WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2025 – 12:09 PM EDT

PDB ID	:	9DFM / pdb_00009dfm
Title	:	Crystal structure of PrnB in complex with tryptamine
Authors	:	Li, B.; Wang, Y.
Deposited on	:	2024-08-30
Resolution	:	2.25 Å(reported)

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

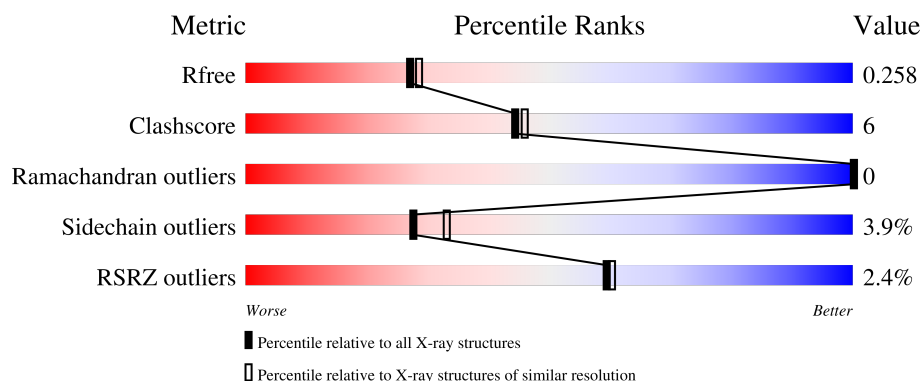|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.25 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		2.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	370	3% 79% 13% • 6%
1	B	370	2% 80% 14% • 6%

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2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6098 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 PrnB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total 2754	C 1770	N 462	O 516	S 6	0	1	0
1	B	347	Total 2747	C 1765	N 460	O 516	S 6	0	0	0

- Molecule 2 is 2-(1H-INDOL-3-YL)ETHANAMINE (CCD ID: TSS) (formula: $C_{10}H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).
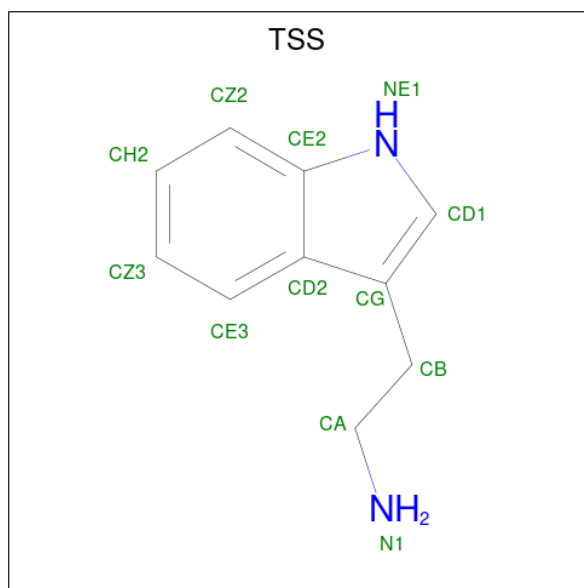
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 24	C 20	N 4	0	1
2	B	1	Total 12	C 10	N 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	210	Total	O	0	0
			210	210		
5	B	217	Total	O	0	0
			217	217		

# 3 Residue-property plots ⓘ

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

• Molecule 1: PrnB

Chain A:
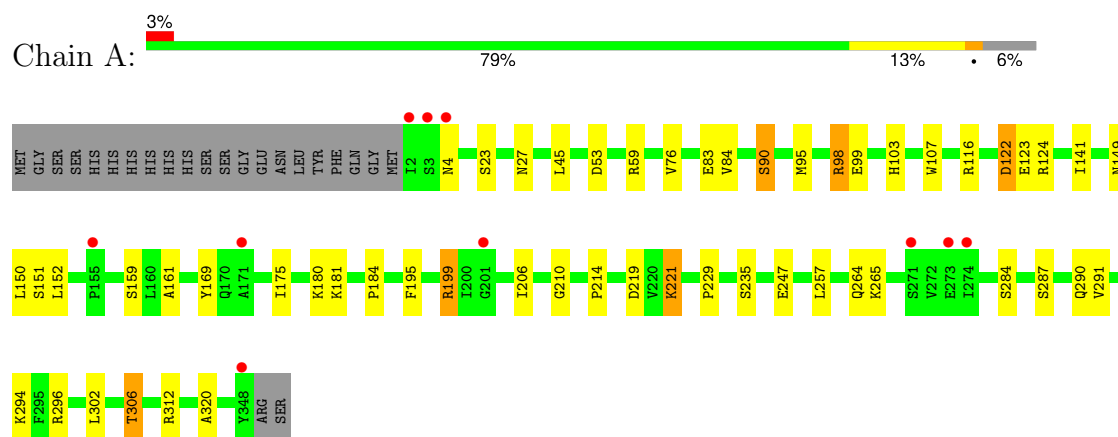
• Molecule 1: PrnB

Chain B:
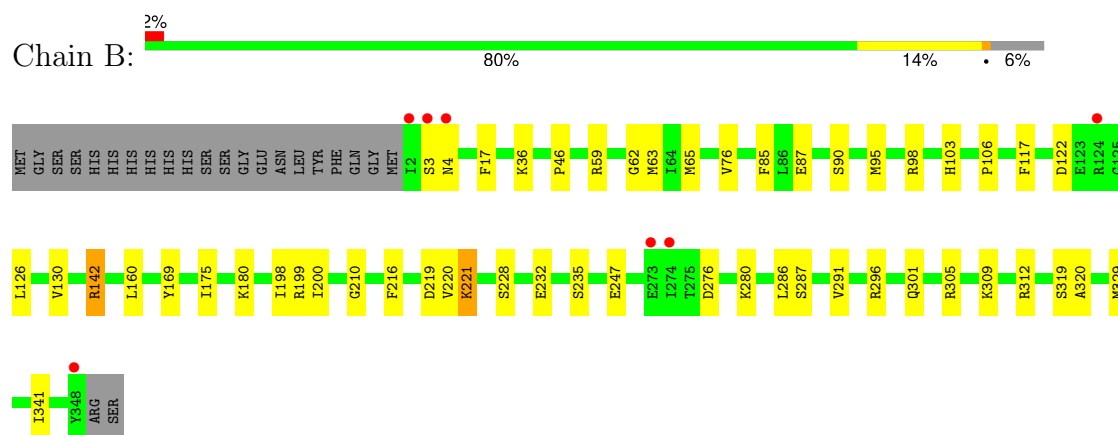
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.74Å 122.36Å 66.47Å 90.00° 94.62° 90.00°	Depositor
Resolution (Å)	46.11 – 2.25 46.11 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.11-2.25) 92.7 (46.11-2.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.206 , 0.260 0.205 , 0.258	Depositor DCC
R_{free} test set	50545 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6098	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: HEM, GOL, TSS

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	0.44	2/2819 (0.1%)	0.59	0/3827
1	B	0.44	1/2808 (0.0%)	0.58	0/3812
All	All	0.44	3/5627 (0.1%)	0.59	0/7639

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLU	CB-CG	6.50	1.64	1.52
1	A	247	GLU	CB-CG	5.92	1.63	1.52
1	A	247	GLU	CD-OE2	5.04	1.31	1.25

There are no bond angle outliers.

