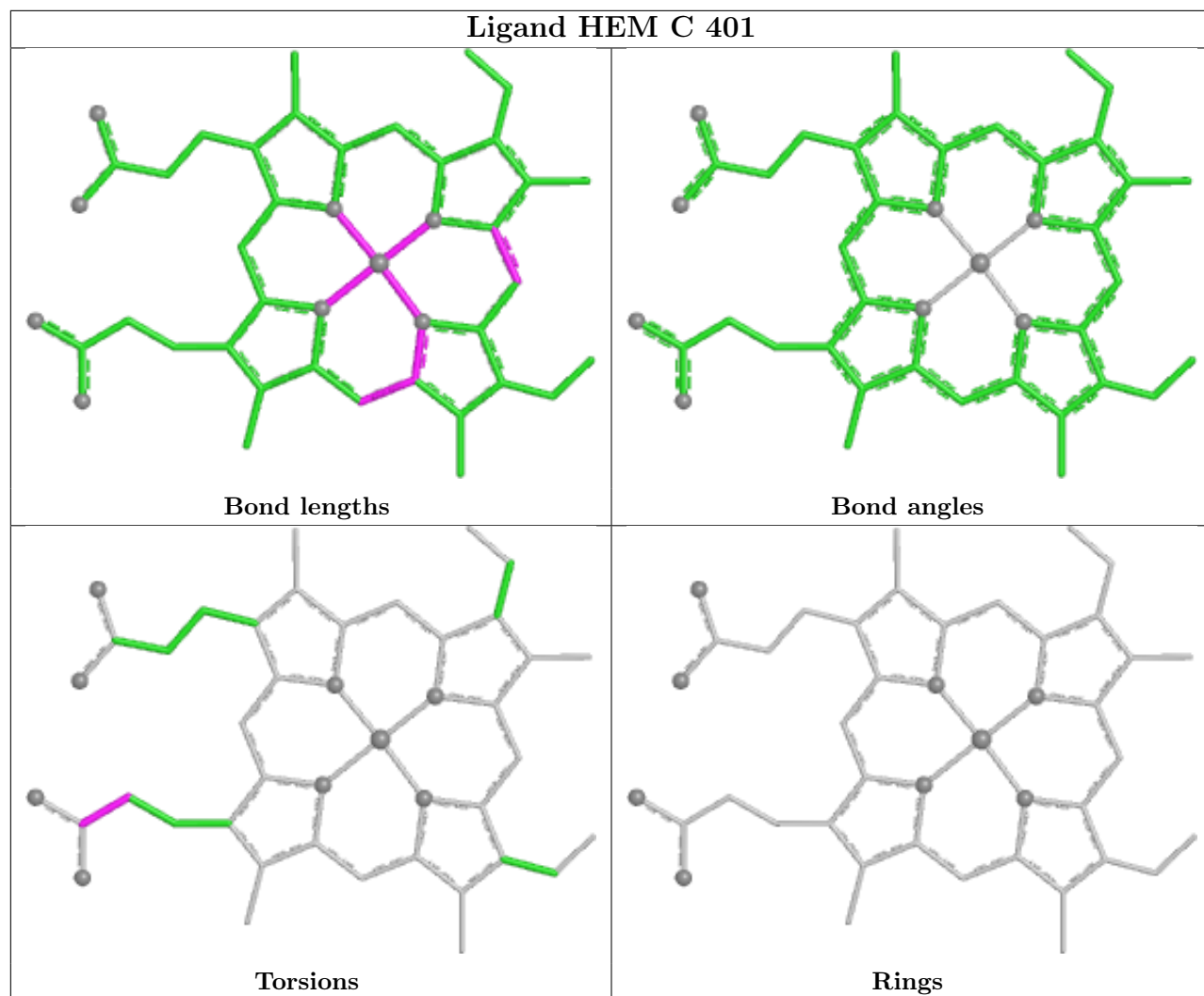
There are no ring outliers.

