



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:13 AM EDT

PDB ID : 7W1A / pdb_00007w1a
Title : Crystal Structure of MPH-E in complex with GMP and Azithromycin
Authors : Qi, Q.; Kuang, L.; Jiang, Y.
Deposited on : 2021-11-19
Resolution : 2.17 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

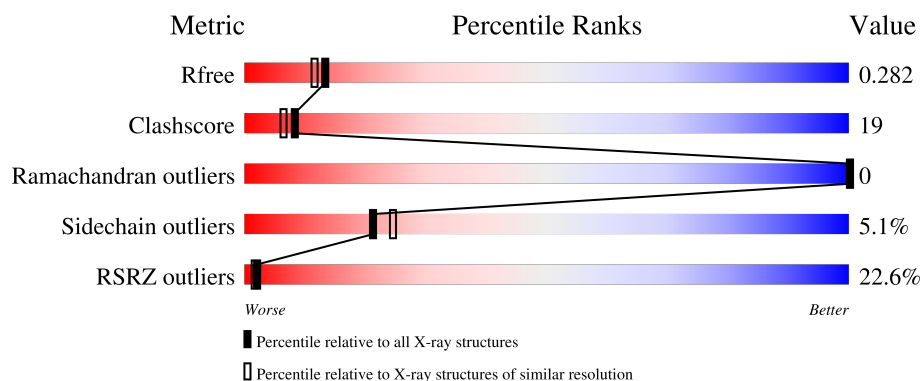
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	302	22% 63% 30% 5%
1	B	302	21% 64% 29% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4836 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.

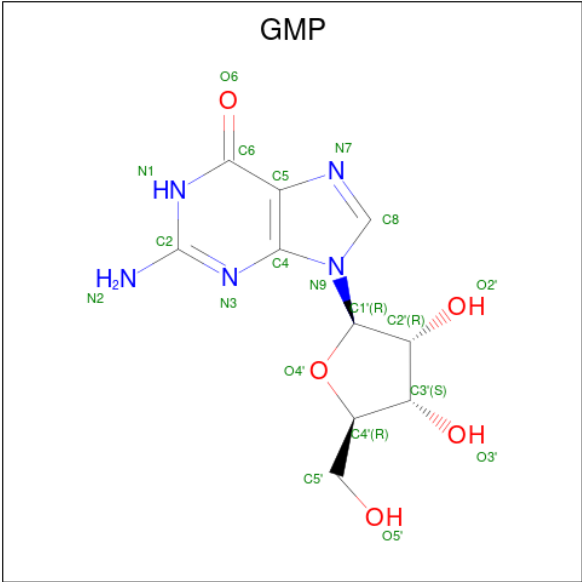
- Molecule 1 is a protein called Macrolide 2'-phosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	287	Total	C	N	O	S	0	0	0
			2308	1484	385	432	7			
1	A	287	Total	C	N	O	S	0	0	0
			2315	1483	386	439	7			

There are 16 discrepancies between the modelled and reference sequences:

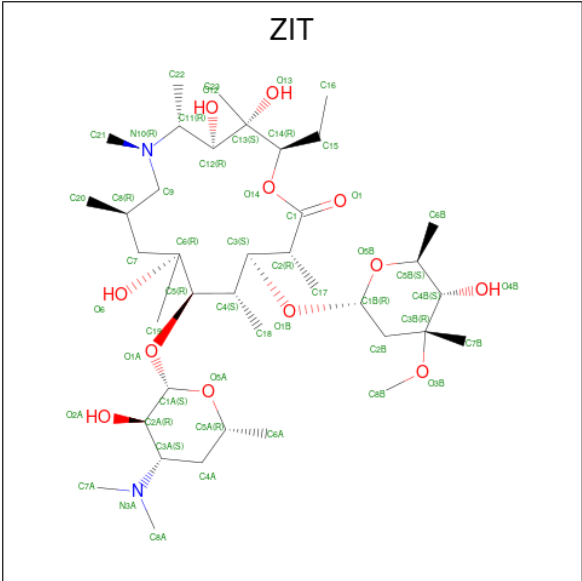
Chain	Residue	Modelled	Actual	Comment	Reference
B	295	LEU	-	expression tag	UNP A5Y459
B	296	GLU	-	expression tag	UNP A5Y459
B	297	HIS	-	expression tag	UNP A5Y459
B	298	HIS	-	expression tag	UNP A5Y459
B	299	HIS	-	expression tag	UNP A5Y459
B	300	HIS	-	expression tag	UNP A5Y459
B	301	HIS	-	expression tag	UNP A5Y459
B	302	HIS	-	expression tag	UNP A5Y459
A	295	LEU	-	expression tag	UNP A5Y459
A	296	GLU	-	expression tag	UNP A5Y459
A	297	HIS	-	expression tag	UNP A5Y459
A	298	HIS	-	expression tag	UNP A5Y459
A	299	HIS	-	expression tag	UNP A5Y459
A	300	HIS	-	expression tag	UNP A5Y459
A	301	HIS	-	expression tag	UNP A5Y459
A	302	HIS	-	expression tag	UNP A5Y459

- Molecule 2 is GUANOSINE (CCD ID: GMP) (formula: C₁₀H₁₃N₅O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			20	10	5	5		
2	A	1	Total	C	N	O	0	0
			20	10	5	5		

- Molecule 3 is AZITHROMYCIN (CCD ID: ZIT) (formula: C₃₈H₇₂N₂O₁₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			52	38	2	12		

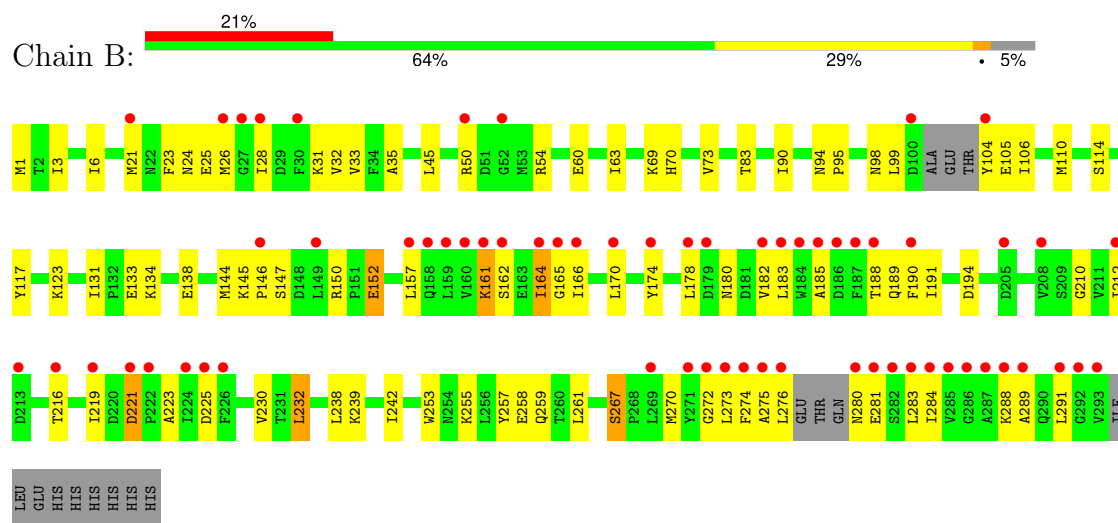
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	37	Total	O	0	0
			37	37		
4	A	32	Total	O	0	0
			32	32		