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	2754	0	2770	32	0
1	B	2747	0	2763	29	0
2	A	24	0	24	4	0
2	B	12	0	12	5	0
3	A	30	0	40	0	0
3	B	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	3	0
4	B	43	0	30	3	0
5	A	210	0	0	6	0
5	B	217	0	0	3	0
All	All	6098	0	5693	67	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 6.

All (67) 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:124:ARG:HH12	1:A:181:LYS:HE2	1.55	0.72
1:A:116:ARG:NH1	1:A:123:GLU:HB3	2.17	0.59
1:A:27:ASN:ND2	5:A:511:HOH:O	2.36	0.58
1:A:210:GLY:H	2:A:401[A]:TSS:HA2	1.69	0.57
2:B:1001:TSS:HE3	2:B:1001:TSS:N1	2.19	0.57
1:A:152:LEU:HD21	1:A:265:LYS:HG3	1.87	0.56
1:B:62:GLY:HA2	1:B:65:MET:HE2	1.88	0.56
4:B:1002:HEM:HMB1	4:B:1002:HEM:HBB2	1.87	0.55
1:A:90:SER:HB2	1:A:95:MET:O	2.05	0.55
1:B:142:ARG:NH1	5:B:1106:HOH:O	2.36	0.55
1:B:59:ARG:HB2	1:B:103:HIS:HB3	1.89	0.55
2:B:1001:TSS:HE3	2:B:1001:TSS:HN11	1.72	0.54
1:B:309:LYS:HD2	1:B:312:ARG:CZ	2.38	0.54
1:B:3:SER:HB3	1:B:106:PRO:O	2.09	0.53
1:B:216:PHE:O	1:B:220:VAL:HG23	2.09	0.53
1:B:90:SER:HB2	1:B:95:MET:O	2.09	0.52
1:A:124:ARG:NH1	1:A:181:LYS:HE2	2.24	0.52
2:B:1001:TSS:HB1	4:B:1002:HEM:C1B	2.45	0.52
1:A:116:ARG:HH11	1:A:123:GLU:HB3	1.76	0.51
1:A:161:ALA:HB3	1:A:284:SER:HB2	1.93	0.51
1:B:287:SER:O	1:B:291:VAL:HG23	2.13	0.49
1:A:84:VAL:HG13	5:A:578:HOH:O	2.12	0.49
1:A:287:SER:O	1:A:291:VAL:HG23	2.13	0.49
1:A:219:ASP:OD2	1:A:296:ARG:NH2	2.44	0.49
1:A:149:ASN:O	1:A:150:LEU:HD23	2.12	0.48
1:A:302:LEU:O	1:A:306:THR:HG23	2.13	0.48
1:B:210:GLY:H	2:B:1001:TSS:CE3	2.27	0.48
1:A:195:PHE:CZ	2:A:401[B]:TSS:HZ2	2.49	0.47
1:A:229:PRO:O	5:A:502:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HG3	1:A:99:GLU:N	2.30	0.47
1:B:221:LYS:HZ3	1:B:221:LYS:HG2	1.50	0.47
1:B:320:ALA:HB3	4:B:1002:HEM:CGA	2.43	0.47
1:B:219:ASP:OD2	1:B:296:ARG:NH2	2.46	0.47
1:B:198:ILE:HG22	1:B:200:ILE:HG13	1.97	0.47
1:B:232:GLU:HB3	1:B:329:MET:CE	2.44	0.47
1:B:319:SER:H	2:B:1001:TSS:HD1	1.80	0.47
1:B:17:PHE:CD1	1:B:36:LYS:HE3	2.50	0.46
1:A:103:HIS:HA	1:A:107:TRP:HB2	1.97	0.46
1:A:76:VAL:HG11	1:A:83:GLU:HG3	1.96	0.46
1:A:59:ARG:HB2	1:A:103:HIS:HB3	1.98	0.46
1:A:199:ARG:NH1	5:A:521:HOH:O	2.46	0.46
1:B:126:LEU:O	1:B:130:VAL:HG22	2.16	0.46
1:B:286:LEU:HB2	1:B:341:ILE:HG21	1.98	0.45
1:A:320:ALA:HB3	4:A:407:HEM:CGA	2.47	0.45
1:B:276:ASP:O	1:B:280:LYS:HG3	2.17	0.45
1:A:53:ASP:OD1	5:A:503:HOH:O	2.21	0.45
2:A:401[A]:TSS:HB1	4:A:407:HEM:C4B	2.52	0.45
1:B:46:PRO:HG3	1:B:85:PHE:CZ	2.52	0.45
1:A:206:ILE:HD12	5:A:519:HOH:O	2.18	0.44
1:B:63:MET:HG2	1:B:117:PHE:CZ	2.54	0.43
1:B:175:ILE:HD12	1:B:175:ILE:HA	1.84	0.43
1:A:141:ILE:HD11	1:A:214:PRO:HB2	1.99	0.43
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.87	0.43
1:A:184:PRO:HB3	1:A:306:THR:HG22	2.00	0.43
2:A:401[A]:TSS:HB1	4:A:407:HEM:NB	2.34	0.43
1:B:142:ARG:HG2	5:B:1106:HOH:O	2.17	0.43
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.89	0.43
1:A:4:ASN:OD1	1:A:4:ASN:N	2.51	0.42
1:A:290:GLN:O	1:A:294:LYS:HG3	2.19	0.42
1:B:87:GLU:OE2	5:B:1101:HOH:O	2.22	0.42
1:B:232:GLU:HB3	1:B:329:MET:HE3	2.02	0.42
1:A:122:ASP:OD1	1:A:122:ASP:N	2.53	0.41
1:B:180:LYS:HB3	1:B:180:LYS:HE2	1.86	0.41
1:A:306:THR:O	1:A:312:ARG:HA	2.21	0.41
1:B:76:VAL:HG21	1:B:200:ILE:HG12	2.02	0.41
1:A:221:LYS:HZ3	1:A:221:LYS:HG2	1.66	0.40
1:B:301:GLN:O	1:B:305:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	346/370 (94%)	342 (99%)	4 (1%)	0	100	100
1	B	345/370 (93%)	337 (98%)	8 (2%)	0	100	100
All	All	691/740 (93%)	679 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	309/328 (94%)	294 (95%)	15 (5%)	21	23
1	B	308/328 (94%)	299 (97%)	9 (3%)	37	46
All	All	617/656 (94%)	593 (96%)	24 (4%)	27	33