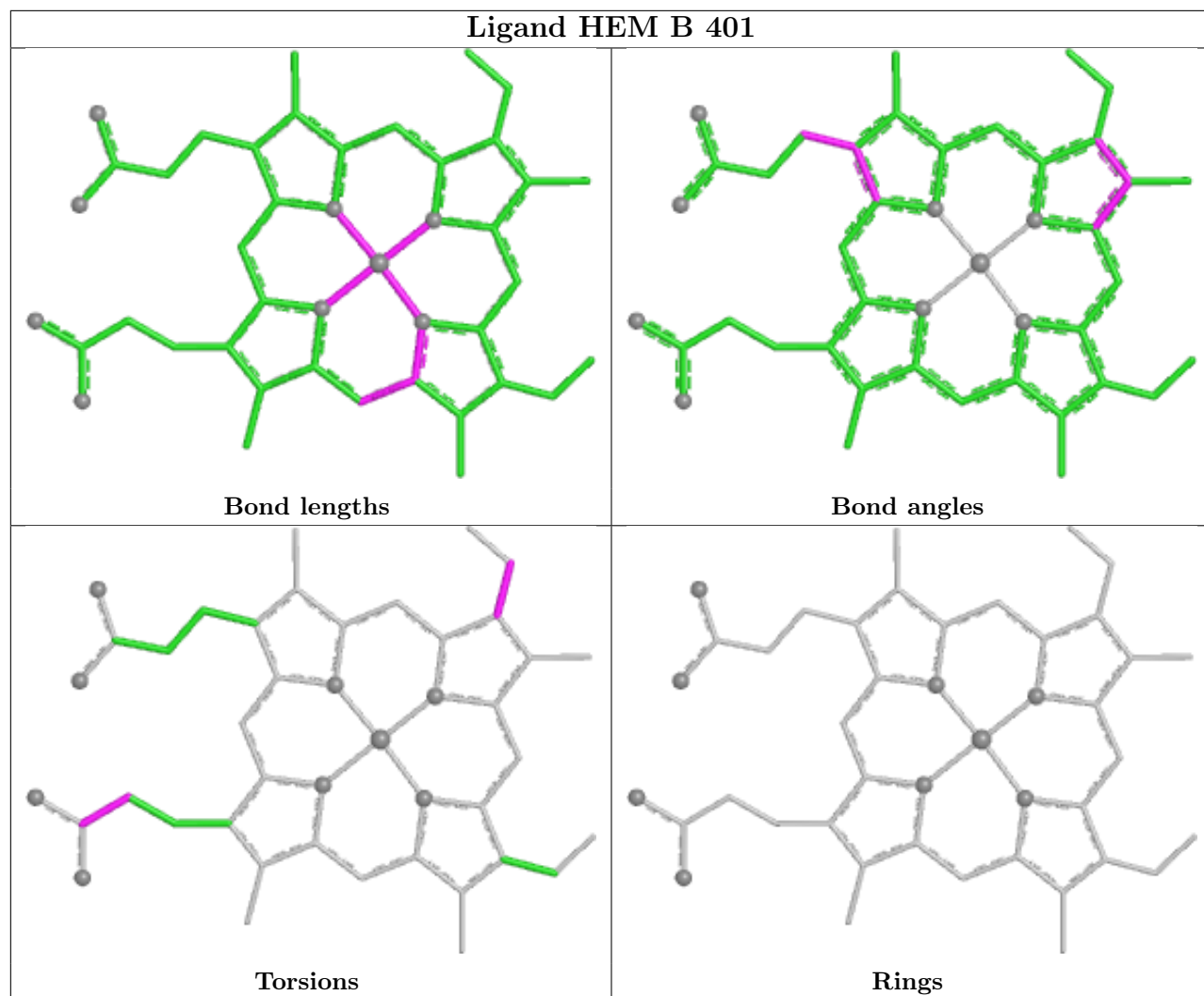
8 monomers are involved in 15 short contacts:

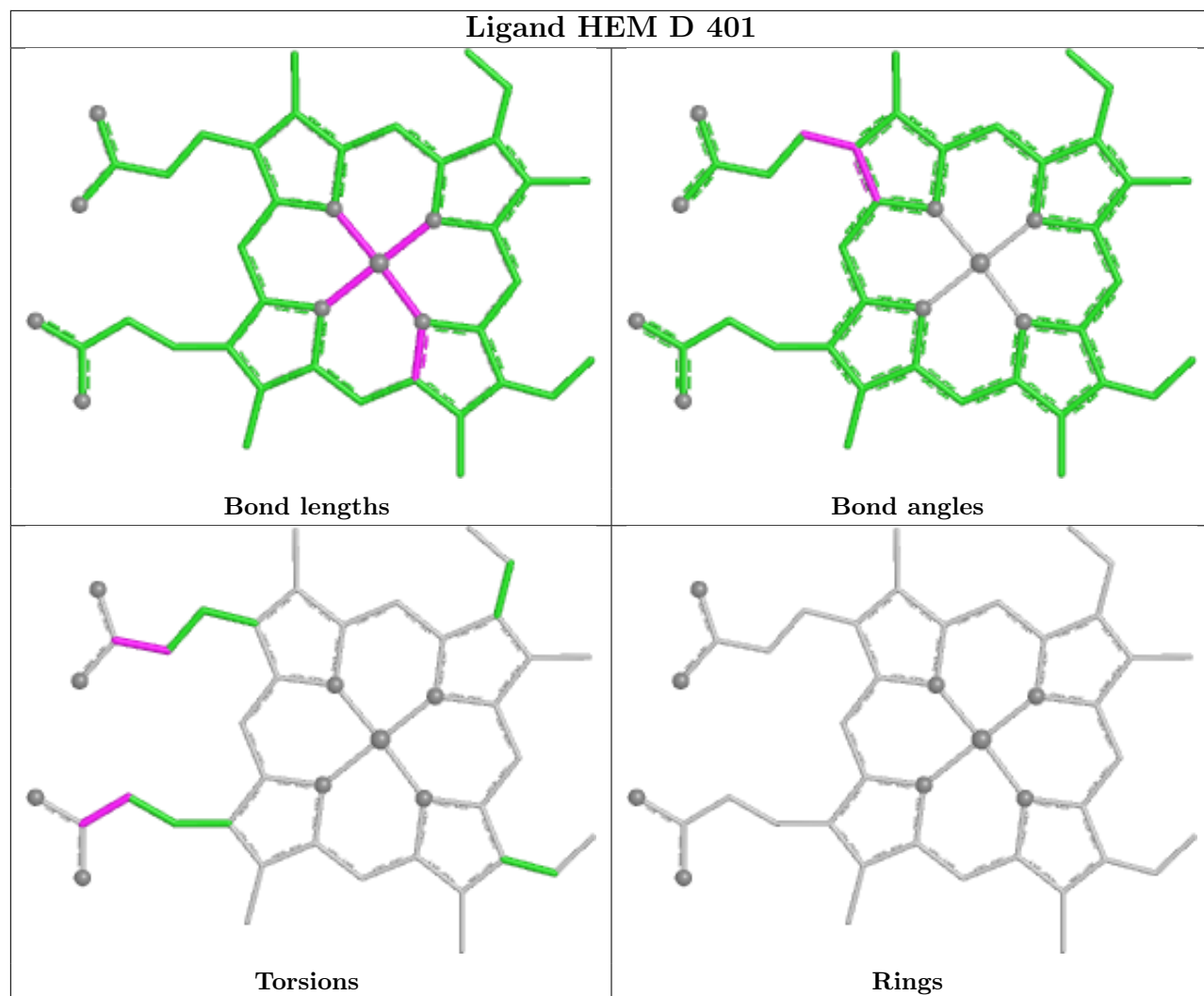
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	1	0
2	C	401	HEM	3	0
2	B	401	HEM	2	0
2	D	401	HEM	2	0
3	D	402	5PK	2	0
3	B	402	5PK	2	0
3	C	402	5PK	5	0
3	A	402	5PK	2	0

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.