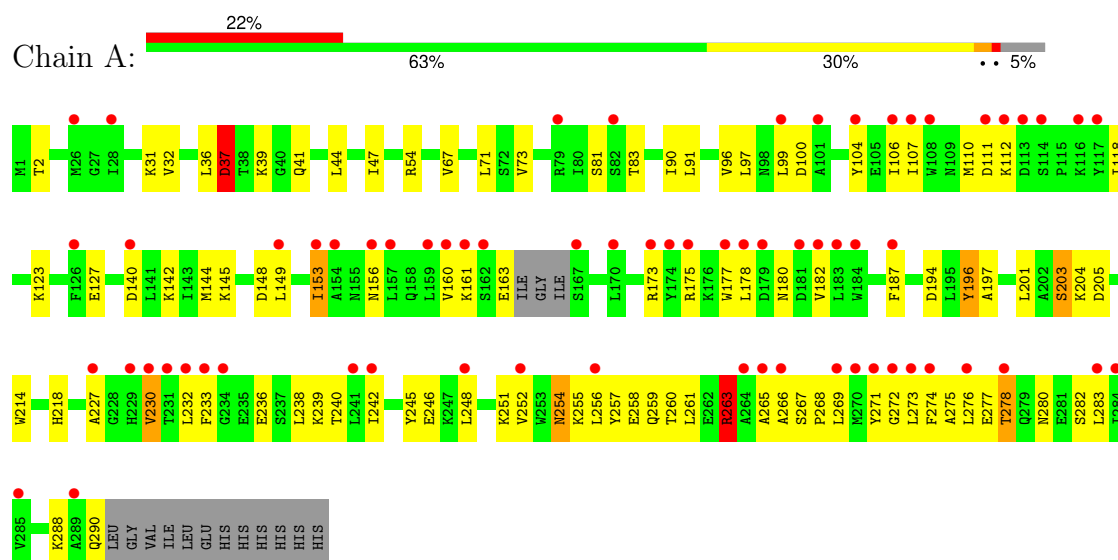
3 Residue-property plots

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: Macrolide 2'-phosphotransferase



• Molecule 1: Macrolide 2'-phosphotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.01Å 45.85Å 89.68Å 90.00° 105.71° 90.00°	Depositor
Resolution (Å)	40.49 – 2.17 40.49 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.49-2.17) 98.9 (40.49-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.254 , 0.283 0.255 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (5.88%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4836	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: GMP, ZIT

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	0.73	1/2361 (0.0%)	0.84	2/3194 (0.1%)
1	B	0.76	0/2353	0.95	3/3181 (0.1%)
All	All	0.74	1/4714 (0.0%)	0.89	5/6375 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ASP	CB-CG	-6.32	1.36	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ILE	N-CA-C	7.47	118.77	111.67
1	B	165	GLY	CA-C-O	-6.30	117.19	122.29
1	B	212	ILE	CA-C-O	-5.35	115.07	120.69
1	A	36	LEU	CA-C-N	5.02	130.10	120.97
1	A	36	LEU	C-N-CA	5.02	130.10	120.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain
1	A	175	ARG	Sidechain
1	A	263	ARG	Sidechain
1	B	50	ARG	Sidechain

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	2315	0	2327	100	0
1	B	2308	0	2335	85	0
2	A	20	0	13	1	0
2	B	20	0	13	1	0
3	A	52	0	72	18	0
3	B	52	0	72	14	0
4	A	32	0	0	1	0
4	B	37	0	0	0	0
All	All	4836	0	4832	184	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 19.