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	45	LEU
1	A	90	SER
1	A	98	ARG
1	A	122	ASP
1	A	151	SER
1	A	159	SER
1	A	169	TYR

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Mol	Chain	Res	Type
1	A	180	LYS
1	A	199	ARG
1	A	221	LYS
1	A	235	SER
1	A	257	LEU
1	A	264	GLN
1	A	306	THR
1	B	4	ASN
1	B	98	ARG
1	B	122	ASP
1	B	142	ARG
1	B	169	TYR
1	B	199	ARG
1	B	221	LYS
1	B	228	SER
1	B	235	SER

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	GOL	B	1005	-	5,5,5	0.95	0	5,5,5	1.11	0
3	GOL	A	406	-	5,5,5	1.01	0	5,5,5	0.88	0
3	GOL	B	1003	-	5,5,5	1.27	0	5,5,5	1.02	0
4	HEM	B	1002	1,2	42,50,50	1.60	6 (14%)	46,82,82	1.56	8 (17%)
2	TSS	B	1001	4	12,13,13	1.08	2 (16%)	12,17,17	1.08	2 (16%)
2	TSS	A	401[A]	4	12,13,13	1.07	0	12,17,17	0.83	0
3	GOL	A	403	-	5,5,5	0.70	0	5,5,5	1.07	0
3	GOL	A	402	-	5,5,5	0.97	0	5,5,5	0.92	0
2	TSS	A	401[B]	-	12,13,13	1.08	0	12,17,17	0.81	0
4	HEM	A	407	1,2	42,50,50	1.58	7 (16%)	46,82,82	1.61	13 (28%)
3	GOL	A	404	-	5,5,5	0.90	0	5,5,5	1.17	0
3	GOL	B	1004	-	5,5,5	1.03	0	5,5,5	1.02	0
3	GOL	A	405	-	5,5,5	0.93	0	5,5,5	1.08	0

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	GOL	B	1005	-	-	4/4/4/4	-
3	GOL	A	406	-	-	4/4/4/4	-
3	GOL	B	1003	-	-	0/4/4/4	-
4	HEM	B	1002	1,2	-	5/12/54/54	-
2	TSS	B	1001	4	-	1/3/3/3	0/2/2/2
2	TSS	A	401[A]	4	-	1/3/3/3	0/2/2/2
3	GOL	A	403	-	-	4/4/4/4	-
3	GOL	A	402	-	-	4/4/4/4	-
2	TSS	A	401[B]	-	-	1/3/3/3	0/2/2/2
4	HEM	A	407	1,2	-	6/12/54/54	-
3	GOL	A	404	-	-	1/4/4/4	-
3	GOL	B	1004	-	-	2/4/4/4	-
3	GOL	A	405	-	-	1/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	HEM	C3C-C2C	-4.39	1.34	1.40
4	A	407	HEM	C3C-CAC	3.65	1.55	1.47
4	A	407	HEM	C3C-C2C	-3.61	1.35	1.40
4	B	1002	HEM	C3C-CAC	3.36	1.55	1.47
4	A	407	HEM	C3C-C4C	3.29	1.46	1.41
4	A	407	HEM	CAB-C3B	3.09	1.55	1.47
4	B	1002	HEM	CAB-C3B	3.02	1.55	1.47
4	B	1002	HEM	C3C-C4C	2.62	1.45	1.41
4	A	407	HEM	CMB-C2B	2.40	1.55	1.50
4	B	1002	HEM	FE-NB	2.33	2.11	1.98
4	B	1002	HEM	FE-ND	2.29	2.10	1.98
4	A	407	HEM	FE-ND	2.19	2.10	1.98
2	B	1001	TSS	CD1-NE1	-2.12	1.32	1.36
4	A	407	HEM	FE-NB	2.12	2.09	1.98
2	B	1001	TSS	CD2-CE2	-2.11	1.37	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	407	HEM	C4C-CHD-C1D	3.71	127.45	122.56
4	B	1002	HEM	C4C-CHD-C1D	3.44	127.10	122.56
4	A	407	HEM	C4D-ND-C1D	3.16	108.94	105.21
4	A	407	HEM	CMA-C3A-C4A	-3.16	123.83	128.46
4	B	1002	HEM	C4D-ND-C1D	2.93	108.68	105.21
4	B	1002	HEM	C3B-C2B-C1B	2.86	108.56	106.41
4	B	1002	HEM	C1B-NB-C4B	2.76	108.47	105.21
4	A	407	HEM	CMC-C2C-C3C	2.57	129.81	124.68
4	A	407	HEM	C4A-C3A-C2A	2.54	108.76	107.00
4	A	407	HEM	C2D-C1D-ND	-2.53	106.98	109.90
4	B	1002	HEM	CMC-C2C-C3C	2.48	129.64	124.68
4	A	407	HEM	C1B-NB-C4B	2.43	108.09	105.21
4	B	1002	HEM	CMA-C3A-C4A	-2.41	124.92	128.46
4	B	1002	HEM	C3D-C4D-ND	-2.26	107.69	110.17
4	A	407	HEM	CAA-CBA-CGA	-2.25	107.77	113.83
2	B	1001	TSS	CE3-CD2-CE2	2.16	121.03	118.17
4	A	407	HEM	O1A-CGA-CBA	-2.11	116.40	123.09
4	B	1002	HEM	C2B-C1B-NB	-2.10	107.43	109.84
4	A	407	HEM	O2A-CGA-CBA	2.08	120.56	114.00
4	A	407	HEM	C3D-C4D-ND	-2.05	107.93	110.17
2	B	1001	TSS	CA-CB-CG	-2.04	108.55	112.85
4	A	407	HEM	C1D-C2D-C3D	2.03	109.11	106.98
4	A	407	HEM	O2D-CGD-CBD	2.02	120.37	114.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	TSS	N1-CA-CB-CG
2	A	401[B]	TSS	N1-CA-CB-CG
2	B	1001	TSS	N1-CA-CB-CG
3	A	402	GOL	C1-C2-C3-O3
3	A	406	GOL	C1-C2-C3-O3
3	B	1005	GOL	O1-C1-C2-O2
3	B	1005	GOL	O1-C1-C2-C3
3	B	1005	GOL	C1-C2-C3-O3
3	A	402	GOL	O1-C1-C2-O2
3	A	406	GOL	O1-C1-C2-O2
3	B	1005	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	406	GOL	O1-C1-C2-C3
3	B	1004	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	A	406	GOL	O2-C2-C3-O3
3	A	403	GOL	O1-C1-C2-O2
3	B	1004	GOL	O2-C2-C3-O3
4	A	407	HEM	C3A-C2A-CAA-CBA
4	A	407	HEM	C1A-C2A-CAA-CBA
4	A	407	HEM	C3D-CAD-CBD-CGD
4	B	1002	HEM	CAA-CBA-CGA-O2A
3	A	404	GOL	C1-C2-C3-O3
3	A	405	GOL	C1-C2-C3-O3
4	B	1002	HEM	CAA-CBA-CGA-O1A
4	A	407	HEM	CAA-CBA-CGA-O2A
4	A	407	HEM	CAA-CBA-CGA-O1A
4	B	1002	HEM	C3D-CAD-CBD-CGD
4	B	1002	HEM	CAD-CBD-CGD-O1D
4	A	407	HEM	CAD-CBD-CGD-O1D
4	B	1002	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	HEM	3	0