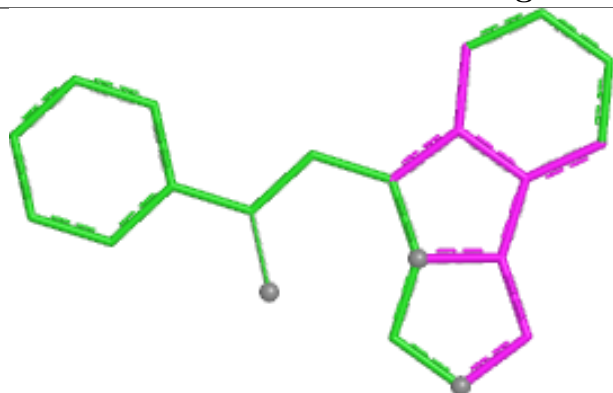




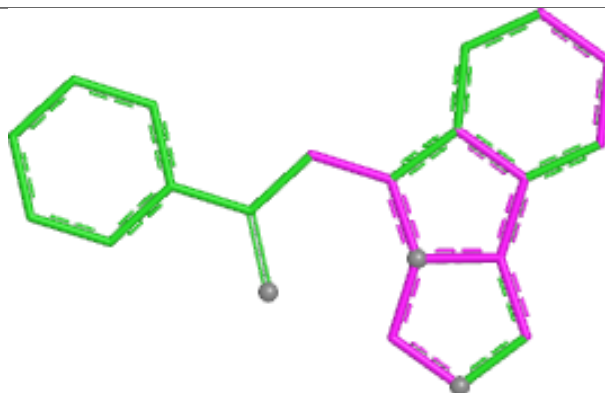




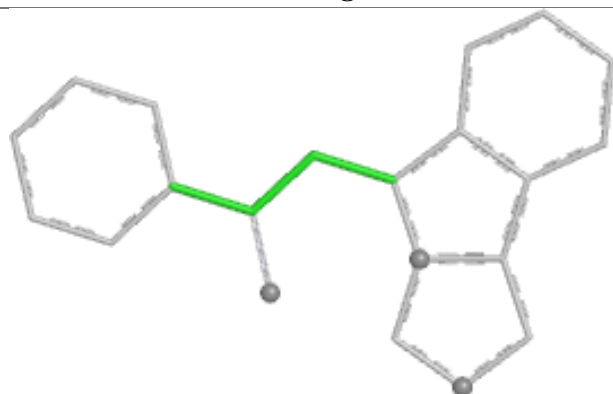
Ligand 5PK D 402



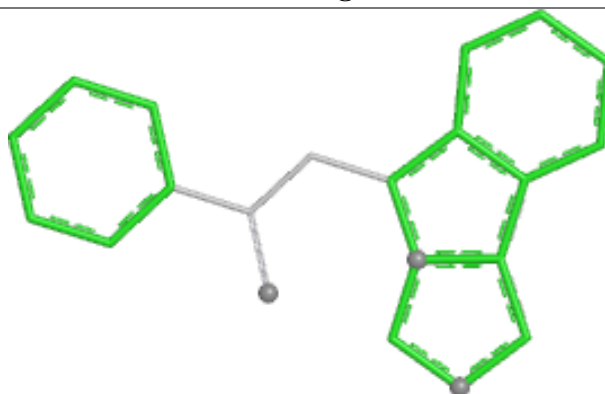
Bond lengths



Bond angles

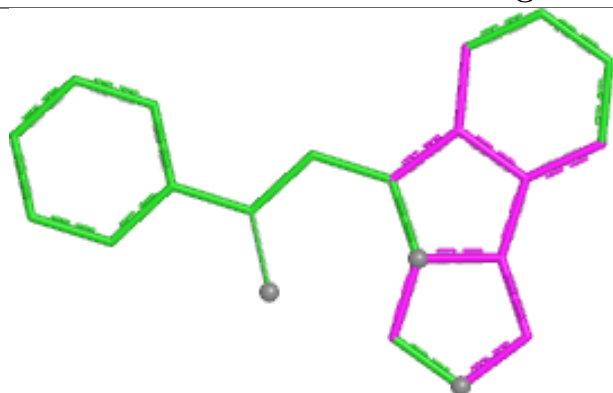


Torsions

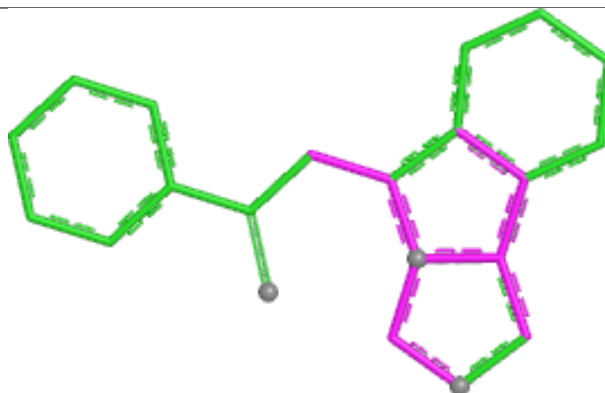


Rings

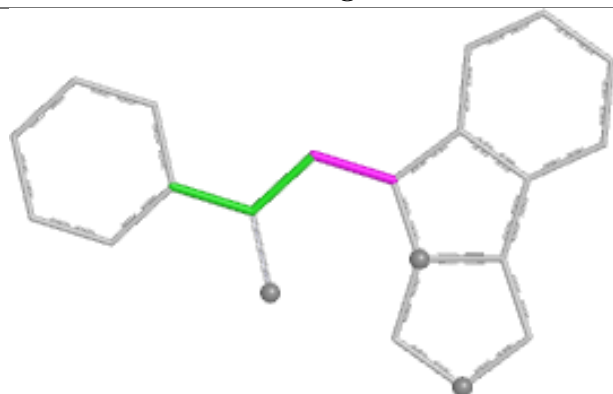
Ligand 5PK B 402



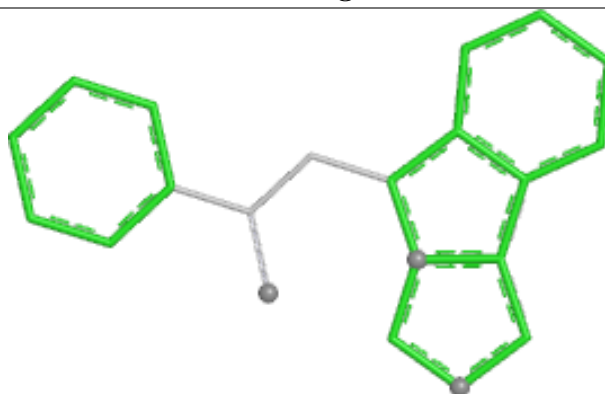
Bond lengths



Bond angles

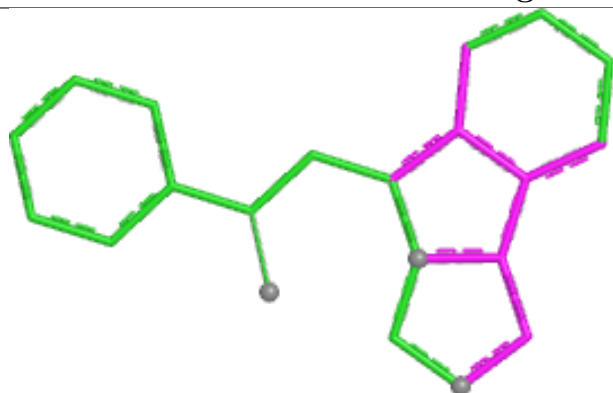


Torsions

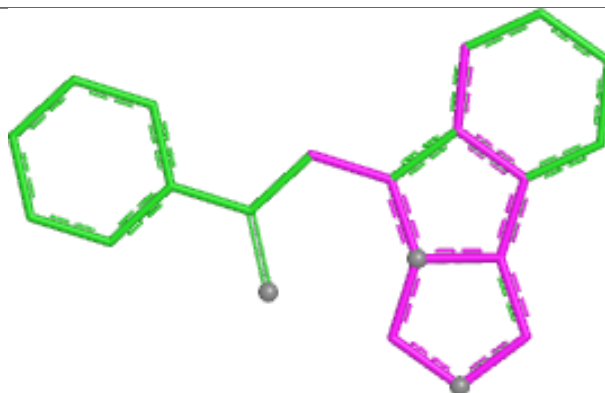


Rings