All (184) 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:271:TYR:CZ	3:A:402:ZIT:H201	1.80	1.15
1:B:232:LEU:CD2	3:B:402:ZIT:H161	1.77	1.14
1:B:232:LEU:HD21	3:B:402:ZIT:H161	1.33	1.07
1:A:271:TYR:CE1	3:A:402:ZIT:C20	2.47	0.98
1:A:156:ASN:HB3	1:A:273:LEU:HD11	1.48	0.96
1:A:271:TYR:CE1	3:A:402:ZIT:H201	2.02	0.94
1:A:271:TYR:CZ	3:A:402:ZIT:C20	2.59	0.85
1:A:271:TYR:HB2	3:A:402:ZIT:H191	1.59	0.83
1:A:156:ASN:O	1:A:160:VAL:HG23	1.78	0.82
1:B:270:MET:HE2	1:B:273:LEU:HD21	1.65	0.79
1:B:272:GLY:CA	1:B:288:LYS:HD2	2.13	0.79
1:A:271:TYR:CE1	3:A:402:ZIT:H203	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:HD21	3:B:402:ZIT:C16	2.13	0.78
1:A:271:TYR:HB2	3:A:402:ZIT:C19	2.13	0.78
1:A:268:PRO:HB3	1:A:290:GLN:HB3	1.67	0.77
1:B:150:ARG:HG2	1:B:178:LEU:HD23	1.69	0.75
1:A:271:TYR:CG	3:A:402:ZIT:H191	2.22	0.74
1:A:145:LYS:HD3	1:A:148:ASP:OD2	1.88	0.73
1:B:21:MET:SD	1:B:33:VAL:HG11	2.29	0.73
1:B:99:LEU:HD13	3:B:402:ZIT:C23	2.19	0.72
1:A:149:LEU:O	1:A:153:ILE:HG22	1.90	0.71
1:A:271:TYR:CB	3:A:402:ZIT:H191	2.20	0.71
1:B:21:MET:HG2	1:B:35:ALA:HA	1.74	0.69
1:A:160:VAL:HG21	1:A:269:LEU:CD1	2.23	0.68
1:B:272:GLY:CA	1:B:288:LYS:CD	2.72	0.67
1:B:106:ILE:HD12	1:B:106:ILE:H	1.60	0.66
1:A:257:TYR:CE2	1:A:261:LEU:HD11	2.30	0.66
1:A:255:LYS:HE3	1:A:258:GLU:OE1	1.95	0.66
1:B:281:GLU:HG2	1:B:284:ILE:H	1.60	0.66
1:B:182:VAL:HG22	1:B:255:LYS:HG3	1.78	0.65
1:A:180:ASN:OD1	1:A:182:VAL:HG12	1.97	0.65
1:A:145:LYS:N	1:A:145:LYS:HD2	2.12	0.64
1:A:271:TYR:CD2	3:A:402:ZIT:H213	2.33	0.64
1:A:265:ALA:O	1:A:268:PRO:HD2	1.97	0.64
1:A:100:ASP:HB2	1:A:107:ILE:HD11	1.80	0.63
1:A:160:VAL:HG21	1:A:269:LEU:HD11	1.81	0.63
1:B:194:ASP:HB2	1:B:216:THR:HG21	1.80	0.63
1:B:232:LEU:CD2	3:B:402:ZIT:C16	2.67	0.62
1:A:238:LEU:HD11	1:A:260:THR:HG21	1.82	0.62
1:A:156:ASN:HB3	1:A:273:LEU:CD1	2.29	0.62
1:B:232:LEU:HG	3:B:402:ZIT:C16	2.30	0.61
1:A:32:VAL:HG21	2:A:401:GMP:H5'1	1.83	0.60
1:A:177:TRP:HZ3	1:A:266:ALA:HB2	1.66	0.60
1:B:145:LYS:HD2	1:B:146:PRO:HD3	1.83	0.59
1:B:272:GLY:HA3	1:B:288:LYS:CD	2.33	0.59
1:A:271:TYR:CD2	3:A:402:ZIT:H8	2.38	0.58
1:B:110:MET:HE1	1:B:117:TYR:CG	2.39	0.58
1:A:112:LYS:HE2	1:A:232:LEU:O	2.04	0.58
1:B:232:LEU:CG	3:B:402:ZIT:H161	2.33	0.57
1:B:32:VAL:HG21	2:B:401:GMP:H5'1	1.87	0.57
1:B:273:LEU:HD12	1:B:274:PHE:N	2.21	0.56
1:A:255:LYS:HE3	1:A:255:LYS:HA	1.86	0.56
1:A:97:LEU:CD2	1:A:197:ALA:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:OH	3:A:402:ZIT:H201	2.06	0.56
1:A:71:LEU:HD12	1:A:73:VAL:HG22	1.88	0.55
1:B:6:ILE:HB	1:B:21:MET:HE1	1.88	0.55
1:B:232:LEU:HD23	3:B:402:ZIT:H161	1.83	0.55
1:A:203:SER:HB3	1:A:205:ASP:OD1	2.07	0.55
1:B:275:ALA:O	1:B:280:ASN:N	2.40	0.54
1:B:28:ILE:HG13	3:B:402:ZIT:C8A	2.37	0.54
1:B:24:ASN:HD21	1:B:26:MET:HE3	1.73	0.54
1:B:69:LYS:HB2	1:B:70:HIS:ND1	2.22	0.54
1:A:160:VAL:HG22	1:A:273:LEU:CD2	2.38	0.54
1:A:97:LEU:HD23	1:A:197:ALA:HB3	1.90	0.54
1:A:245:TYR:HA	1:A:248:LEU:HD12	1.90	0.54
1:A:44:LEU:HB2	1:A:90:ILE:HD13	1.91	0.53
1:B:232:LEU:CG	3:B:402:ZIT:C16	2.87	0.53
1:B:273:LEU:HD12	1:B:273:LEU:C	2.33	0.53
1:A:259:GLN:O	1:A:263:ARG:HG2	2.09	0.53
1:B:99:LEU:HD13	3:B:402:ZIT:H231	1.89	0.53
1:B:267:SER:OG	3:B:402:ZIT:O5B	2.27	0.53
1:B:189:GLN:O	1:B:191:ILE:HG23	2.09	0.53
1:B:134:LYS:HE3	1:B:138:GLU:OE2	2.08	0.53
1:A:252:VAL:HG13	1:A:256:LEU:HD23	1.89	0.53
1:B:1:MET:HB2	1:B:31:LYS:HE2	1.91	0.53
1:B:257:TYR:CE2	1:B:261:LEU:HD11	2.44	0.52
1:B:270:MET:CE	1:B:273:LEU:HD21	2.36	0.52
1:B:272:GLY:N	1:B:288:LYS:HD2	2.24	0.52
1:A:142:LYS:O	1:A:218:HIS:HB2	2.09	0.52
1:A:160:VAL:HG11	1:A:269:LEU:HD12	1.91	0.52
1:A:238:LEU:O	1:A:242:ILE:HG13	2.10	0.52
1:A:257:TYR:CZ	1:A:261:LEU:HD11	2.45	0.52
1:A:236:GLU:HA	1:A:239:LYS:HG3	1.92	0.51
1:A:177:TRP:CZ3	1:A:266:ALA:HB2	2.44	0.51
1:A:187:PHE:CG	1:A:251:LYS:HE3	2.45	0.51
1:B:272:GLY:HA2	1:B:288:LYS:HD2	1.92	0.51
1:A:204:LYS:HA	4:A:505:HOH:O	2.11	0.50
1:A:160:VAL:HG22	1:A:273:LEU:HD23	1.93	0.50
1:B:275:ALA:C	1:B:276:LEU:HD23	2.37	0.50
1:A:118:ILE:HG21	1:A:240:THR:HG22	1.92	0.50
1:A:153:ILE:HG12	1:A:178:LEU:HD21	1.94	0.50
1:B:170:LEU:HD22	1:B:174:TYR:CZ	2.46	0.50
1:A:100:ASP:O	1:A:104:TYR:N	2.40	0.50
1:B:190:PHE:HA	1:B:219:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:HA	1:B:63:ILE:HD12	1.93	0.49
