



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:24 AM UTC

PDB ID : 6B11 / pdb_00006b11
Title : Ty1HI in complex with native substrate 23-deoxy-5-O-mycaminosyl-tylonolide (23-DMTL)
Authors : DeMars, M.D.; Sherman, D.H.; Podust, L.M.
Deposited on : 2017-09-15
Resolution : 1.99 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

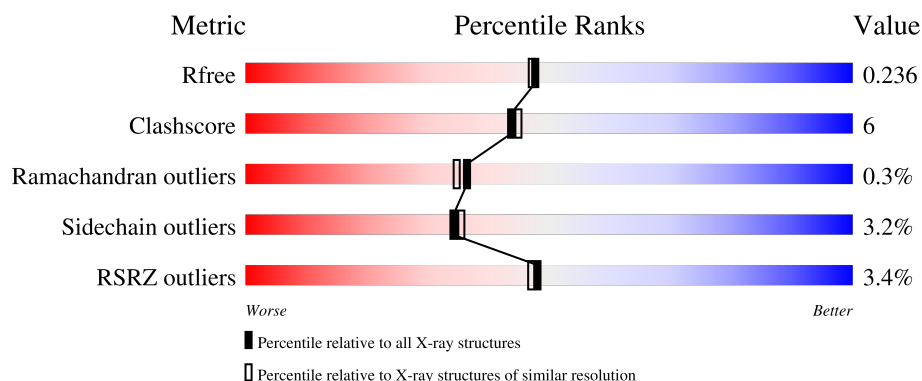
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	440	% 74% 12% • 12%
1	B	440	5% 73% 11% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6422 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 20-oxo-5-O-mycaminosyltylactone 23-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	3	0
			2974	1869	534	561	10			
1	B	383	Total	C	N	O	S	0	4	0
			2933	1849	519	555	10			

There are 40 discrepancies between the modelled and reference sequences:

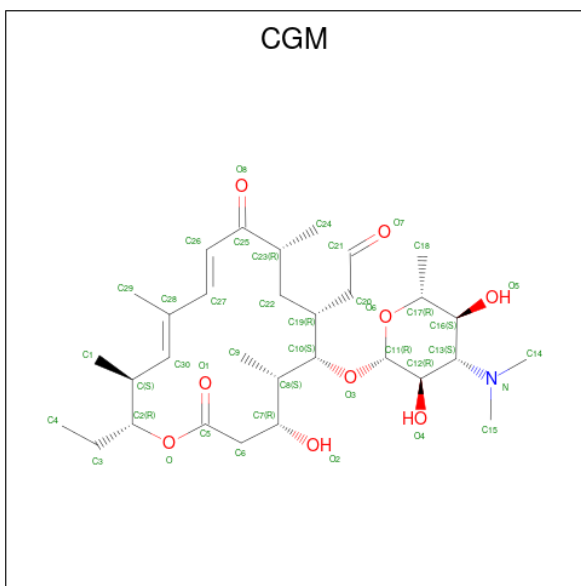
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9ZHQ1
A	-18	GLY	-	expression tag	UNP Q9ZHQ1
A	-17	SER	-	expression tag	UNP Q9ZHQ1
A	-16	SER	-	expression tag	UNP Q9ZHQ1
A	-15	HIS	-	expression tag	UNP Q9ZHQ1
A	-14	HIS	-	expression tag	UNP Q9ZHQ1
A	-13	HIS	-	expression tag	UNP Q9ZHQ1
A	-12	HIS	-	expression tag	UNP Q9ZHQ1
A	-11	HIS	-	expression tag	UNP Q9ZHQ1
A	-10	HIS	-	expression tag	UNP Q9ZHQ1
A	-9	SER	-	expression tag	UNP Q9ZHQ1
A	-8	SER	-	expression tag	UNP Q9ZHQ1
A	-7	GLY	-	expression tag	UNP Q9ZHQ1
A	-6	LEU	-	expression tag	UNP Q9ZHQ1
A	-5	VAL	-	expression tag	UNP Q9ZHQ1
A	-4	PRO	-	expression tag	UNP Q9ZHQ1
A	-3	ARG	-	expression tag	UNP Q9ZHQ1
A	-2	GLY	-	expression tag	UNP Q9ZHQ1
A	-1	SER	-	expression tag	UNP Q9ZHQ1
A	0	HIS	-	expression tag	UNP Q9ZHQ1
B	-19	MET	-	expression tag	UNP Q9ZHQ1
B	-18	GLY	-	expression tag	UNP Q9ZHQ1
B	-17	SER	-	expression tag	UNP Q9ZHQ1
B	-16	SER	-	expression tag	UNP Q9ZHQ1
B	-15	HIS	-	expression tag	UNP Q9ZHQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q9ZHQ1
B	-13	HIS	-	expression tag	UNP Q9ZHQ1
B	-12	HIS	-	expression tag	UNP Q9ZHQ1
B	-11	HIS	-	expression tag	UNP Q9ZHQ1
B	-10	HIS	-	expression tag	UNP Q9ZHQ1
B	-9	SER	-	expression tag	UNP Q9ZHQ1
B	-8	SER	-	expression tag	UNP Q9ZHQ1
B	-7	GLY	-	expression tag	UNP Q9ZHQ1
B	-6	LEU	-	expression tag	UNP Q9ZHQ1
B	-5	VAL	-	expression tag	UNP Q9ZHQ1
B	-4	PRO	-	expression tag	UNP Q9ZHQ1
B	-3	ARG	-	expression tag	UNP Q9ZHQ1
B	-2	GLY	-	expression tag	UNP Q9ZHQ1
B	-1	SER	-	expression tag	UNP Q9ZHQ1
B	0	HIS	-	expression tag	UNP Q9ZHQ1

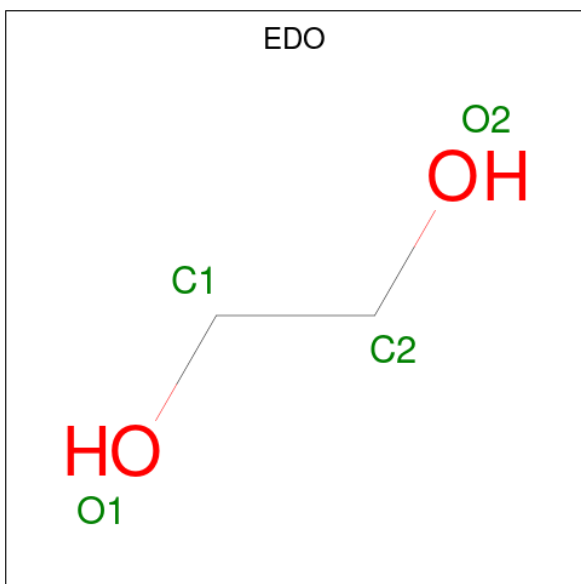
- # HEM

- Molecule 3 is (4R,5S,6S,7R,9R,11E,13E,15S,16R)-16-ethyl-4-hydroxy-5,9,13,15-tetramethyl-2,10-dioxo-7-(2-oxoethyl)-1-oxacyclohexadeca-11,13-dien-6-yl 3,6-dideoxy-3-(dimethylamino)

)-beta-D-glucopyranoside (CCD ID: CGM) (formula: C₃₁H₅₁NO₉).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 82	C 62	N 2	O 18	0	1
3	B	1	Total 41	C 31	N 1	O 9	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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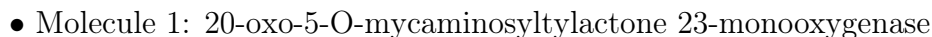
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	84	Total O 84 84	0	0

- Molecule 1: 20-oxo-5-O-mycaminosyltylactone 23-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.73Å 109.24Å 150.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.47 – 1.99 88.32 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (88.47-1.99) 95.9 (88.32-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.240 0.197 , 0.236	Depositor DCC
R_{free} test set	3507 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6422	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, EDO, CGM, CSO