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	TSS	5	0
2	A	401[A]	TSS	3	0
2	A	401[B]	TSS	1	0
4	A	407	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HEM B 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand TSS B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand TSS A 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand TSS A 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 407

Bond lengths

Bond angles

Torsions

Rings
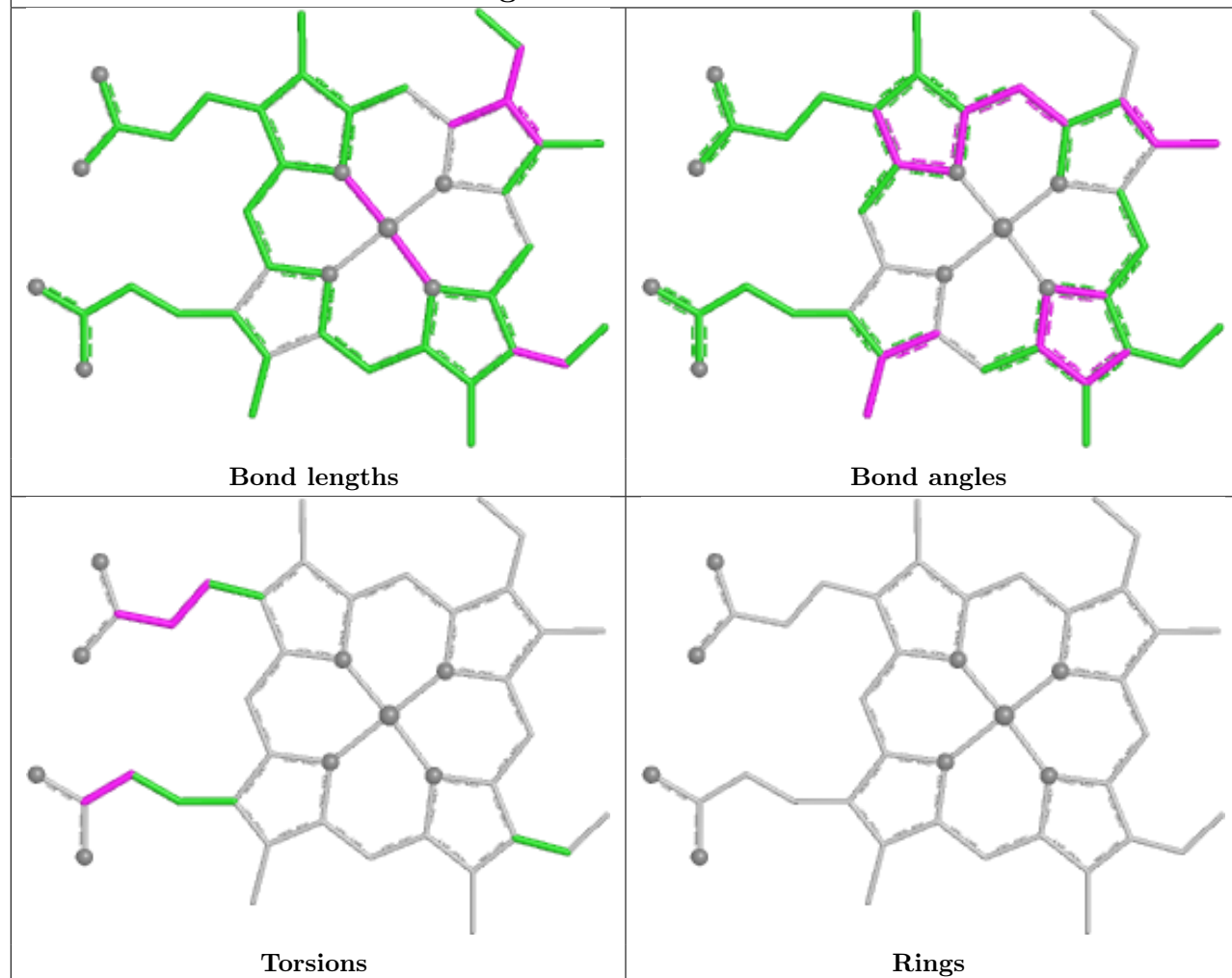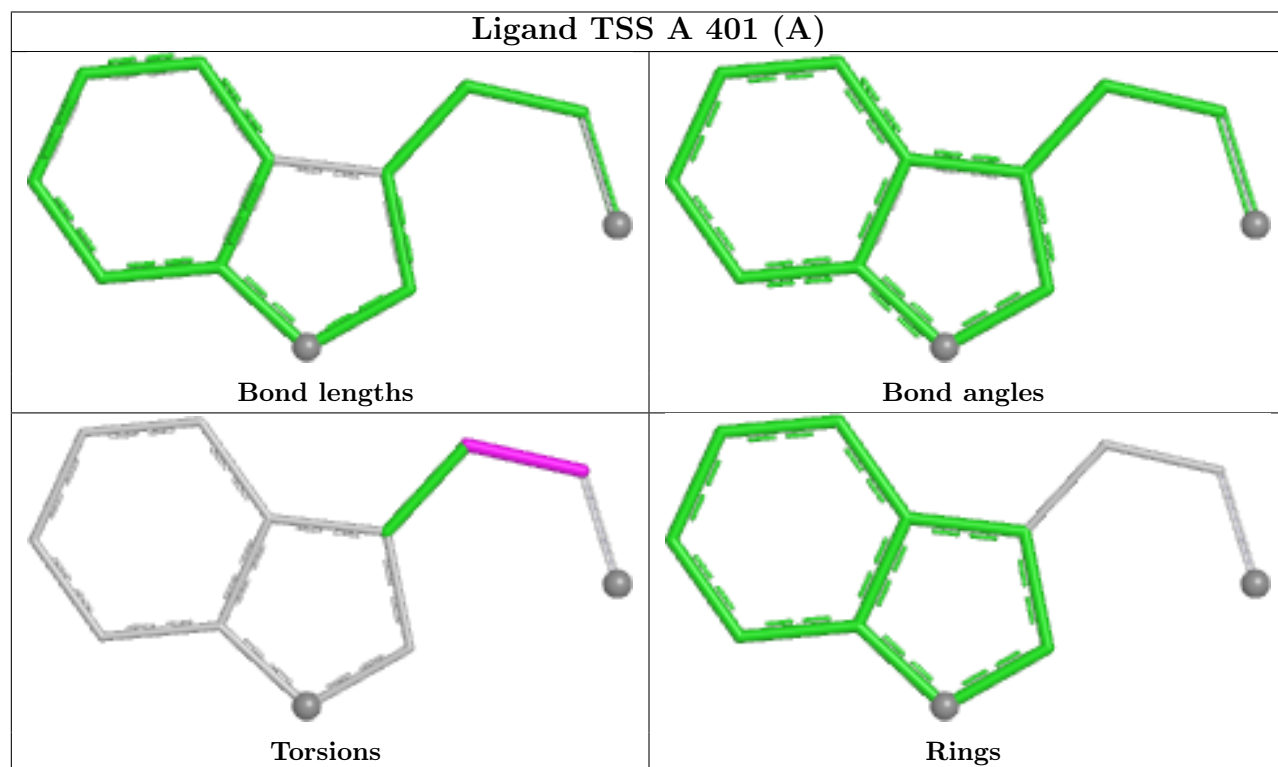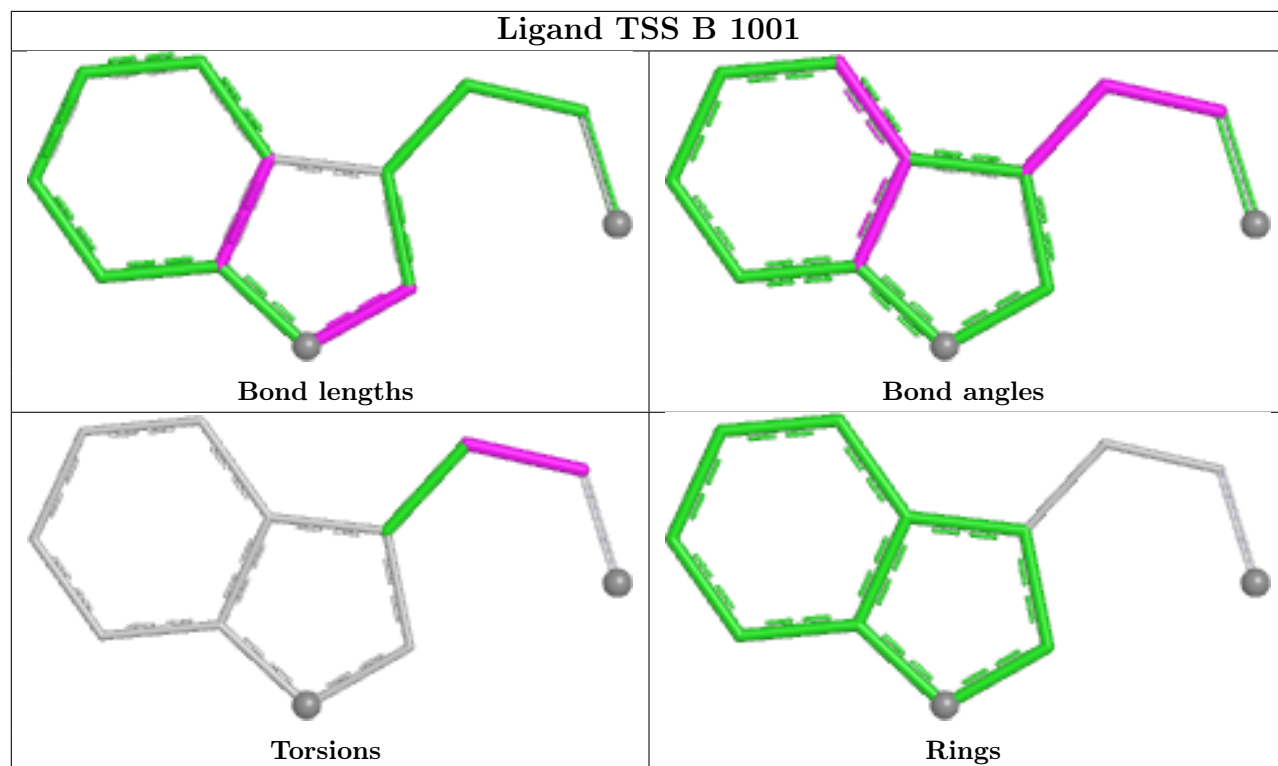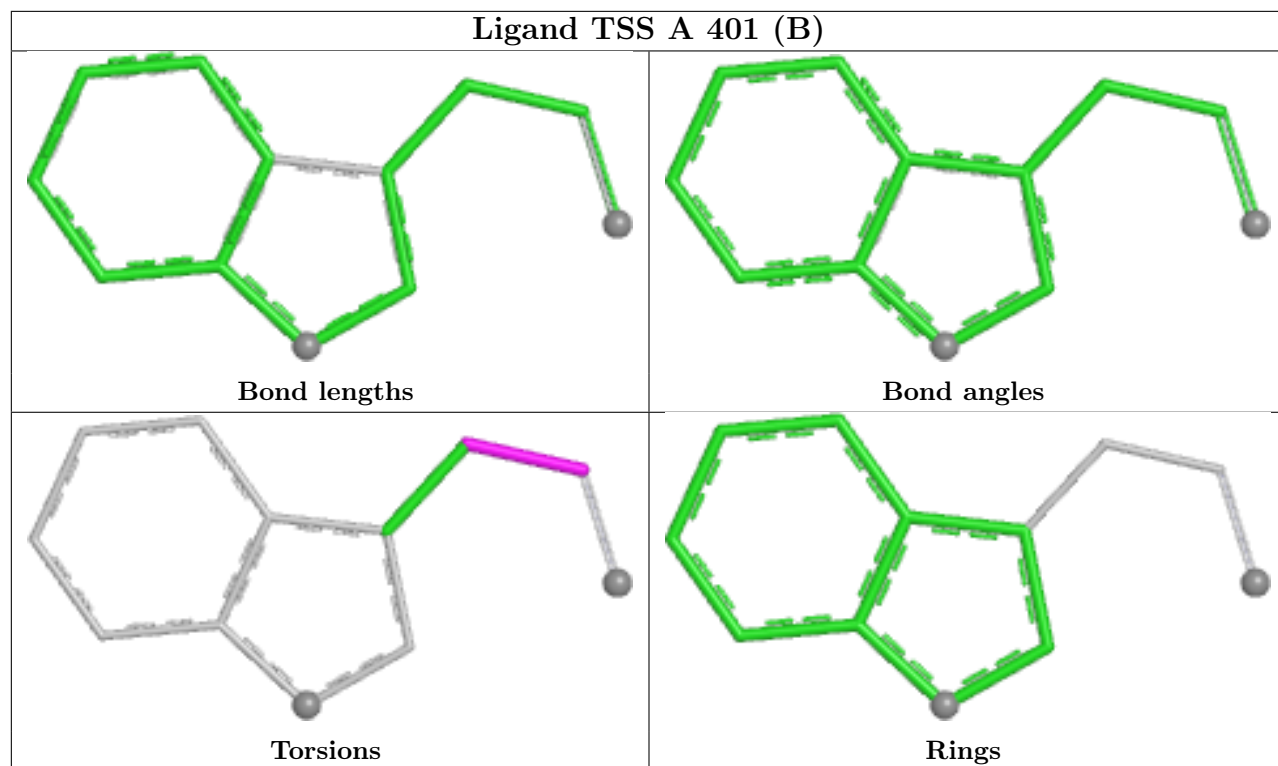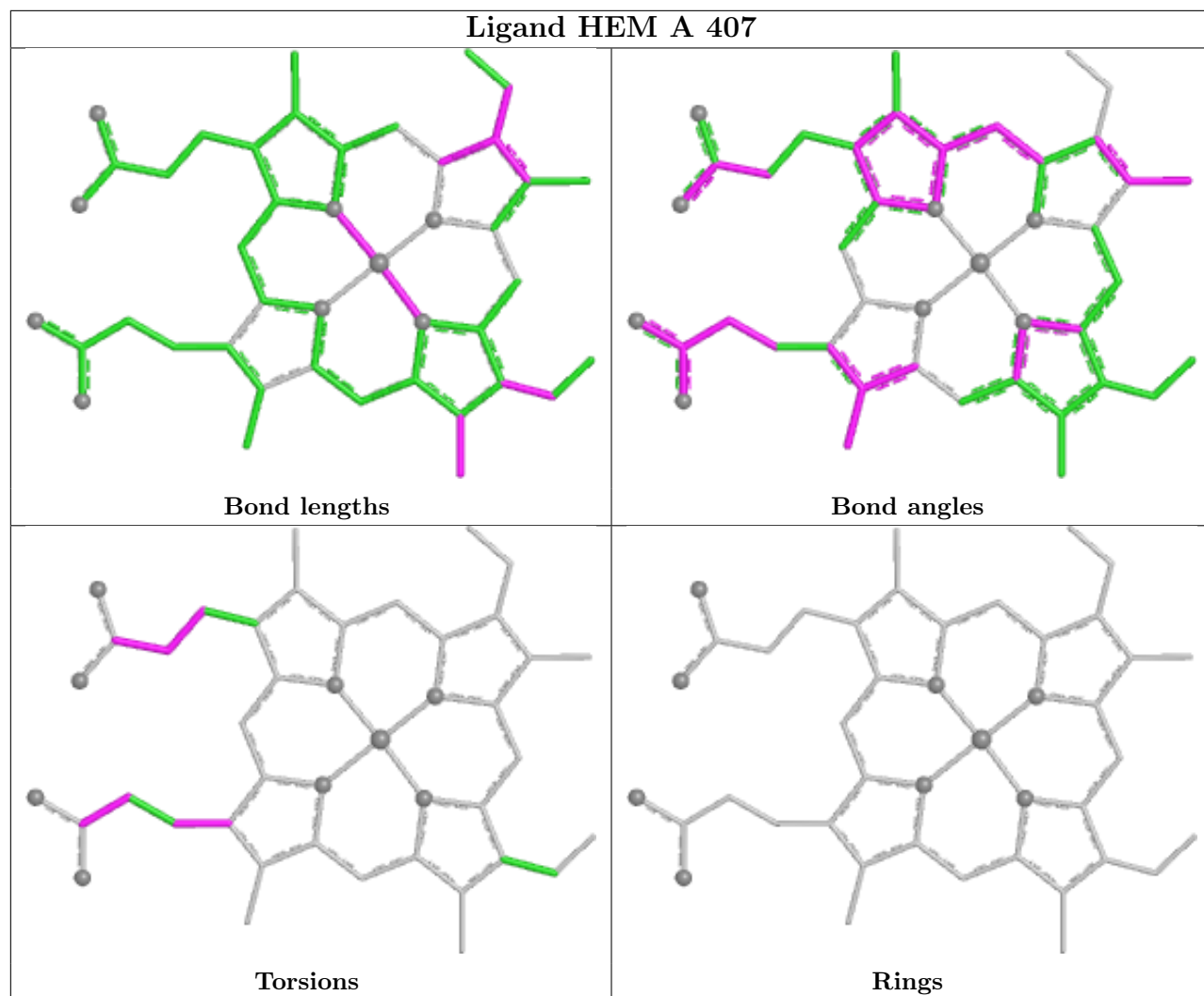
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	347/370 (93%)	0.36	10 (2%)	54	54	19, 31, 53, 69	1 (0%)
1	B	347/370 (93%)	0.35	7 (2%)	64	64	19, 31, 51, 75	0
All	All	694/740 (93%)	0.35	17 (2%)	59	60	19, 31, 52, 75	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	4.8
1	B	2	ILE	4.1
1	A	3	SER	4.0
1	B	273	GLU	3.7
1	B	348	TYR	3.3
1	A	274	ILE	2.7
1	A	348	TYR	2.6
1	A	271	SER	2.6
1	A	273	GLU	2.5
1	A	4	ASN	2.4
1	B	274	ILE	2.3
1	A	201	GLY	2.3
1	B	4	ASN	2.2
1	A	155	PRO	2.2
1	B	124	ARG	2.1
1	B	3	SER	2.1
1	A	171	ALA	2.1