1:B:28:ILE:HG13	3:B:402:ZIT:H8A3	1.93	0.49
1:A:257:TYR:O	1:A:261:LEU:HG	2.13	0.49
1:B:238:LEU:O	1:B:242:ILE:HG13	2.12	0.49
1:B:21:MET:SD	1:B:33:VAL:CG1	3.00	0.49
1:A:123:LYS:O	1:A:127:GLU:HG3	2.12	0.49
1:A:271:TYR:CE2	3:A:402:ZIT:H8	2.48	0.48
1:A:144:MET:HB3	1:A:149:LEU:CD2	2.43	0.48
1:A:106:ILE:HD11	3:A:402:ZIT:H151	1.94	0.48
1:A:112:LYS:HE2	1:A:233:PHE:HA	1.95	0.48
1:A:97:LEU:HD13	1:A:106:ILE:HG23	1.96	0.48
1:A:37:ASP:HB3	1:A:39:LYS:H	1.77	0.48
1:B:104:TYR:CD1	1:B:105:GLU:N	2.82	0.48
1:B:110:MET:HE3	1:B:114:SER:HB3	1.96	0.47
1:A:230:VAL:CG2	1:A:238:LEU:HD13	2.43	0.47
1:A:160:VAL:HG21	1:A:269:LEU:HD12	1.94	0.47
1:B:133:GLU:HG3	1:B:219:ILE:HD13	1.97	0.47
1:A:272:GLY:O	1:A:276:LEU:HG	2.14	0.47
1:A:106:ILE:C	1:A:107:ILE:HG13	2.39	0.47
1:B:183:LEU:HD22	1:B:259:GLN:CA	2.45	0.47
1:B:157:LEU:O	1:B:157:LEU:HD12	2.15	0.46
1:A:160:VAL:CG2	1:A:269:LEU:HD11	2.46	0.46
1:A:271:TYR:CE2	3:A:402:ZIT:H213	2.50	0.46
1:B:150:ARG:O	1:B:178:LEU:HD21	2.16	0.46
1:A:163:GLU:O	1:A:288:LYS:NZ	2.45	0.46
1:B:3:ILE:HG23	1:B:21:MET:HE2	1.97	0.46
1:B:183:LEU:HD21	1:B:258:GLU:HB3	1.98	0.45
1:B:6:ILE:CD1	1:B:23:PHE:HE2	2.29	0.45
1:A:271:TYR:CD1	3:A:402:ZIT:H203	2.49	0.45
1:A:254:ASN:OD1	1:A:254:ASN:N	2.50	0.45
1:A:111:ASP:O	1:A:112:LYS:C	2.60	0.45
1:A:275:ALA:O	1:A:278:THR:HG22	2.16	0.45
1:A:31:LYS:HG2	1:A:47:ILE:HB	1.98	0.45
1:A:37:ASP:HB2	1:A:41:GLN:O	2.16	0.45
1:B:288:LYS:O	1:B:289:ALA:C	2.60	0.45
1:B:183:LEU:HD22	1:B:259:GLN:HA	2.00	0.44
1:B:257:TYR:O	1:B:261:LEU:HG	2.17	0.44
1:A:99:LEU:CD2	1:A:106:ILE:HD13	2.47	0.44
1:A:145:LYS:N	1:A:145:LYS:CD	2.79	0.44
1:A:259:GLN:HA	1:A:259:GLN:OE1	2.17	0.44
1:B:26:MET:HE1	1:B:98:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ALA:HB2	1:B:253:TRP:CZ2	2.53	0.44
1:B:73:VAL:HB	1:B:210:GLY:HA2	2.00	0.44
1:B:221:ASP:OD2	1:B:223:ALA:HB3	2.17	0.44
1:B:232:LEU:HG	3:B:402:ZIT:H163	1.99	0.44
1:B:150:ARG:CG	1:B:178:LEU:HD23	2.42	0.44
1:A:280:ASN:HB3	1:A:283:LEU:HD12	1.99	0.43
1:A:54:ARG:HB2	1:A:83:THR:HG22	2.00	0.43
1:A:182:VAL:HG13	1:A:255:LYS:HG3	1.99	0.43
1:B:54:ARG:HB2	1:B:83:THR:HG22	2.01	0.43
1:A:160:VAL:CG2	1:A:273:LEU:HD21	2.48	0.43
1:B:123:LYS:HE3	1:A:205:ASP:OD2	2.19	0.43
1:A:238:LEU:HD22	1:A:257:TYR:HD1	1.84	0.43
1:B:194:ASP:HB2	1:B:216:THR:CG2	2.48	0.43
1:B:239:LYS:HD2	1:B:257:TYR:CE1	2.53	0.43
1:A:230:VAL:HB	1:A:238:LEU:HD12	2.01	0.43
1:A:194:ASP:CG	3:A:402:ZIT:H7A2	2.43	0.43
1:A:227:ALA:O	1:A:230:VAL:HG12	2.18	0.43
1:B:33:VAL:HB	1:B:45:LEU:HB2	2.01	0.43
1:A:246:GLU:HG2	1:A:252:VAL:HG21	2.00	0.43
1:B:288:LYS:O	1:B:291:LEU:N	2.52	0.42
1:B:230:VAL:HG23	1:B:238:LEU:HB2	2.01	0.42
1:B:110:MET:HE1	1:B:117:TYR:CB	2.50	0.42
1:B:272:GLY:HA2	1:B:288:LYS:CD	2.45	0.42
1:B:164:ILE:HD12	1:B:288:LYS:HD3	2.01	0.42
1:B:272:GLY:HA3	1:B:288:LYS:CE	2.48	0.42
1:A:274:PHE:O	1:A:278:THR:N	2.51	0.42
1:A:99:LEU:HD21	1:A:106:ILE:HD13	2.01	0.42
1:B:70:HIS:CD2	1:B:131:ILE:HG12	2.54	0.42
1:B:161:LYS:HG3	1:B:166:ILE:HG22	2.01	0.42
1:A:187:PHE:CD1	1:A:251:LYS:HE3	2.55	0.42
1:B:144:MET:HE1	1:B:152:GLU:CD	2.43	0.42
1:A:230:VAL:HG23	1:A:238:LEU:CD1	2.50	0.42
1:A:230:VAL:HG23	1:A:238:LEU:HD13	2.02	0.42
1:B:99:LEU:HD23	1:B:106:ILE:HA	2.02	0.42
1:B:170:LEU:HD22	1:B:174:TYR:OH	2.19	0.42
1:A:96:VAL:HG13	1:A:110:MET:HE2	2.01	0.41
1:A:278:THR:HG23	1:A:280:ASN:N	2.35	0.41
1:A:187:PHE:CD2	1:A:251:LYS:HD3	2.55	0.41
1:B:25:GLU:OE2	1:B:31:LYS:NZ	2.33	0.41
1:A:91:LEU:HD12	1:A:201:LEU:HD11	2.02	0.41
1:A:255:LYS:HA	1:A:255:LYS:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HB3	1:B:95:PRO:HD2	2.03	0.41
1:B:180:ASN:OD1	1:B:180:ASN:N	2.53	0.41
1:A:187:PHE:CE2	1:A:251:LYS:HG2	2.56	0.41
1:B:6:ILE:HD11	1:B:23:PHE:HE2	1.87	0.40
1:B:146:PRO:HG3	1:B:188:THR:HG23	2.03	0.40
1:A:67:VAL:HG11	1:A:214:TRP:CZ3	2.56	0.40
1:A:160:VAL:CG2	1:A:273:LEU:CD2	3.00	0.40
1:A:196:TYR:HB3	3:A:402:ZIT:C8B	2.52	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	283/302 (94%)	275 (97%)	8 (3%)	0	100	100
1	B	281/302 (93%)	269 (96%)	12 (4%)	0	100	100
All	All	564/604 (93%)	544 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/266 (95%)	238 (94%)	15 (6%)	18	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	252/266 (95%)	241 (96%)	11 (4%)	25	31
All	All	505/532 (95%)	479 (95%)	26 (5%)	21	24