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	1.35	11/3020 (0.4%)	1.16	4/4113 (0.1%)
1	B	1.24	9/2979 (0.3%)	1.14	12/4063 (0.3%)
All	All	1.30	20/5999 (0.3%)	1.15	16/8176 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ARG	CA-C	-7.97	1.42	1.52
1	B	378	GLU	N-CA	7.69	1.55	1.46
1	A	255	LEU	C-O	-7.14	1.15	1.24
1	A	350	PHE	C-O	-7.09	1.15	1.24
1	B	161	LEU	CA-C	-6.64	1.43	1.52
1	B	275	LEU	CA-C	-6.33	1.44	1.52
1	A	292	LEU	C-O	-6.01	1.18	1.24
1	B	346	GLU	C-O	-5.87	1.21	1.23
1	A	151	ASP	CA-C	-5.74	1.45	1.52
1	A	272	VAL	CA-C	-5.46	1.45	1.52
1	A	101	ASP	C-O	-5.38	1.17	1.24
1	A	169	MET	N-CA	5.38	1.52	1.46
1	B	382	ALA	CA-C	-5.33	1.46	1.52
1	B	416	LEU	CA-C	-5.27	1.46	1.52
1	B	154	ALA	N-CA	5.25	1.52	1.46
1	B	272	VAL	CA-C	-5.16	1.46	1.52
1	A	284	GLU	CA-C	-5.14	1.46	1.52
1	B	274	VAL	N-CA	5.12	1.52	1.46
1	A	283	ARG	N-CA	5.04	1.52	1.46
1	A	98	SER	N-CA	5.03	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	LEU	CA-C-N	-7.28	112.82	120.03
1	B	94	LEU	C-N-CA	-7.28	112.82	120.03
1	B	292	LEU	CA-C-N	-7.17	111.39	119.28
1	B	292	LEU	C-N-CA	-7.17	111.39	119.28
1	A	241	GLY	N-CA-C	-6.57	103.45	112.25
1	B	138	ARG	CA-C-N	-6.56	112.23	119.19
1	B	138	ARG	C-N-CA	-6.56	112.23	119.19
1	B	56	GLU	CA-C-N	5.90	126.31	119.47
1	B	56	GLU	C-N-CA	5.90	126.31	119.47
1	A	168	PRO	CA-C-N	-5.47	113.33	120.44
1	A	168	PRO	C-N-CA	-5.47	113.33	120.44
1	A	229	ASP	N-CA-C	5.41	117.51	110.53
1	B	416	LEU	CA-C-N	-5.38	114.38	119.76
1	B	416	LEU	C-N-CA	-5.38	114.38	119.76
1	B	84	ASP	N-CA-C	5.26	117.23	109.50
1	B	75	GLN	N-CA-C	5.17	116.92	111.28

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	2974	0	2939	32	0
1	B	2933	0	2868	36	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	82	0	0	3	0
3	B	41	0	0	0	0
4	A	56	0	84	10	0
4	B	16	0	24	0	0
5	A	150	0	0	4	0
5	B	84	0	0	2	0
All	All	6422	0	5975	74	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 (74) 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:169:MET:HE1	1:B:382:ALA:HB2	1.29	1.14
1:A:394[B]:ARG:HH21	4:A:507:EDO:H21	1.43	0.83
1:B:169:MET:HE1	1:B:382:ALA:CB	2.10	0.80
1:B:169:MET:CE	1:B:382:ALA:HB2	2.12	0.78
1:B:75:GLN:O	1:B:79:ARG:HG3	1.87	0.74
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.69	0.74
1:B:88:SER:OG	1:B:114:ASP:OD2	2.08	0.70
1:A:35:TRP:CD2	1:A:36:PRO:HA	2.28	0.69
1:A:76[B]:ASP:OD1	4:A:504:EDO:H21	1.92	0.68
1:B:71:LEU:O	5:B:601:HOH:O	2.11	0.67
1:B:319:ILE:O	1:B:320:ASP:C	2.41	0.63
1:A:86:ARG:HH12	4:A:505:EDO:H12	1.62	0.63
1:B:183:GLU:H	1:B:183:GLU:CD	2.07	0.63
3:A:502[A]:CGM:C30	3:A:502[A]:CGM:C5	2.78	0.61
1:B:321:GLY:O	1:B:322:HIS:ND1	2.34	0.60
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.84	0.60
1:B:33:ILE:HG23	1:B:61:ALA:HB2	1.84	0.58
1:A:60:ARG:HG2	1:A:70:TRP:CZ3	2.39	0.58
1:B:151[B]:ASP:OD1	5:B:602:HOH:O	2.17	0.57
1:A:267:MET:HG3	1:A:379:LEU:HD11	1.86	0.57
1:A:223:THR:HG22	1:A:240:ARG:HH22	1.70	0.57
1:B:145:VAL:CG2	1:B:169:MET:HE2	2.35	0.56
1:A:86:ARG:HH12	4:A:505:EDO:C1	2.18	0.56
1:A:302:TYR:OH	4:A:503:EDO:H12	2.05	0.56
1:B:319:ILE:O	1:B:321:GLY:N	2.38	0.56
1:B:131:LEU:O	1:B:135:ARG:HG3	2.06	0.55
1:B:316:ASP:HA	1:B:324:ILE:O	2.05	0.55
1:A:350:PHE:H	4:A:516:EDO:H21	1.71	0.55
1:B:178:LEU:O	1:B:232:LEU:HB2	2.06	0.55
3:A:502[B]:CGM:C4	5:A:666:HOH:O	2.54	0.55
1:A:118:HIS:CD2	1:A:367:HIS:CE1	2.96	0.54
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.89	0.54
1:B:35:TRP:CD2	1:B:36:PRO:HA	2.41	0.54
1:B:57:PRO:HG3	1:B:74:ARG:NH2	2.22	0.54
1:A:91:PRO:O	5:A:601:HOH:O	2.18	0.53
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.38	0.53
1:A:350:PHE:H	4:A:516:EDO:C2	2.22	0.52
1:A:41[B]:CSO:OD	1:A:43:PHE:N	2.35	0.52
1:B:320:ASP:OD1	1:B:321:GLY:N	2.43	0.52
1:B:33:ILE:HG23	1:B:61:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:O	1:B:70:TRP:HA	2.13	0.49
1:B:356:ALA:O	1:B:357:ARG:HB2	2.11	0.48
1:A:86:ARG:HH22	4:A:505:EDO:H12	1.78	0.48
1:A:131:LEU:HB2	1:B:187:TYR:CE1	2.50	0.47
1:A:267:MET:CG	1:A:379:LEU:HD11	2.45	0.46
1:A:240:ARG:C	1:A:241:GLY:O	2.58	0.45
3:A:502[A]:CGM:C4	5:A:666:HOH:O	2.65	0.45
1:A:161:LEU:CD2	1:A:272:VAL:HG11	2.47	0.44
1:A:394[B]:ARG:HH21	4:A:507:EDO:C2	2.22	0.44
1:B:55:GLU:C	1:B:57:PRO:HD3	2.43	0.44
1:B:369:CYS:HB2	2:B:501:HEM:NA	2.32	0.44
1:A:76[B]:ASP:OD1	4:A:504:EDO:C2	2.65	0.44
1:B:76:ASP:OD1	1:B:77:HIS:N	2.50	0.44
1:B:145:VAL:HG22	1:B:169:MET:HE2	1.99	0.44
1:A:368:GLN:O	1:A:369:CYS:C	2.61	0.44
1:B:320:ASP:O	1:B:321:GLY:C	2.61	0.43
1:B:56:GLU:N	1:B:57:PRO:HD3	2.33	0.43
1:B:98:SER:HB2	1:B:99:PRO:HD2	2.01	0.42
1:A:215:LEU:HD12	1:A:253:ALA:HB1	2.02	0.42
1:B:318:GLU:CB	1:B:323:THR:HG22	2.50	0.42
1:B:177:LEU:O	1:B:177:LEU:HD12	2.19	0.42
1:A:150:ASP:OD1	1:A:389:ARG:NH2	2.45	0.42
1:A:69:VAL:HG21	1:A:331:VAL:HG23	2.02	0.41
1:A:98:SER:HB2	1:A:99:PRO:HD2	2.01	0.41
1:A:217:ARG:NH1	5:A:609:HOH:O	2.46	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.87	0.41
1:A:131:LEU:O	1:A:132:ARG:C	2.63	0.41
1:B:183:GLU:CD	1:B:183:GLU:N	2.77	0.41
1:A:179:ASP:HB2	1:A:230:GLY:HA3	2.02	0.41
1:B:86:ARG:HA	1:B:314:THR:OG1	2.21	0.41
1:B:317:ILE:O	1:B:323:THR:HA	2.21	0.40
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.97	0.40
1:A:88:SER:OG	1:A:114:ASP:OD2	2.23	0.40
1:A:285:LEU:HD22	1:A:292:LEU:HD13	2.04	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	382/440 (87%)	372 (97%)	10 (3%)	0	100	100
1	B	381/440 (87%)	365 (96%)	14 (4%)	2 (0%)	24	21
All	All	763/880 (87%)	737 (97%)	24 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	GLY
1	B	320	ASP