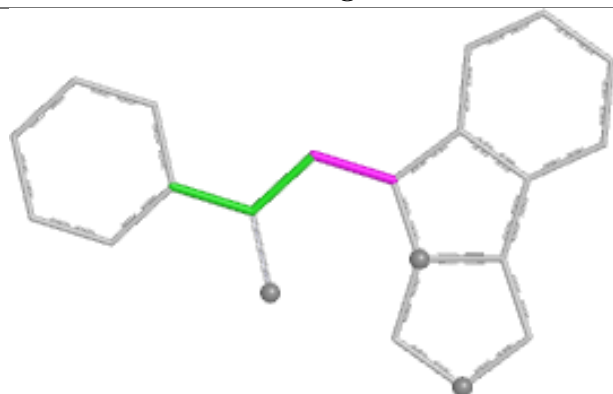
Ligand 5PK C 402



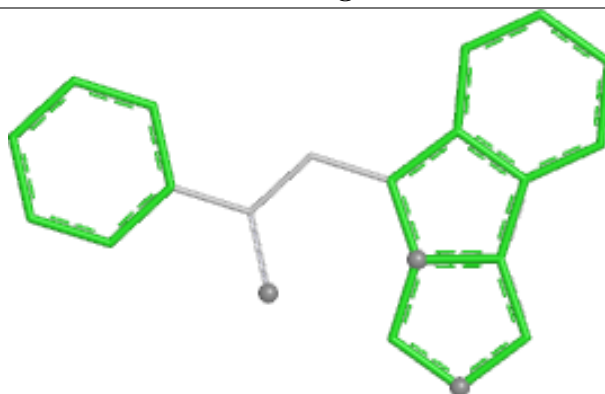
Bond lengths



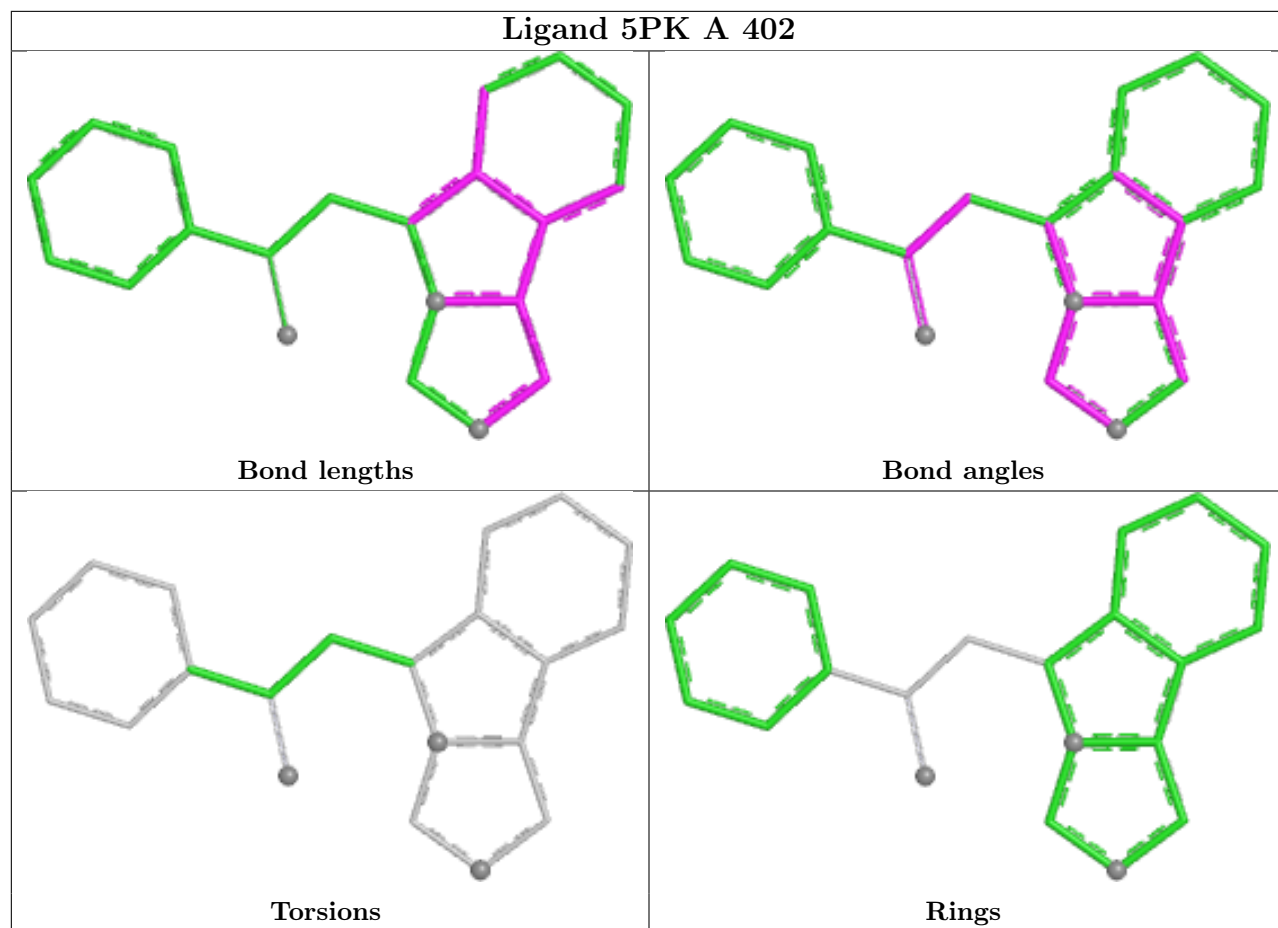
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	328/365 (89%)	-1.02	0 100 100	29, 48, 73, 89	1 (0%)
1	B	326/365 (89%)	-0.99	0 100 100	30, 49, 75, 94	1 (0%)
1	C	344/365 (94%)	-0.99	0 100 100	30, 47, 74, 92	1 (0%)
1	D	331/365 (90%)	-1.01	0 100 100	33, 48, 76, 91	0
All	All	1329/1460 (91%)	-1.00	0 100 100	29, 48, 75, 94	3 (0%)

There are no RSRZ outliers to report.

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