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

Mol	Chain	Res	Type
1	B	90	ILE
1	B	147	SER
1	B	152	GLU
1	B	161	LYS
1	B	162	SER
1	B	164	ILE
1	B	221	ASP
1	B	225	ASP
1	B	232	LEU
1	B	267	SER
1	B	283	LEU
1	A	2	THR
1	A	37	ASP
1	A	81	SER
1	A	140	ASP
1	A	153	ILE
1	A	161	LYS
1	A	196	TYR
1	A	203	SER
1	A	230	VAL
1	A	254	ASN
1	A	263	ARG
1	A	267	SER
1	A	277	GLU
1	A	278	THR
1	A	282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	GLN
1	A	7	GLN
1	A	98	ASN
1	A	156	ASN
1	A	229	HIS

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Mol	Chain	Res	Type
1	A	290	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GMP	B	401	-	22,22,22	0.63	0	33,33,33	1.08	3 (9%)
3	ZIT	A	402	-	54,54,54	0.86	4 (7%)	82,83,83	1.78	16 (19%)
2	GMP	A	401	-	22,22,22	0.79	1 (4%)	33,33,33	0.85	1 (3%)
3	ZIT	B	402	-	54,54,54	0.87	4 (7%)	82,83,83	1.78	16 (19%)

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	GMP	B	401	-	-	0/6/22/22	0/3/3/3
3	ZIT	A	402	-	-	2/72/107/107	0/3/3/3
2	GMP	A	401	-	-	0/6/22/22	0/3/3/3
3	ZIT	B	402	-	-	2/72/107/107	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	ZIT	C21-N10	2.26	1.51	1.46
3	B	402	ZIT	C4-C3	-2.25	1.48	1.54
3	A	402	ZIT	C4-C3	-2.23	1.48	1.54
3	A	402	ZIT	C21-N10	2.20	1.51	1.46
2	A	401	GMP	C4-N3	2.15	1.39	1.34
3	B	402	ZIT	O5B-C5B	-2.07	1.39	1.44
3	A	402	ZIT	O5B-C5B	-2.04	1.39	1.44
3	B	402	ZIT	O1A-C5	-2.03	1.39	1.44
3	A	402	ZIT	O1A-C5	-2.01	1.39	1.44

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ZIT	O5B-C5B-C6B	5.09	118.03	106.74
3	B	402	ZIT	O5B-C5B-C6B	5.05	117.94	106.74
3	A	402	ZIT	C1A-O1A-C5	4.91	124.62	116.26
3	B	402	ZIT	C1A-O1A-C5	4.90	124.61	116.26
3	A	402	ZIT	C6-C5-C4	4.86	120.94	113.89
3	B	402	ZIT	C6-C5-C4	4.85	120.91	113.89
3	B	402	ZIT	O5B-C5B-C4B	4.65	118.05	110.04
3	A	402	ZIT	O5B-C5B-C4B	4.61	117.98	110.04
3	B	402	ZIT	C3-C4-C5	4.48	120.51	111.17
3	A	402	ZIT	C3-C4-C5	4.45	120.44	111.17
3	B	402	ZIT	O1A-C5-C6	4.14	111.34	106.40
3	A	402	ZIT	O1A-C5-C6	4.11	111.30	106.40
3	B	402	ZIT	C3B-C2B-C1B	3.80	121.40	114.99
3	A	402	ZIT	C3B-C2B-C1B	3.78	121.38	114.99
3	B	402	ZIT	C23-C13-C12	-3.74	106.66	113.14
3	A	402	ZIT	C23-C13-C12	-3.71	106.71	113.14
3	B	402	ZIT	O5B-C1B-C2B	-3.23	106.05	112.08
3	A	402	ZIT	O5B-C1B-C2B	-3.23	106.05	112.08
3	A	402	ZIT	C1B-O5B-C5B	2.88	121.70	113.82
3	B	402	ZIT	C1B-O5B-C5B	2.85	121.64	113.82
2	B	401	GMP	N2-C2-N3	2.52	124.58	119.67
3	B	402	ZIT	O1B-C3-C4	-2.44	105.36	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ZIT	O1B-C3-C4	-2.43	105.37	108.23
3	A	402	ZIT	C21-N10-C11	2.41	117.93	113.59
3	B	402	ZIT	C21-N10-C11	2.38	117.88	113.59
3	B	402	ZIT	C5A-C4A-C3A	-2.34	106.46	110.46
3	A	402	ZIT	C5A-C4A-C3A	-2.30	106.53	110.46
3	A	402	ZIT	C6B-C5B-C4B	2.25	116.31	112.58
3	B	402	ZIT	C6B-C5B-C4B	2.23	116.28	112.58
2	B	401	GMP	O6-C6-C5	2.23	132.41	126.53
3	B	402	ZIT	O1A-C5-C4	2.19	114.75	111.58
2	A	401	GMP	O6-C6-C5	2.18	132.30	126.53
3	A	402	ZIT	O1A-C5-C4	2.17	114.73	111.58
3	A	402	ZIT	O14-C14-C13	2.12	110.62	107.28
3	B	402	ZIT	O14-C14-C13	2.11	110.61	107.28
2	B	401	GMP	C2-N1-C6	2.04	128.81	125.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	ZIT	C4-C5-C6-C7
3	B	402	ZIT	C4-C5-C6-C19
3	A	402	ZIT	C4-C5-C6-C7
3	A	402	ZIT	C4-C5-C6-C19