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	304/347 (88%)	295 (97%)	9 (3%)	36	38
1	B	296/347 (85%)	285 (96%)	11 (4%)	30	30
All	All	600/694 (86%)	580 (97%)	20 (3%)	34	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	48	GLN
1	A	53	ARG
1	A	143	GLN

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Mol	Chain	Res	Type
1	A	183	GLU
1	A	216	ASP
1	A	220	SER
1	A	240	ARG
1	A	341	GLU
1	B	33	ILE
1	B	47	GLU
1	B	58	ILE
1	B	74	ARG
1	B	157[A]	ASP
1	B	157[B]	ASP
1	B	169	MET
1	B	183	GLU
1	B	322	HIS
1	B	324	ILE
1	B	358	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	124	HIS
1	A	143	GLN
1	A	238	GLN
1	A	322	HIS
1	B	143	GLN
1	B	278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	B	41[A]	1	3,6,7	1.33	0	1,6,8	0.18	0
1	CSO	A	41[A]	1	3,6,7	0.80	0	1,6,8	0.71	0
1	CSO	A	41[B]	1	3,6,7	1.12	0	1,6,8	2.01	1 (100%)
1	CSO	B	41[B]	1	3,6,7	0.70	0	1,6,8	1.39	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
1	CSO	B	41[A]	1	-	1/1/5/7	-
1	CSO	A	41[A]	1	-	0/1/5/7	-
1	CSO	A	41[B]	1	-	0/1/5/7	-
1	CSO	B	41[B]	1	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	41[B]	CSO	CB-CA-C	-2.01	105.35	110.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	41[A]	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	41[B]	CSO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

23 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
4	EDO	A	509	-	3,3,3	0.26	0	2,2,2	0.69	0
3	CGM	A	502[B]	-	42,42,42	1.01	2 (4%)	51,59,59	1.44	7 (13%)
4	EDO	A	513	-	3,3,3	0.79	0	2,2,2	0.30	0
4	EDO	A	507	-	3,3,3	0.29	0	2,2,2	0.73	0
3	CGM	A	502[A]	-	42,42,42	1.00	2 (4%)	51,59,59	1.31	7 (13%)
3	CGM	B	502	-	42,42,42	0.85	2 (4%)	51,59,59	1.56	9 (17%)
4	EDO	B	503	-	3,3,3	0.40	0	2,2,2	0.71	0
4	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	A	506	-	3,3,3	0.60	0	2,2,2	0.39	0
4	EDO	A	505	-	3,3,3	0.33	0	2,2,2	1.11	0
4	EDO	A	516	-	3,3,3	0.50	0	2,2,2	0.40	0
4	EDO	A	515	-	3,3,3	0.69	0	2,2,2	0.11	0
4	EDO	B	505	-	3,3,3	0.40	0	2,2,2	0.53	0
4	EDO	A	512	-	3,3,3	0.63	0	2,2,2	0.47	0
4	EDO	A	510	-	3,3,3	0.54	0	2,2,2	0.49	0
2	HEM	A	501	1	50,50,50	1.51	7 (14%)	67,82,82	2.29	23 (34%)
4	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.62	0
4	EDO	A	503	-	3,3,3	0.10	0	2,2,2	0.76	0
2	HEM	B	501	1	50,50,50	1.54	8 (16%)	67,82,82	2.03	18 (26%)
4	EDO	A	511	-	3,3,3	0.33	0	2,2,2	0.73	0
4	EDO	A	514	-	3,3,3	0.36	0	2,2,2	0.68	0
4	EDO	A	508	-	3,3,3	0.29	0	2,2,2	0.80	0
4	EDO	B	506	-	3,3,3	1.34	0	2,2,2	0.23	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
4	EDO	A	509	-	-	1/1/1/1	-
3	CGM	A	502[B]	-	-	10/54/74/74	0/1/2/2
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
3	CGM	A	502[A]	-	-	6/54/74/74	0/1/2/2
3	CGM	B	502	-	-	4/54/74/74	0/1/2/2
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	A	516	-	-	1/1/1/1	-
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
2	HEM	A	501	1	-	1/14/54/54	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
2	HEM	B	501	1	-	0/14/54/54	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	A	514	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1B-NB	-4.31	1.32	1.40
2	B	501	HEM	C4B-NB	-4.26	1.30	1.38
3	A	502[A]	CGM	O-C5	3.99	1.45	1.34
3	A	502[B]	CGM	O-C5	3.96	1.45	1.34
2	B	501	HEM	FE-NB	3.40	2.05	1.94
3	A	502[A]	CGM	O-C2	-3.30	1.40	1.46
3	B	502	CGM	O-C2	-3.27	1.40	1.46
3	A	502[B]	CGM	O-C2	-3.24	1.40	1.46
2	B	501	HEM	C3C-C4C	-3.10	1.40	1.46
2	A	501	HEM	FE-NC	3.08	2.05	1.95
2	A	501	HEM	FE-NB	3.05	2.04	1.94
3	B	502	CGM	O-C5	2.80	1.42	1.34
2	A	501	HEM	C4D-ND	-2.72	1.35	1.40
2	B	501	HEM	FE-ND	-2.68	1.86	1.94
2	B	501	HEM	C1B-NB	-2.65	1.35	1.40
2	B	501	HEM	C1C-NC	-2.57	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1C-C2C	-2.57	1.40	1.45
2	A	501	HEM	C1B-C2B	-2.40	1.39	1.44
2	A	501	HEM	CMD-C2D	2.38	1.55	1.50
2	B	501	HEM	FE-NC	2.15	2.02	1.95
2	A	501	HEM	C3C-C4C	-2.04	1.42	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C4B-NB	-7.18	104.31	109.47
2	B	501	HEM	CHC-C4B-NB	5.95	130.83	124.42
2	A	501	HEM	C1B-NB-C4B	5.29	111.47	105.21
2	A	501	HEM	CHC-C4B-NB	4.65	129.42	124.42
2	B	501	HEM	CHD-C1D-ND	4.53	129.30	124.42
2	B	501	HEM	CHD-C1D-C2D	-4.50	117.93	125.03
2	B	501	HEM	CHD-C4C-NC	4.46	129.31	124.45
2	A	501	HEM	CHD-C1D-C2D	-4.41	118.06	125.03
3	B	502	CGM	C26-C27-C28	-4.41	119.71	126.23
2	B	501	HEM	CHA-C4D-C3D	-4.25	117.40	125.23
2	A	501	HEM	CHB-C1B-NB	4.21	129.57	124.37
3	B	502	CGM	O-C2-C3	-4.10	100.36	106.90
3	B	502	CGM	O7-C21-C20	-4.10	113.44	125.38
2	B	501	HEM	C4C-CHD-C1D	-4.00	117.52	126.02
2	B	501	HEM	C1B-NB-C4B	3.98	109.92	105.21
2	A	501	HEM	CHD-C1D-ND	3.92	128.64	124.42
2	A	501	HEM	C4C-CHD-C1D	-3.90	117.72	126.02
2	B	501	HEM	CHA-C4D-ND	3.74	129.00	124.37
2	A	501	HEM	CHD-C4C-NC	3.72	128.50	124.45
2	A	501	HEM	O2A-CGA-CBA	3.70	125.70	114.00
2	A	501	HEM	CHA-C4D-C3D	-3.69	118.42	125.23
3	A	502[B]	CGM	C2-O-C5	-3.35	111.43	117.81
3	B	502	CGM	C2-C-C30	-3.29	104.37	110.33
2	B	501	HEM	C3B-C4B-NB	-3.26	107.13	109.47
3	A	502[B]	CGM	O7-C21-C20	-3.15	116.20	125.38
2	A	501	HEM	CAB-C3B-C2B	-3.11	118.31	128.43
3	A	502[B]	CGM	O-C5-C6	3.10	116.98	111.43
2	A	501	HEM	O2A-CGA-O1A	-3.05	115.50	123.33
2	B	501	HEM	C1A-CHA-C4D	-2.95	119.30	126.25
3	A	502[B]	CGM	C1-C-C2	-2.93	107.49	111.78
2	B	501	HEM	C3D-C4D-ND	2.92	113.37	110.17
2	A	501	HEM	C4A-CHB-C1B	-2.90	119.42	126.25
3	A	502[A]	CGM	C29-C28-C27	2.90	122.52	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[B]	CGM	C29-C28-C27	2.88	122.48	118.09
2	A	501	HEM	CHA-C4D-ND	2.84	127.89	124.37
2	A	501	HEM	C3B-C2B-C1B	2.78	108.50	106.41
2	A	501	HEM	C3D-C4D-ND	2.77	113.21	110.17
2	B	501	HEM	C3B-C2B-C1B	-2.77	104.33	106.41
2	A	501	HEM	C2D-C1D-ND	2.76	113.09	109.90
3	B	502	CGM	O3-C10-C8	-2.73	105.02	108.23
3	B	502	CGM	O2-C7-C8	-2.69	104.24	110.09
3	A	502[A]	CGM	O7-C21-C20	-2.66	117.64	125.38
2	A	501	HEM	CMB-C2B-C1B	2.64	129.16	125.03
3	A	502[A]	CGM	C11-O3-C10	-2.57	111.89	117.98
2	A	501	HEM	CMB-C2B-C3B	-2.52	122.33	128.43
2	A	501	HEM	CAC-C3C-C4C	-2.51	118.83	124.82
2	A	501	HEM	C4D-ND-C1D	-2.42	102.34	105.21
2	B	501	HEM	CAD-C3D-C4D	2.37	128.82	124.70
3	A	502[B]	CGM	C11-C12-C13	2.36	113.00	109.20
3	A	502[B]	CGM	C9-C8-C7	-2.35	107.34	111.09
2	B	501	HEM	O2A-CGA-O1A	-2.35	117.30	123.33
3	A	502[A]	CGM	C11-O6-C17	-2.34	109.64	113.63
2	A	501	HEM	CAB-C3B-C4B	2.30	134.57	124.39
2	B	501	HEM	C2D-C1D-ND	2.30	112.56	109.90
3	B	502	CGM	O2-C7-C6	-2.27	103.98	109.45
2	A	501	HEM	C1A-CHA-C4D	-2.17	121.14	126.25
2	B	501	HEM	O2A-CGA-CBA	2.17	120.86	114.00
2	B	501	HEM	C4D-ND-C1D	-2.16	102.65	105.21
3	A	502[A]	CGM	O3-C10-C19	2.14	114.79	109.23
3	B	502	CGM	C24-C23-C25	2.13	114.30	110.59
3	B	502	CGM	C7-C6-C5	-2.10	109.42	114.02
2	B	501	HEM	CMA-C3A-C4A	2.05	128.54	125.42
3	A	502[A]	CGM	C14-N-C15	-2.05	104.48	110.49
3	A	502[A]	CGM	C1-C-C2	-2.04	108.80	111.78