3	5PK	D	402	21/21	0.98	0.06	51,53,56,57	0
2	HEM	B	401	43/43	0.99	0.04	41,43,51,53	0
3	5PK	A	402	21/21	0.99	0.05	54,55,60,60	0
3	5PK	B	402	21/21	0.99	0.05	50,51,57,58	0

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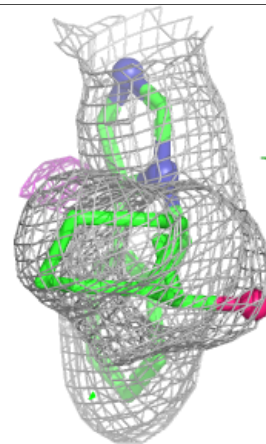
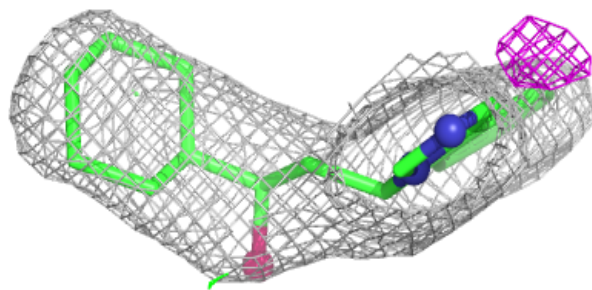
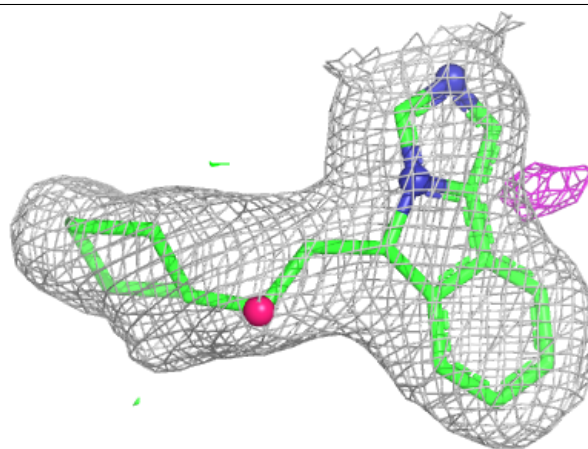
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5PK	C	402	21/21	0.99	0.05	54,54,60,61	0
2	HEM	A	401	43/43	0.99	0.04	43,45,51,53	0
2	HEM	C	401	43/43	1.00	0.03	40,42,48,50	0
2	HEM	D	401	43/43	1.00	0.03	42,44,50,53	0