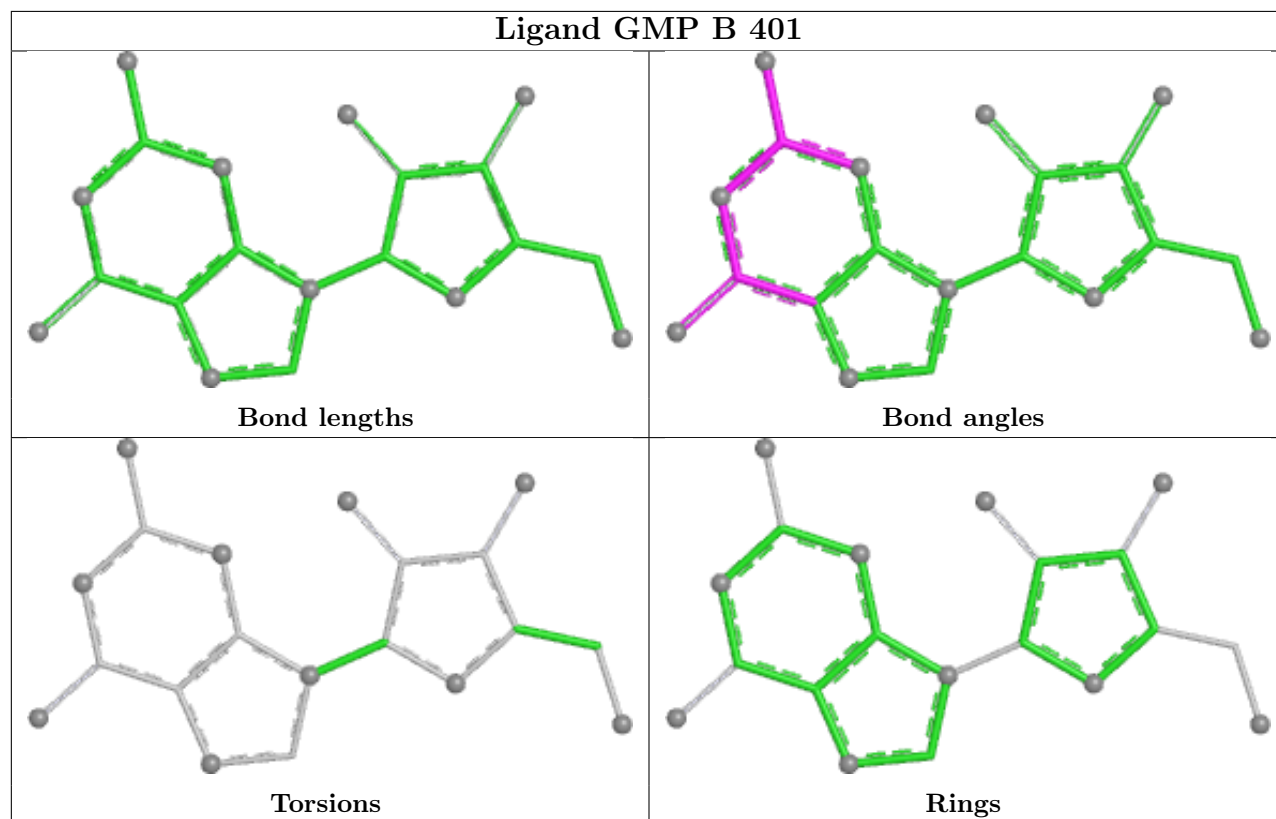
There are no ring outliers.

4 monomers are involved in 34 short contacts:

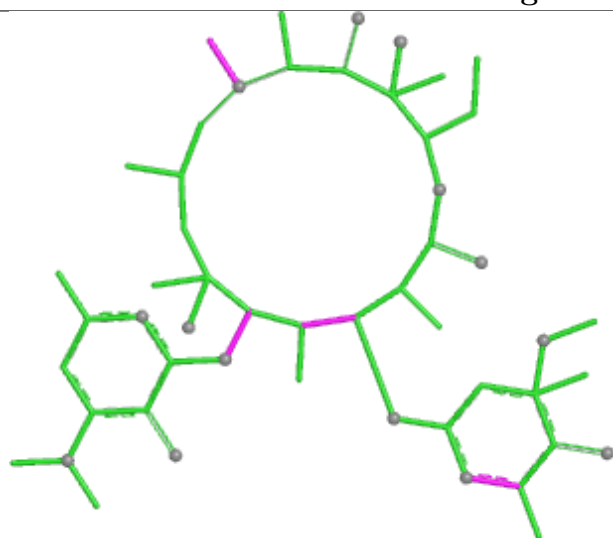
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GMP	1	0
3	A	402	ZIT	18	0
2	A	401	GMP	1	0
3	B	402	ZIT	14	0

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

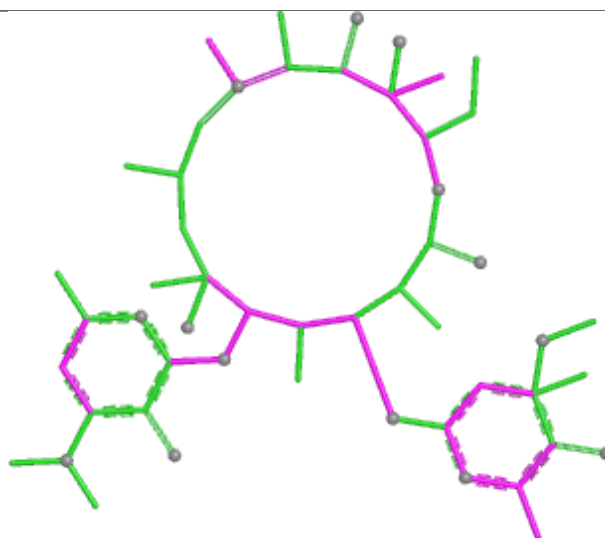
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