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[B]	CGM	C-C2-C3-C4
3	A	502[B]	CGM	O-C2-C3-C4
3	A	502[B]	CGM	C10-C19-C20-C21
3	B	502	CGM	C19-C20-C21-O7
4	A	513	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C4B-C3B-CAB-CBB
4	A	506	EDO	O1-C1-C2-O2
4	A	511	EDO	O1-C1-C2-O2
4	A	514	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
3	A	502[B]	CGM	C19-C20-C21-O7
4	A	508	EDO	O1-C1-C2-O2
4	A	505	EDO	O1-C1-C2-O2
3	A	502[B]	CGM	C22-C19-C20-C21
4	A	507	EDO	O1-C1-C2-O2
3	A	502[B]	CGM	C19-C10-C8-C9
3	B	502	CGM	C19-C10-C8-C9
3	A	502[A]	CGM	C19-C20-C21-O7
3	A	502[A]	CGM	C12-C11-O3-C10
3	A	502[A]	CGM	O6-C11-O3-C10
4	A	509	EDO	O1-C1-C2-O2
4	A	515	EDO	O1-C1-C2-O2
3	A	502[A]	CGM	C22-C19-C20-C21
3	A	502[A]	CGM	C19-C10-C8-C9
3	A	502[B]	CGM	C19-C10-C8-C7
4	A	504	EDO	O1-C1-C2-O2
3	B	502	CGM	C12-C11-O3-C10
3	A	502[B]	CGM	O3-C10-C8-C7
3	B	502	CGM	C19-C10-C8-C7
4	A	510	EDO	O1-C1-C2-O2
3	A	502[B]	CGM	C26-C27-C28-C30
4	A	516	EDO	O1-C1-C2-O2
3	A	502[A]	CGM	C24-C23-C25-O8
3	A	502[B]	CGM	C24-C23-C25-O8

There are no ring outliers.

9 monomers are involved in 18 short contacts:

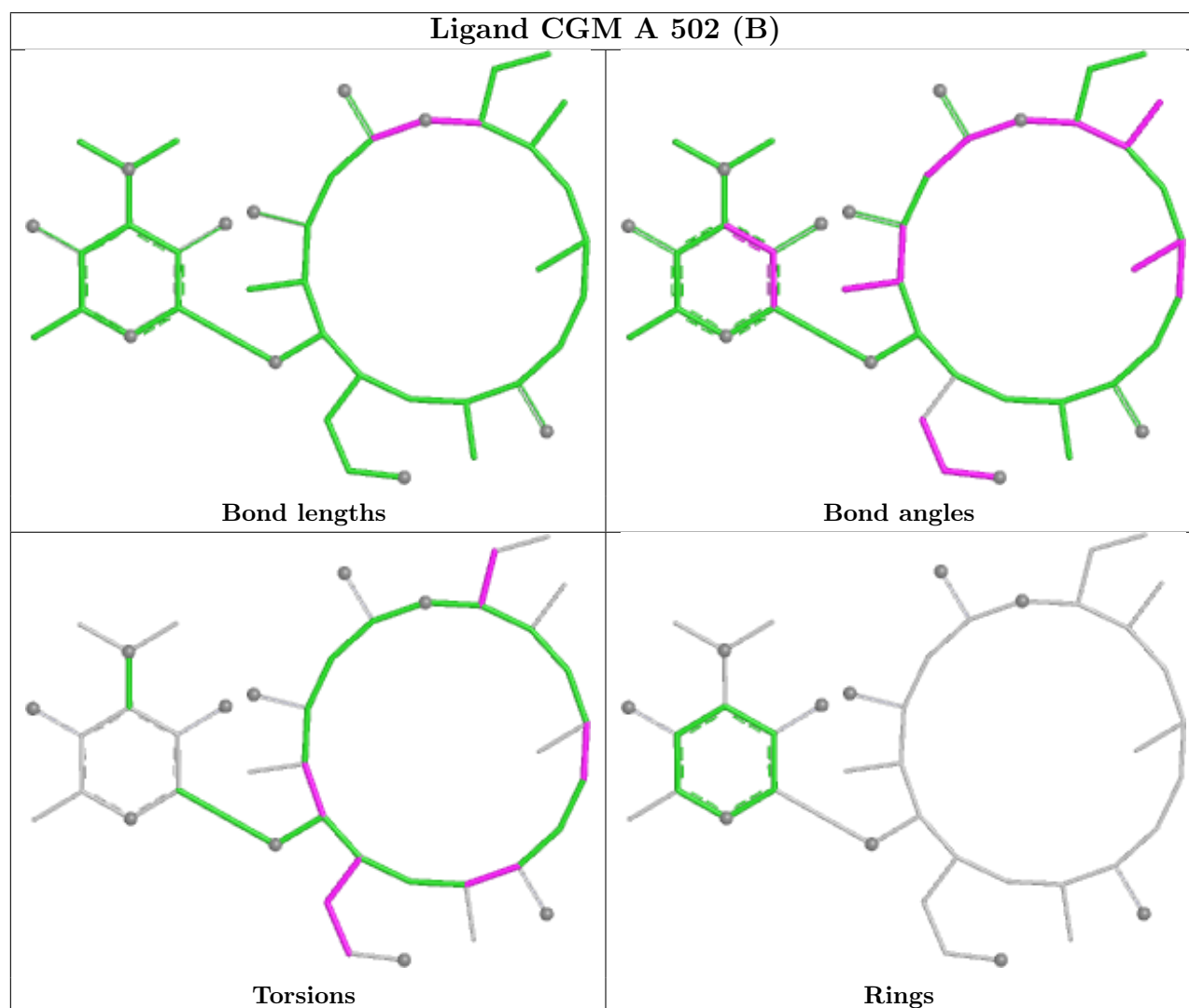
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[B]	CGM	1	0
4	A	507	EDO	2	0
3	A	502[A]	CGM	2	0
4	A	505	EDO	3	0
4	A	516	EDO	2	0
2	A	501	HEM	2	0
4	A	504	EDO	2	0
4	A	503	EDO	1	0