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

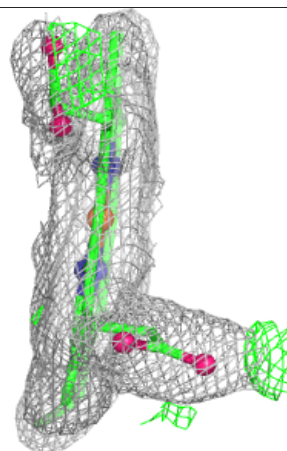
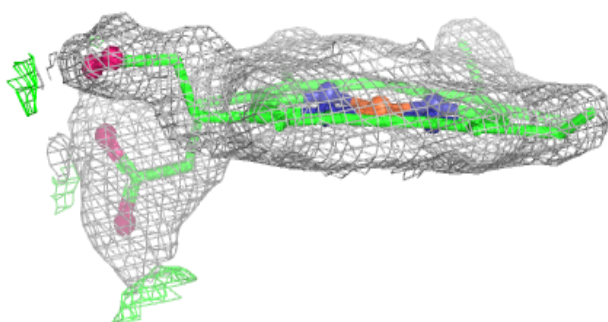
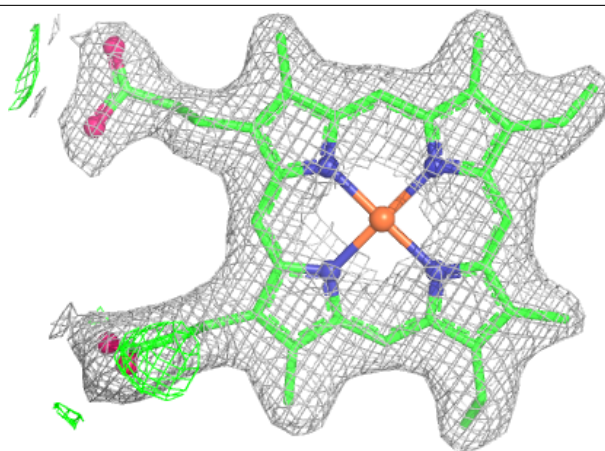
Electron density around 5PK D 402:

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



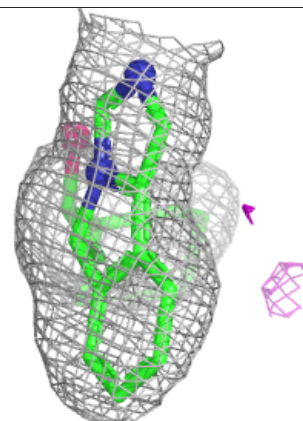
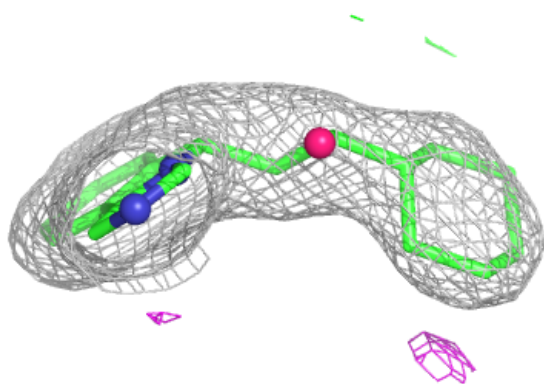
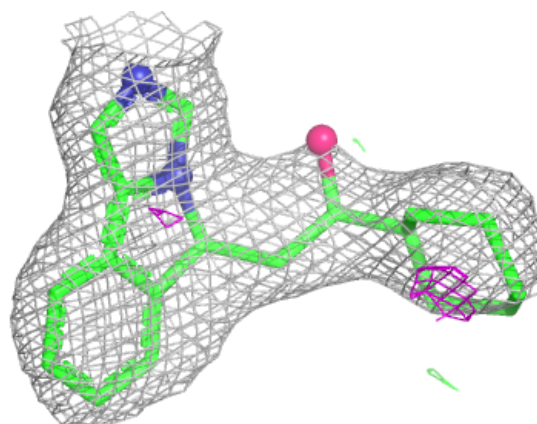
Electron density around HEM B 401:

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

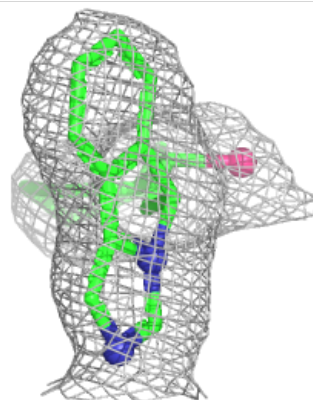
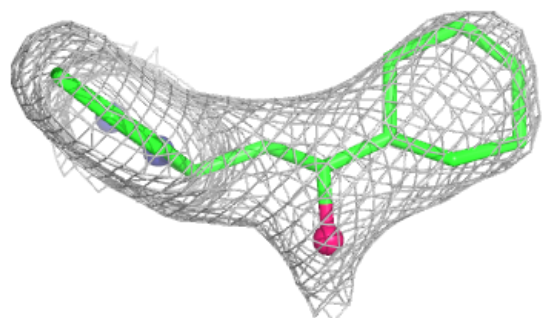
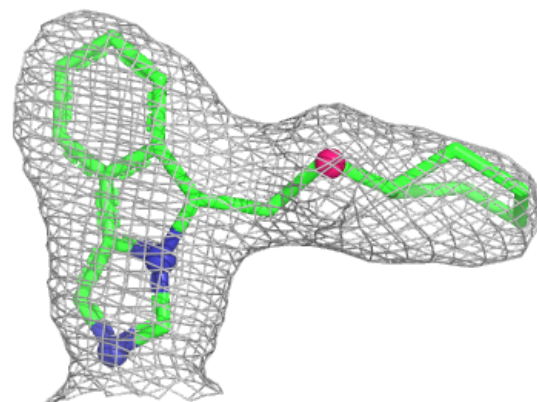


Electron density around 5PK A 402:

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

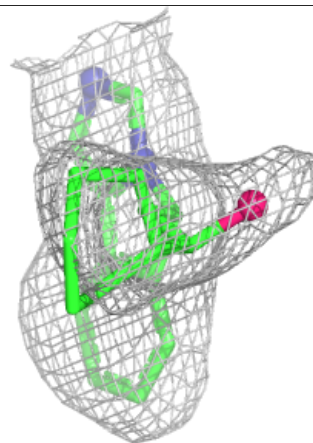
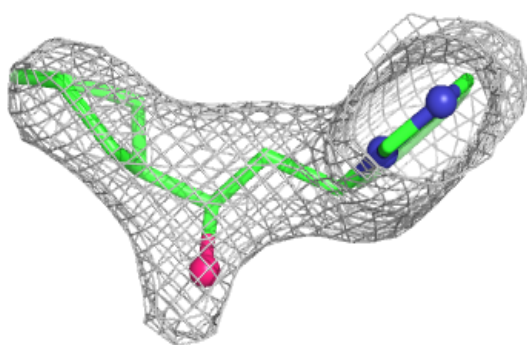
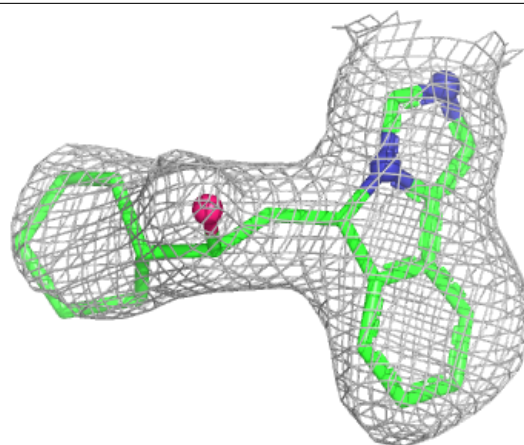
**Electron density around 5PK B 402:**

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



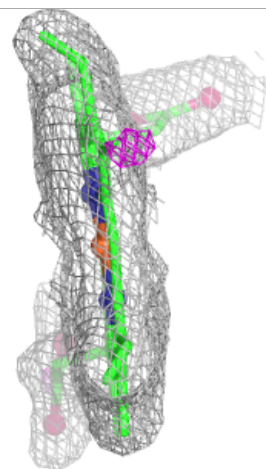
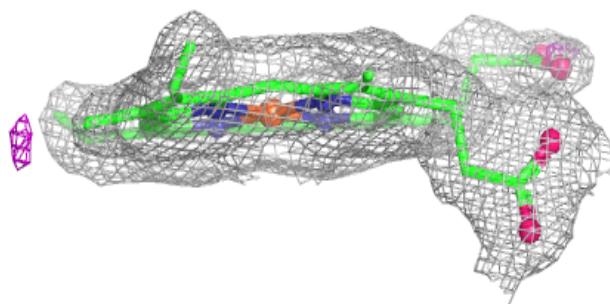
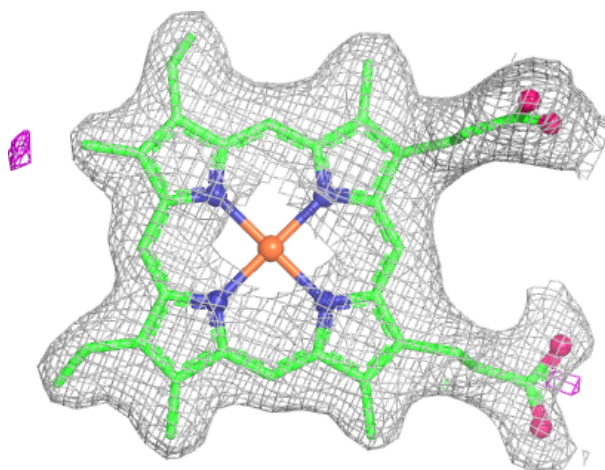
Electron density around 5PK C 402:

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



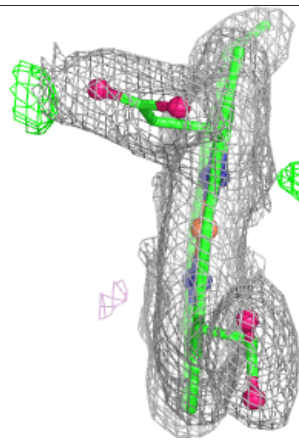
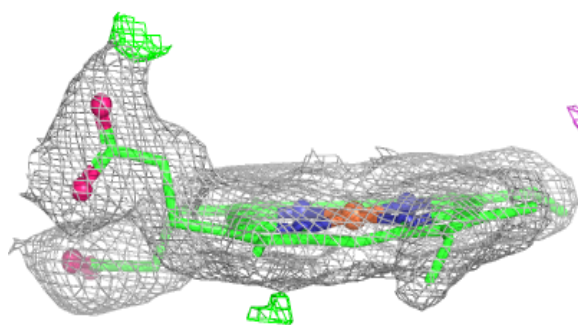
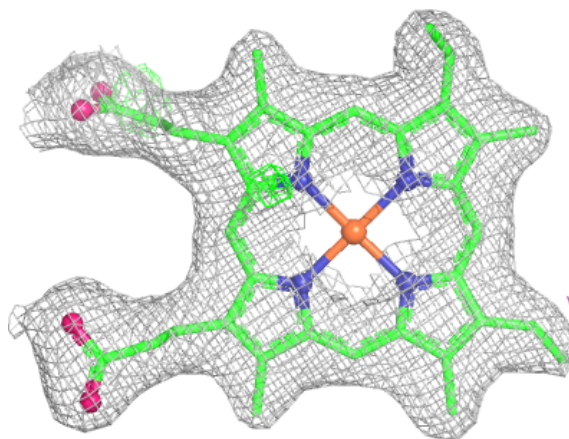
Electron density around HEM A 401:

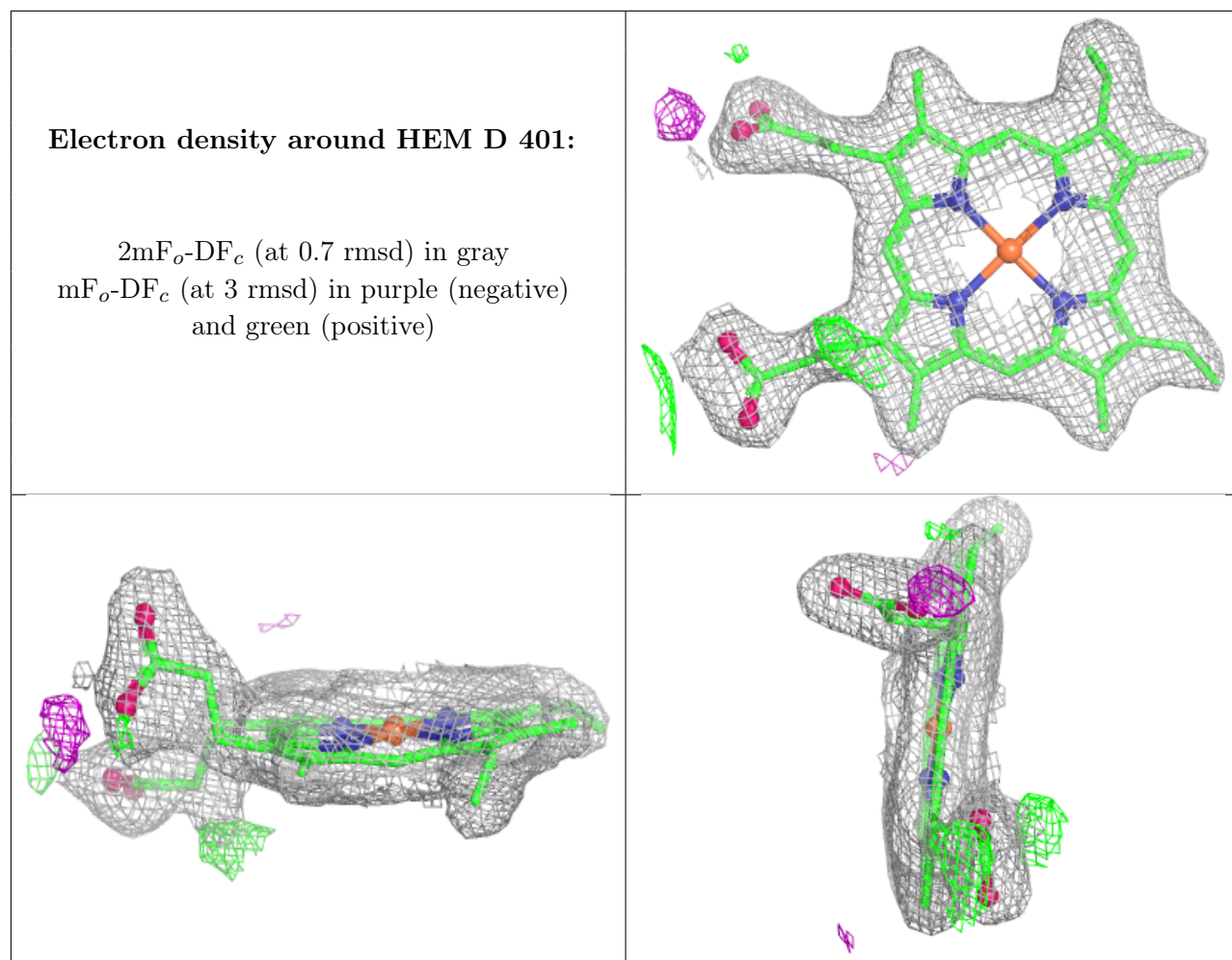
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.