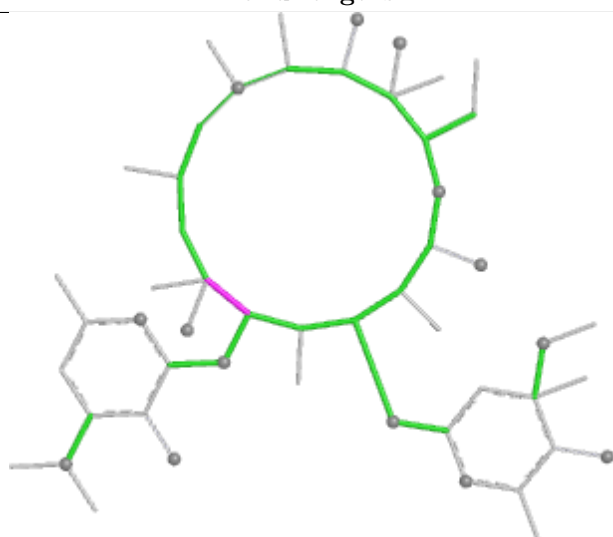
Ligand ZIT A 402



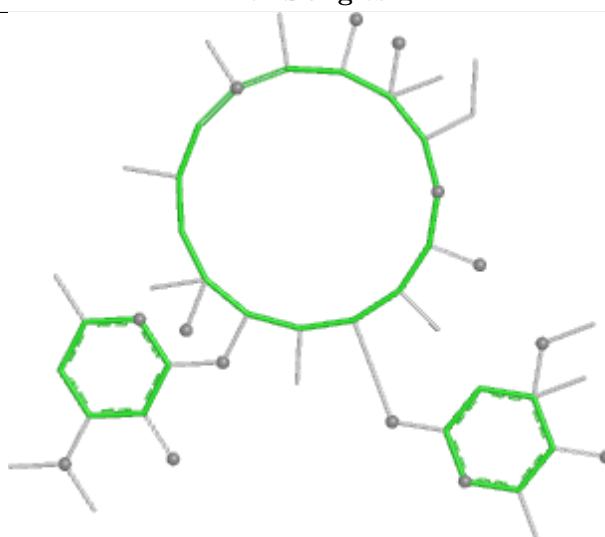
Bond lengths



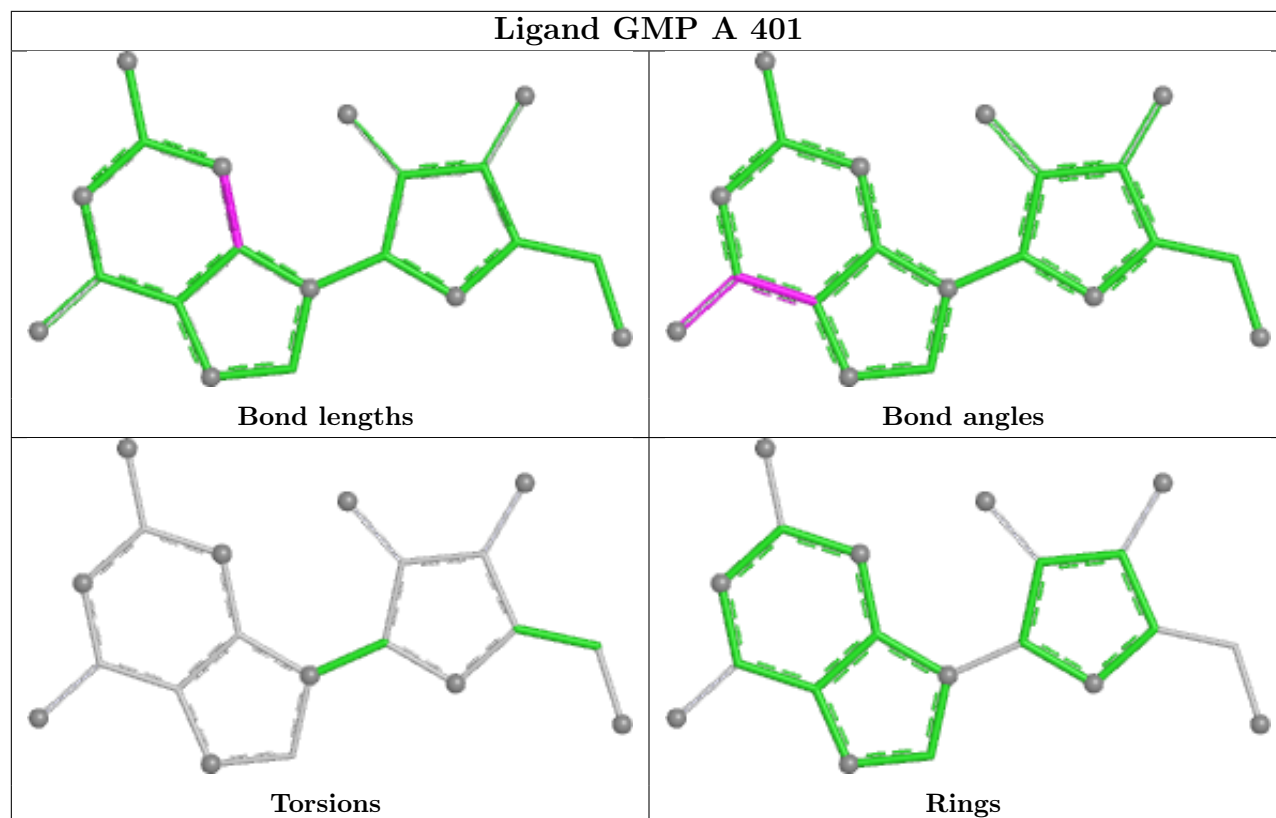
Bond angles

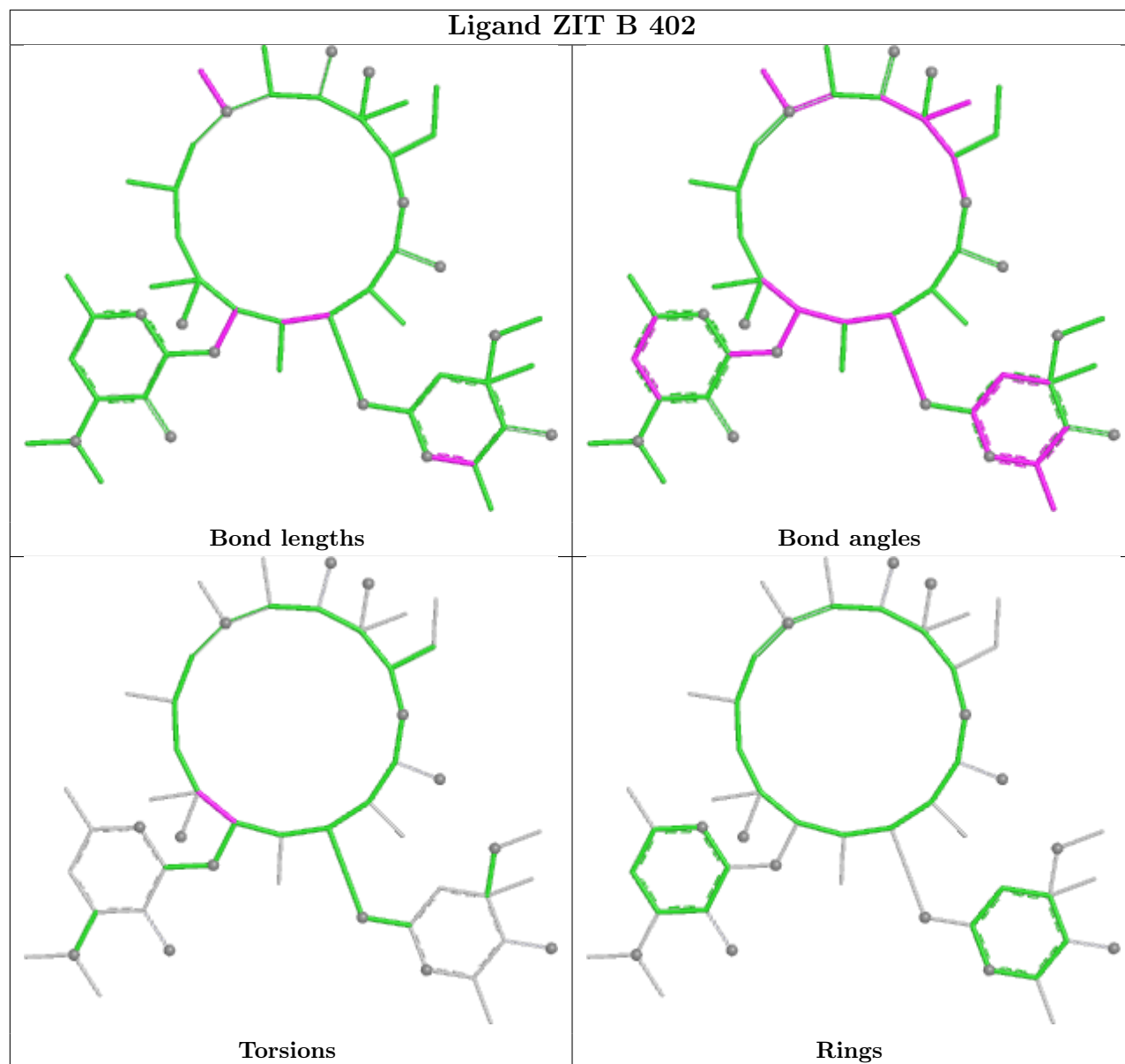


Torsions



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 ⓘ

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	287/302 (95%)	1.28	67 (23%) 2 1	31, 64, 118, 146	0
1	B	287/302 (95%)	1.20	63 (21%) 2 2	30, 58, 102, 135	0
All	All	574/604 (95%)	1.24	130 (22%) 2 2	30, 61, 112, 146	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	VAL	6.7
1	A	273	LEU	6.0
1	B	28	ILE	5.4
1	A	269	LEU	4.7
1	B	288	LYS	4.6
1	A	174	TYR	4.6
1	A	276	LEU	4.5
1	B	205	ASP	4.5
1	A	274	PHE	4.5
1	B	291	LEU	4.3
1	B	164	ILE	4.3
1	A	271	TYR	4.3
1	A	170	LEU	4.2
1	B	21	MET	4.2
1	B	212	ILE	4.2
1	B	187	PHE	4.2
1	B	162	SER	4.1
1	B	161	LYS	4.1
1	B	284	ILE	4.0
1	A	99	LEU	3.9
1	B	271	TYR	3.8
1	B	274	PHE	3.8
1	A	248	LEU	3.8
1	B	174	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	184	TRP	3.7
1	A	265	ALA	3.7
1	A	232	LEU	3.6
1	B	183	LEU	3.6
1	B	170	LEU	3.6
1	B	27	GLY	3.6
1	A	233	PHE	3.6
1	A	264	ALA	3.6
1	B	292	GLY	3.6
1	B	160	VAL	3.5
1	B	185	ALA	3.5
1	A	167	SER	3.5
1	A	242	ILE	3.5
1	A	284	ILE	3.4
1	B	104	TYR	3.4
1	B	52	GLY	3.4
1	A	177	TRP	3.4
1	B	269	LEU	3.3
1	A	108	TRP	3.3
1	A	283	LEU	3.3
1	B	26	MET	3.3
1	A	266	ALA	3.3
1	A	157	LEU	3.3
1	A	114	SER	3.2
1	A	159	LEU	3.2
1	B	149	LEU	3.2
1	B	285	VAL	3.1
1	A	289	ALA	3.1
1	A	234	GLY	3.1
1	A	113	ASP	3.1
1	B	166	ILE	3.1