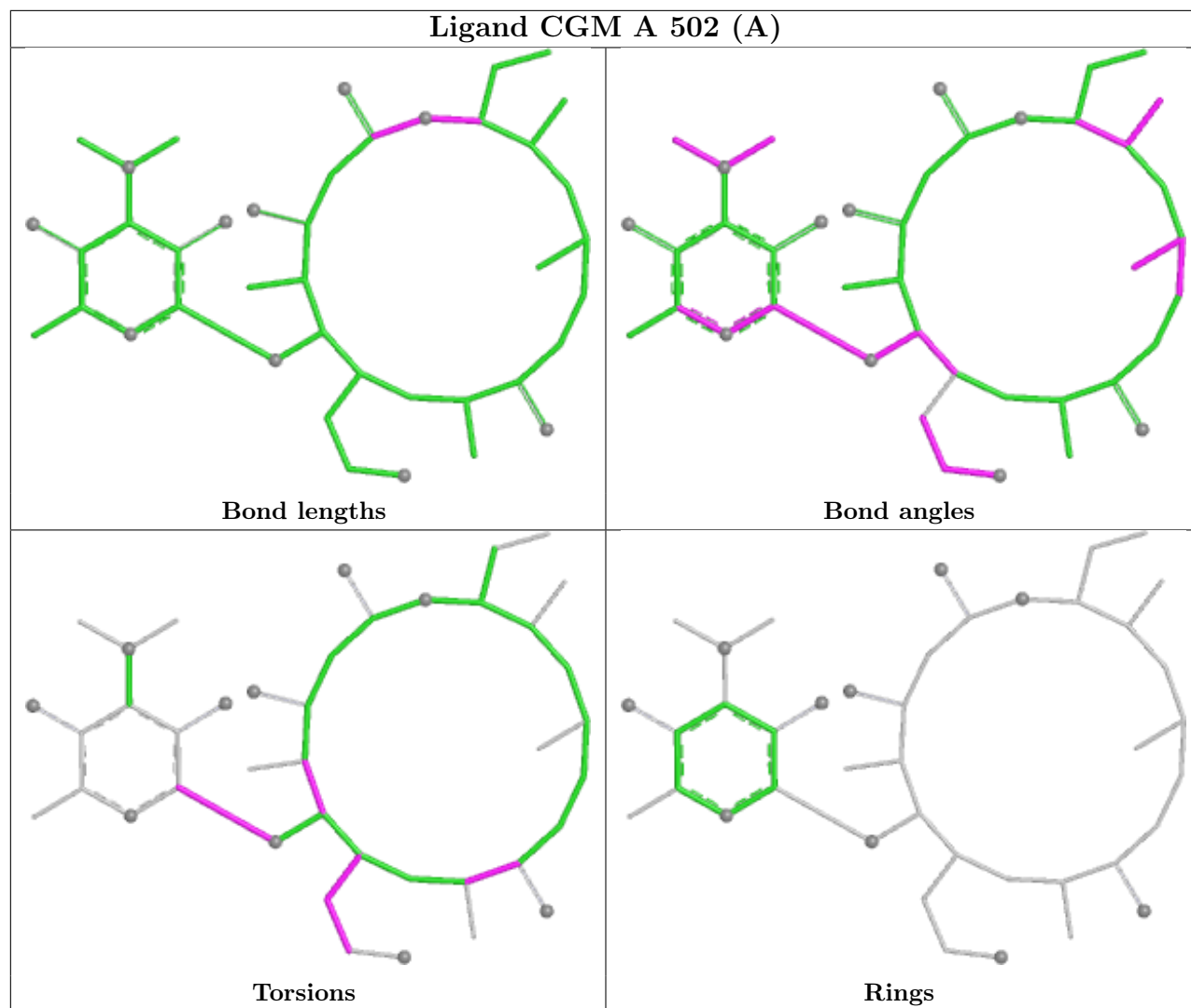
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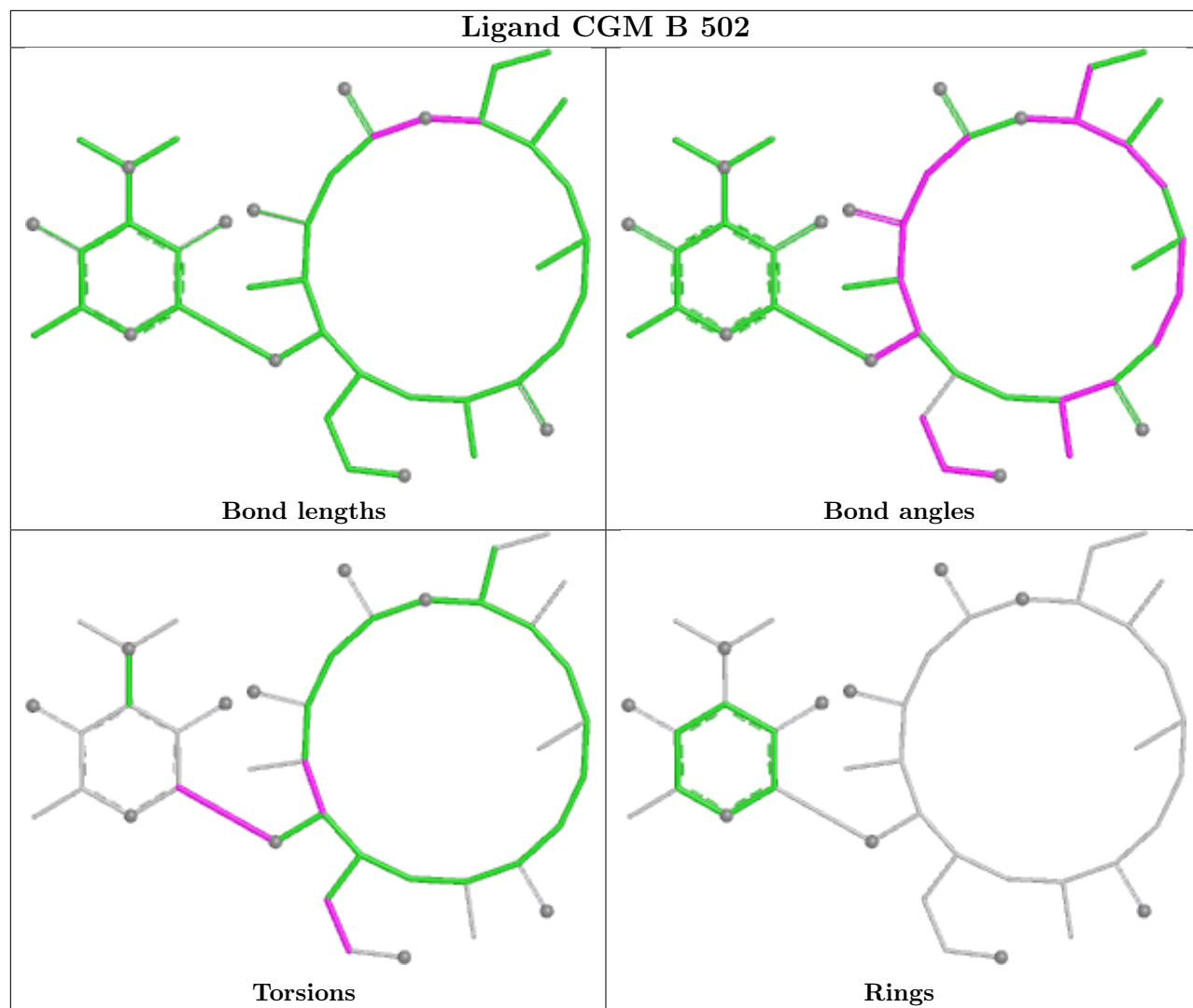
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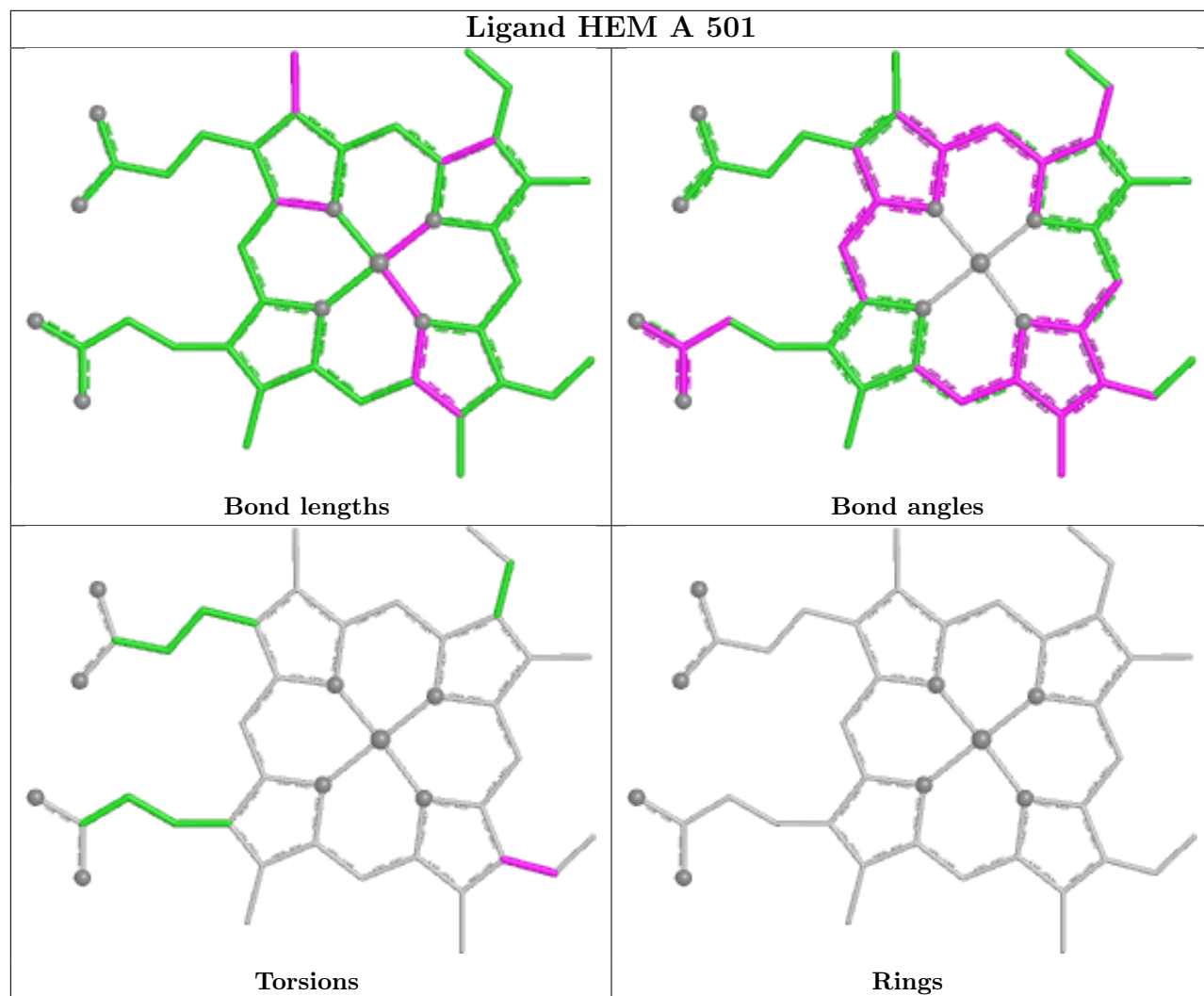
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0