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

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

6.3 Carbohydrates (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, 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	GOL	B	1003	6/6	0.68	0.23	59,60,64,73	0
3	GOL	B	1004	6/6	0.69	0.20	49,55,59,60	0
3	GOL	B	1005	6/6	0.71	0.21	40,48,52,53	0
3	GOL	A	402	6/6	0.74	0.18	39,43,45,49	0
2	TSS	A	401[B]	12/12	0.77	0.23	25,31,32,35	12
2	TSS	A	401[A]	12/12	0.77	0.23	23,31,32,35	12
3	GOL	A	406	6/6	0.77	0.18	52,54,58,59	0
2	TSS	B	1001	12/12	0.83	0.18	32,36,41,42	0
3	GOL	A	403	6/6	0.86	0.13	35,39,45,47	0
3	GOL	A	405	6/6	0.89	0.11	36,40,48,51	0
3	GOL	A	404	6/6	0.90	0.13	40,47,50,60	0
4	HEM	A	407	43/43	0.97	0.08	21,25,30,33	0
4	HEM	B	1002	43/43	0.98	0.08	20,26,30,32	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 TSS A 401 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
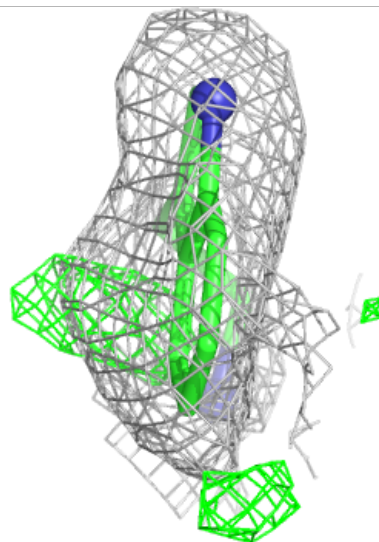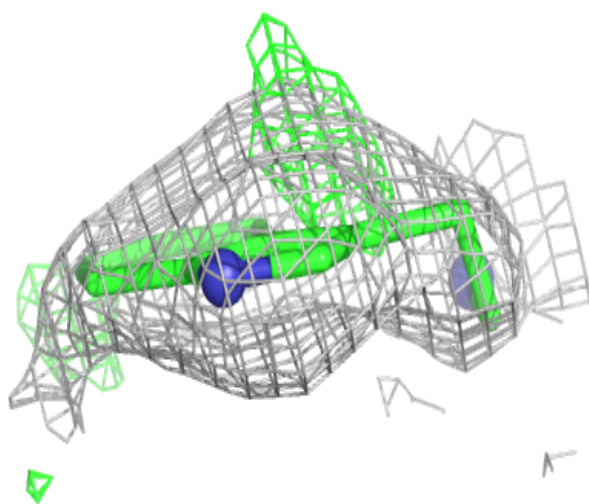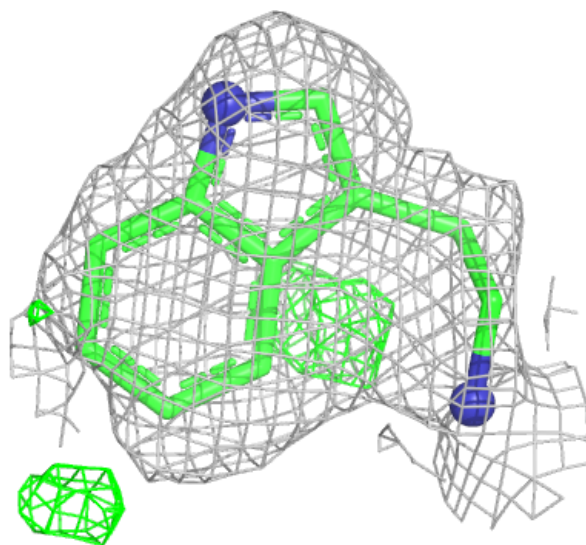and green (positive)
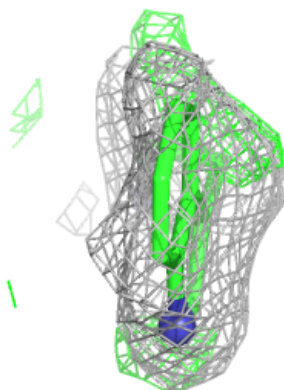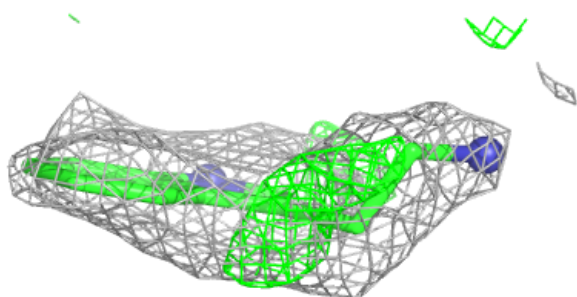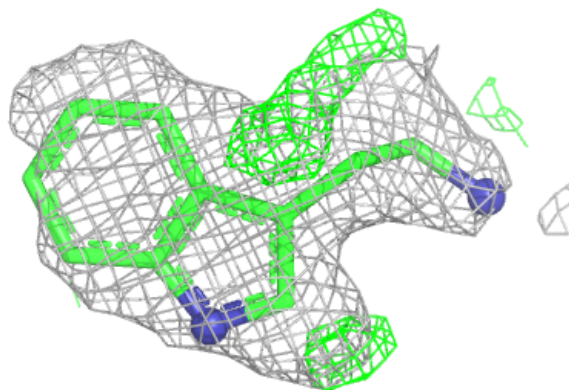
Electron density around TSS A 401 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
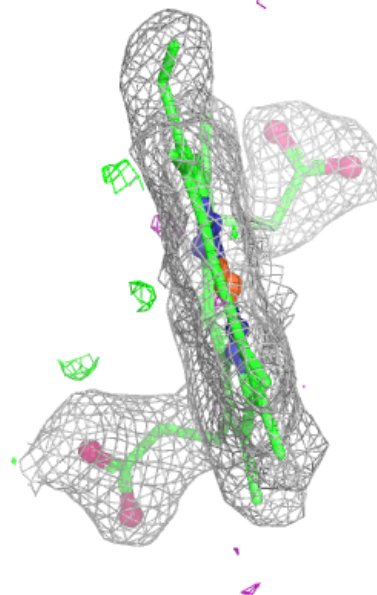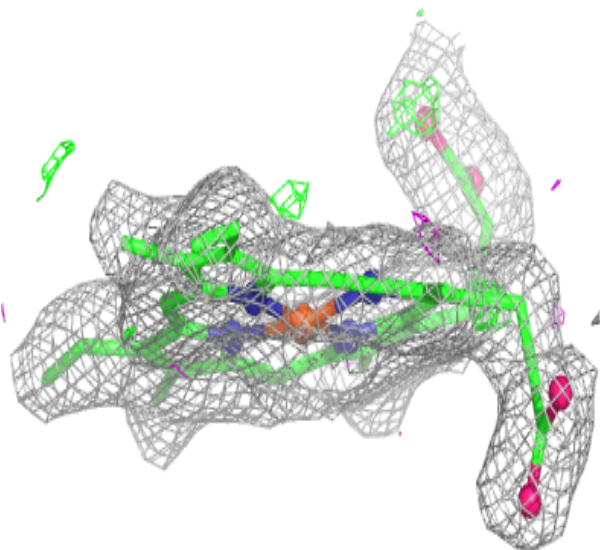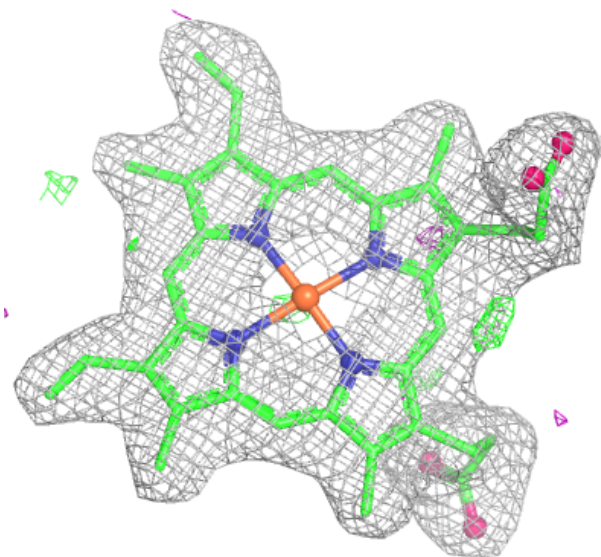and green (positive)
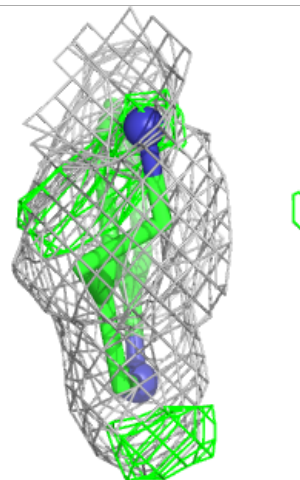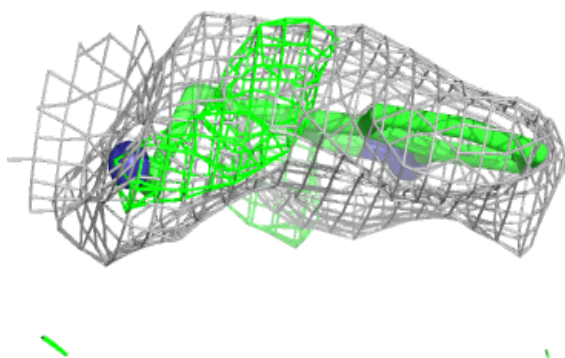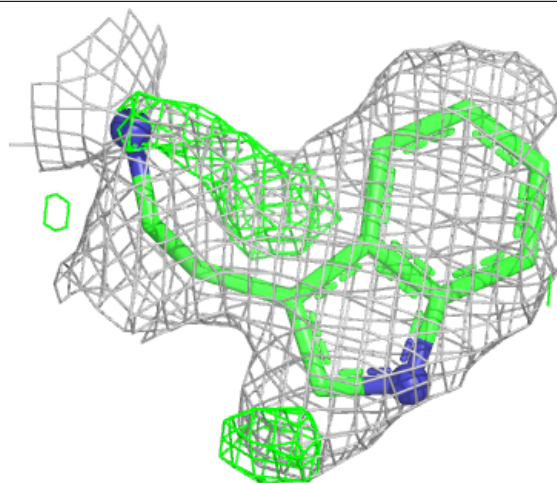
Electron density around TSS B 1001:

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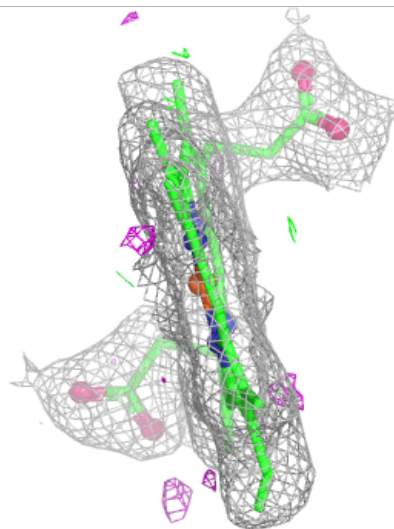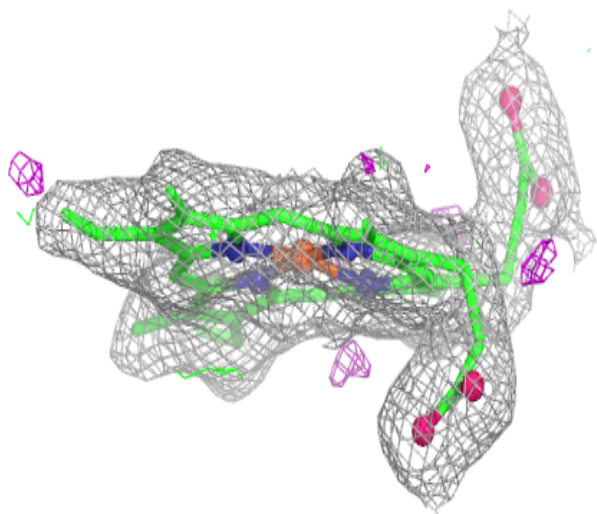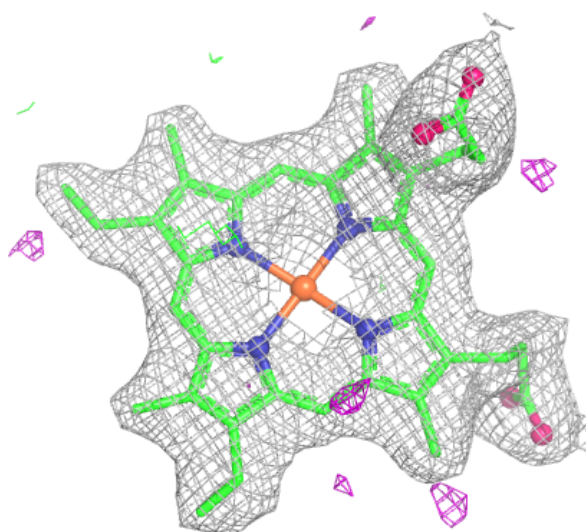mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM A 407:

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

Electron density around HEM B 1002:

$2mF_o-DF_c$ (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.