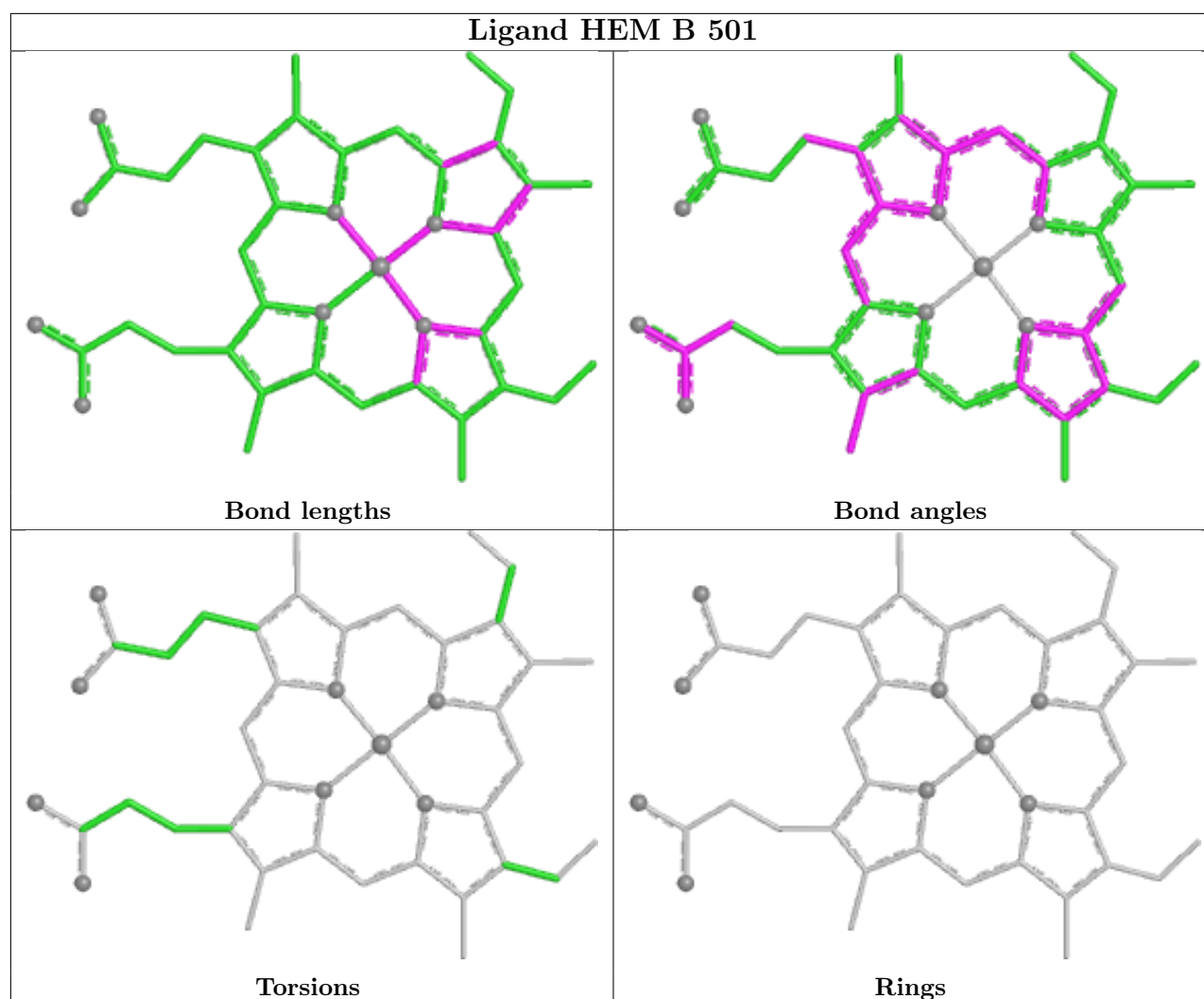
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	384/440 (87%)	0.14	4 (1%) 79 79	17, 41, 63, 94	2 (0%)
1	B	382/440 (86%)	0.49	22 (5%) 29 27	18, 48, 80, 111	3 (0%)
All	All	766/880 (87%)	0.31	26 (3%) 48 47	17, 44, 75, 111	5 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ASP	4.6
1	B	319	ILE	4.2
1	A	33	ILE	4.1
1	A	223	THR	4.1
1	A	228	GLY	3.9
1	B	222	LYS	3.9
1	B	33	ILE	3.2
1	B	32	SER	3.1
1	B	324	ILE	3.0
1	B	356	ALA	2.9
1	B	321	GLY	2.9
1	B	322	HIS	2.9
1	B	323	THR	2.8
1	B	70	TRP	2.7
1	B	314	THR	2.6
1	B	115	PRO	2.5
1	B	54	ALA	2.4
1	B	67	ALA	2.3
1	B	315	ALA	2.3
1	B	241	GLY	2.3
1	B	55	GLU	2.2
1	B	219	ILE	2.2
1	B	68	PRO	2.2
1	B	317	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLY	2.1
1	B	113	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	41[A]	7/8	0.89	0.09	35,37,42,45	7
1	CSO	A	41[B]	7/8	0.89	0.09	32,36,39,42	7
1	CSO	B	41[A]	7/8	0.89	0.10	36,40,42,43	7
1	CSO	B	41[B]	7/8	0.89	0.10	37,43,45,51	7

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.

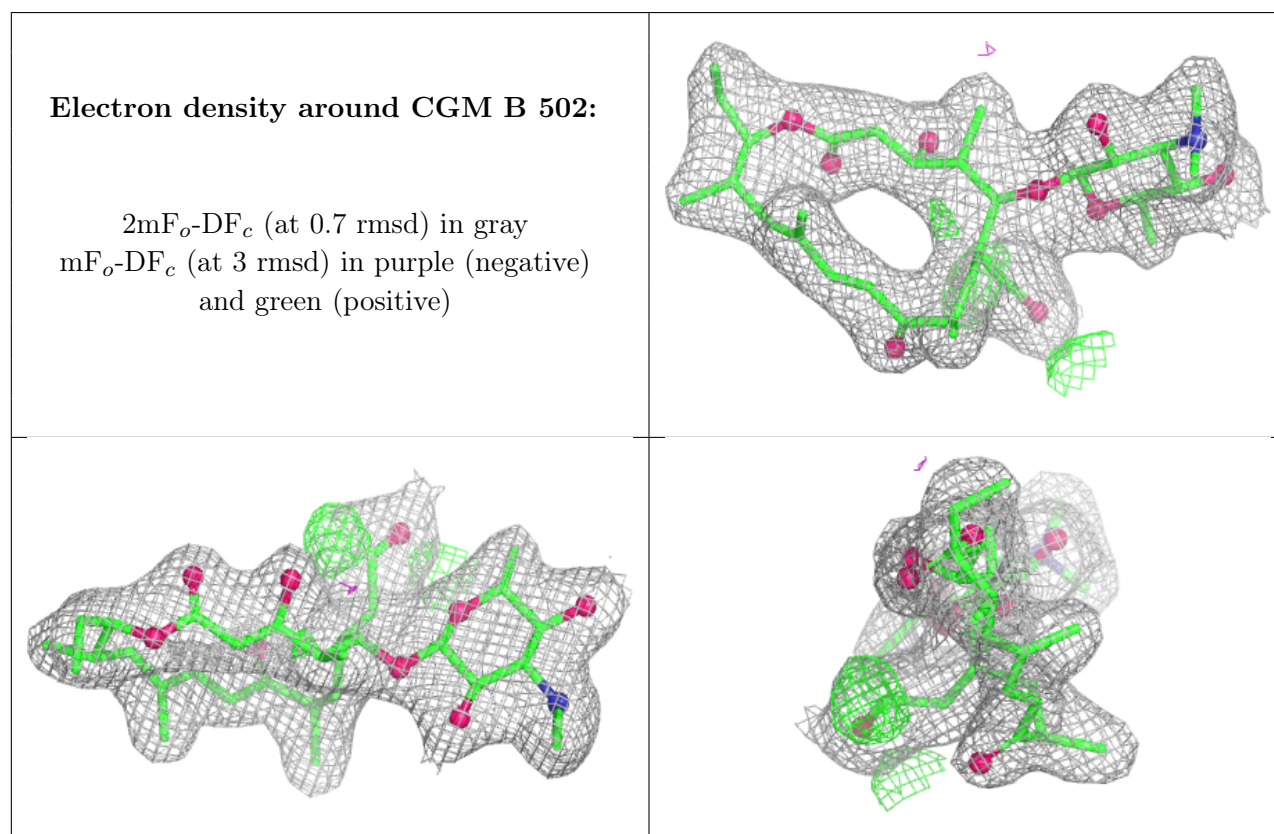
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	511	4/4	0.70	0.15	75,76,76,82	0
4	EDO	A	510	4/4	0.80	0.15	66,75,75,84	0
4	EDO	A	508	4/4	0.84	0.17	64,65,65,66	0
4	EDO	A	505	4/4	0.84	0.14	59,70,72,74	0
4	EDO	A	506	4/4	0.84	0.19	60,60,65,67	0
4	EDO	B	506	4/4	0.85	0.16	46,49,49,56	0
4	EDO	A	513	4/4	0.87	0.17	46,51,53,53	0
4	EDO	A	507	4/4	0.88	0.15	56,56,58,66	0
4	EDO	A	503	4/4	0.89	0.17	39,45,46,63	0
4	EDO	A	514	4/4	0.89	0.14	54,63,63,68	0
4	EDO	B	505	4/4	0.89	0.14	62,64,65,67	0
4	EDO	A	504	4/4	0.89	0.12	60,61,61,62	0

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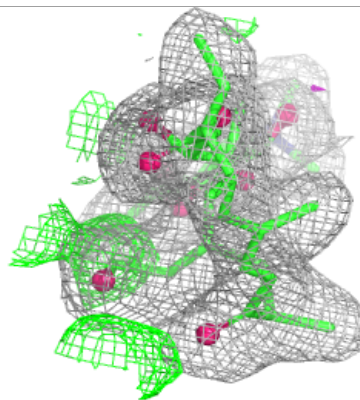
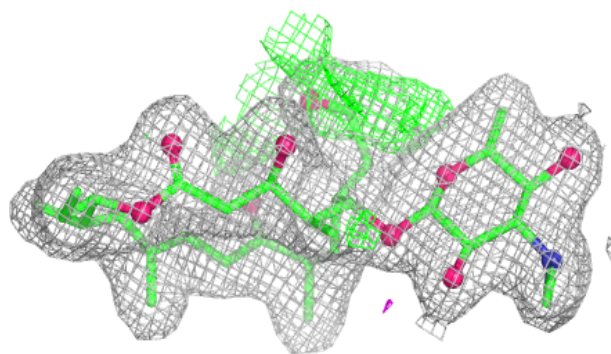
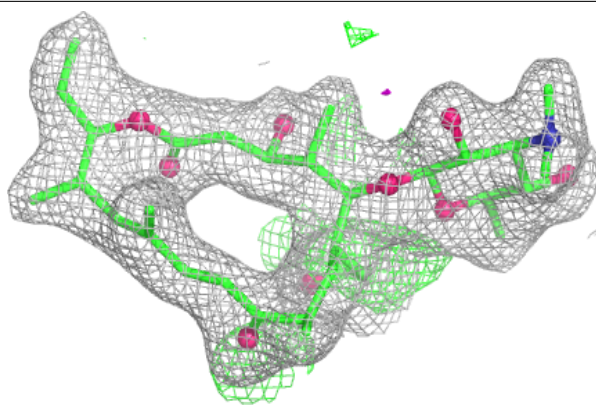
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	503	4/4	0.90	0.12	51,57,57,57	0
4	EDO	A	509	4/4	0.90	0.13	51,56,57,62	0
4	EDO	A	516	4/4	0.90	0.12	48,50,59,67	0
4	EDO	A	515	4/4	0.92	0.14	52,55,56,58	0
4	EDO	A	512	4/4	0.93	0.14	49,57,58,59	0
3	CGM	B	502	41/41	0.94	0.10	38,44,53,57	0
4	EDO	B	504	4/4	0.94	0.12	52,61,63,70	0
3	CGM	A	502[A]	41/41	0.94	0.08	25,34,44,46	41
3	CGM	A	502[B]	41/41	0.94	0.08	25,33,37,38	41
2	HEM	B	501	43/43	0.98	0.07	33,39,46,50	0
2	HEM	A	501	43/43	0.98	0.06	27,31,38,62	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.

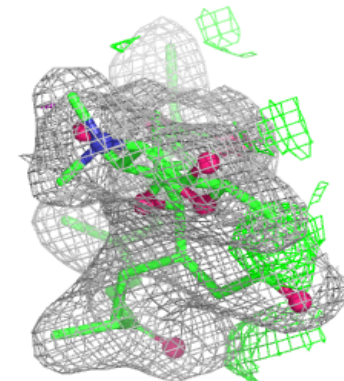
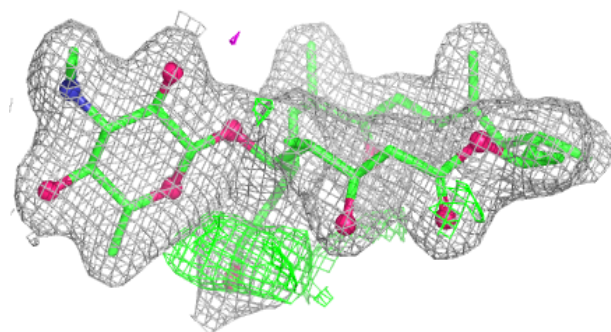
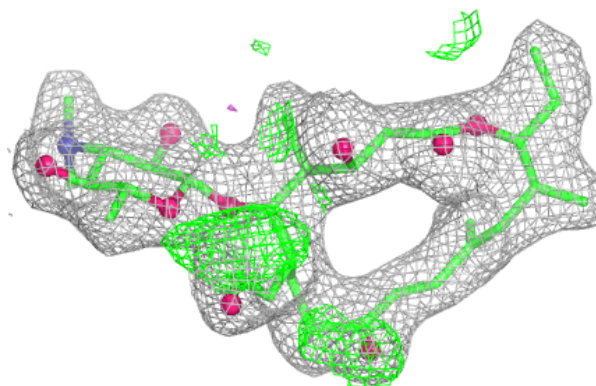


Electron density around CGM A 502 (A):

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

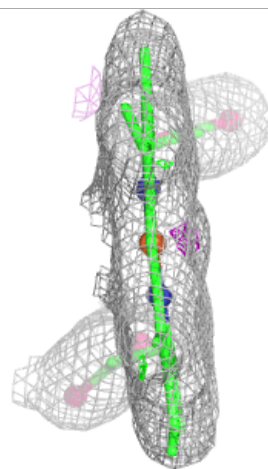
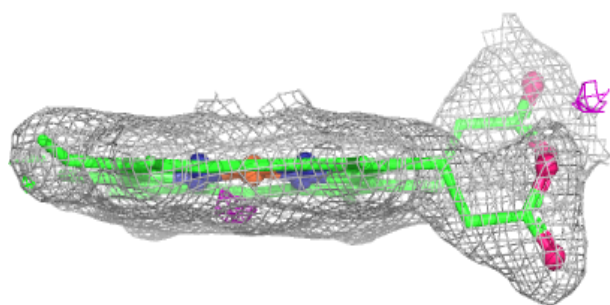
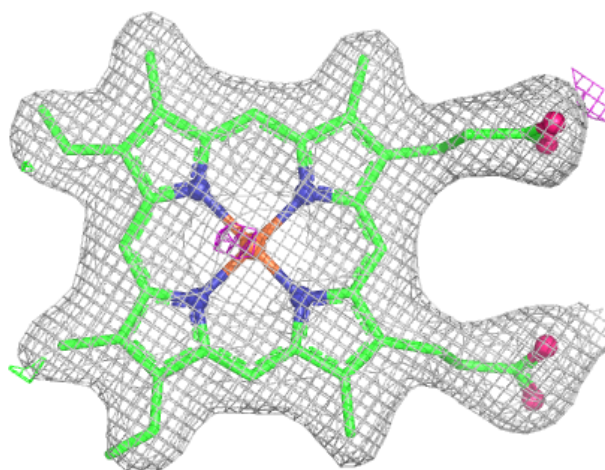
**Electron density around CGM A 502 (B):**

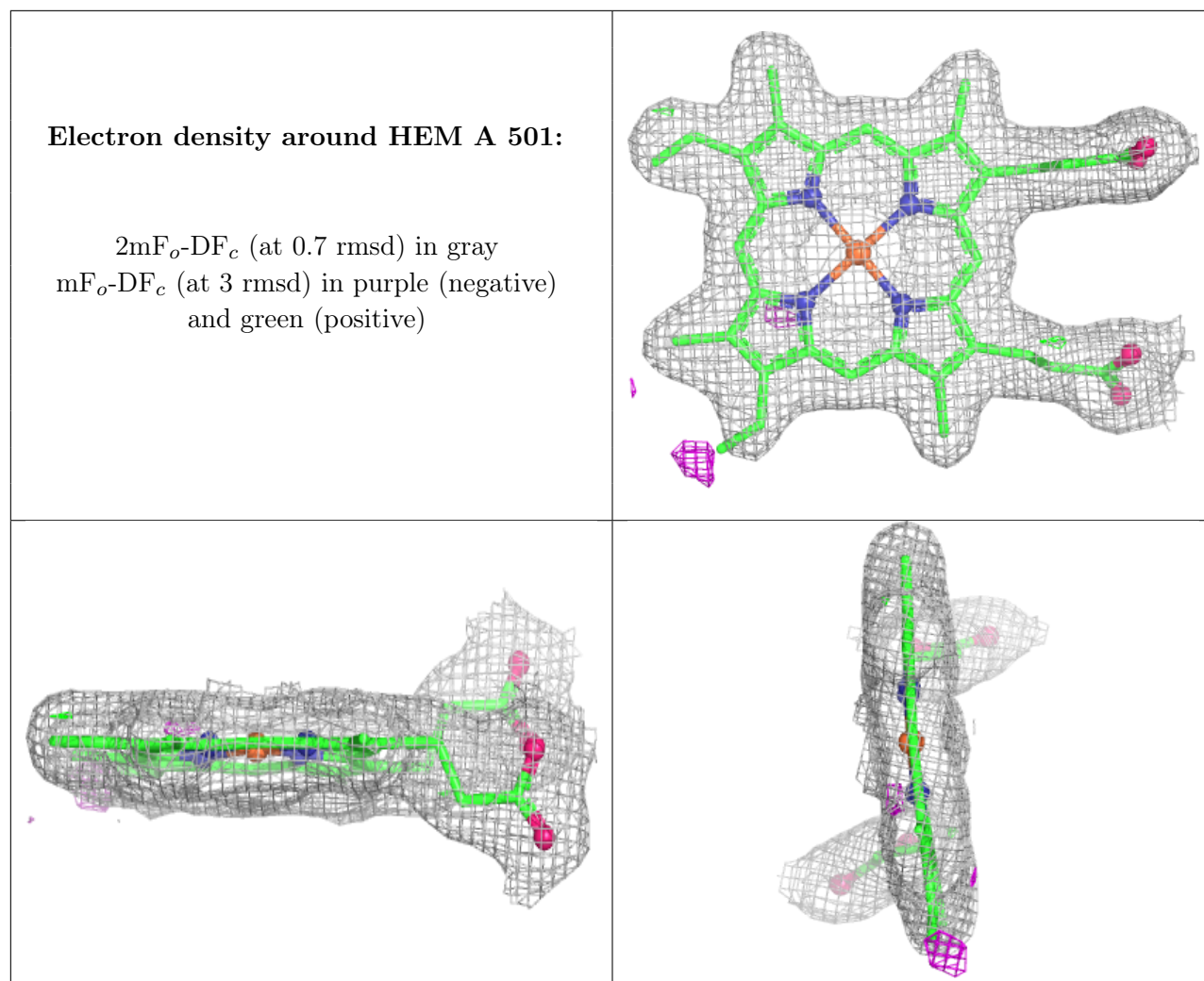
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.