1	A	227	ALA	3.1
1	A	230	VAL	3.1
1	A	26	MET	3.1
1	B	158	GLN	3.1
1	B	190	PHE	3.0
1	A	101	ALA	3.0
1	A	160	VAL	3.0
1	A	285	VAL	3.0
1	B	286	GLY	3.0
1	B	275	ALA	2.9
1	A	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	161	LYS	2.9
1	A	184	TRP	2.9
1	B	182	VAL	2.8
1	A	153	ILE	2.8
1	B	282	SER	2.8
1	B	273	LEU	2.8
1	B	287	ALA	2.7
1	A	28	ILE	2.7
1	B	289	ALA	2.7
1	B	283	LEU	2.7
1	A	82	SER	2.6
1	A	116	LYS	2.6
1	B	219	ILE	2.6
1	B	100	ASP	2.6
1	A	183	LEU	2.6
1	A	182	VAL	2.6
1	B	272	GLY	2.6
1	A	173	ARG	2.6
1	B	280	ASN	2.5
1	A	231	THR	2.5
1	A	187	PHE	2.5
1	B	179	ASP	2.5
1	A	162	SER	2.5
1	B	159	LEU	2.5
1	B	188	THR	2.4
1	B	226	PHE	2.4
1	A	272	GLY	2.4
1	A	278	THR	2.4
1	B	157	LEU	2.4
1	A	149	LEU	2.4
1	A	112	LYS	2.4
1	A	270	MET	2.4
1	B	222	PRO	2.4
1	B	186	ASP	2.3
1	A	106	ILE	2.3
1	A	229	HIS	2.3
1	B	225	ASP	2.3
1	A	156	ASN	2.3
1	A	104	TYR	2.3
1	A	179	ASP	2.3
1	A	154	ALA	2.3
1	A	181	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	2.3
1	B	281	GLU	2.2
1	B	50	ARG	2.2
1	A	111	ASP	2.2
1	A	79	ARG	2.2
1	A	126	PHE	2.2
1	B	213	ASP	2.2
1	A	252	VAL	2.2
1	B	165	GLY	2.2
1	A	175	ARG	2.2
1	B	221	ASP	2.2
1	B	30	PHE	2.1
1	B	224	ILE	2.1
1	A	256	LEU	2.1
1	A	117	TYR	2.1
1	B	208	VAL	2.1
1	B	178	LEU	2.1
1	B	146	PRO	2.1
1	A	107	ILE	2.1
1	A	241	LEU	2.0
1	B	216	THR	2.0
1	A	140	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZIT	A	402	52/52	0.73	0.25	74,98,109,111	0

Continued on next page...

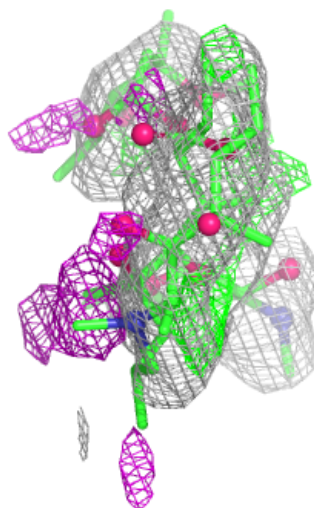
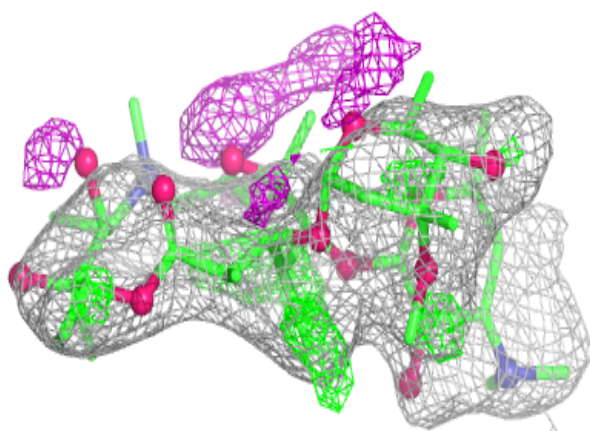
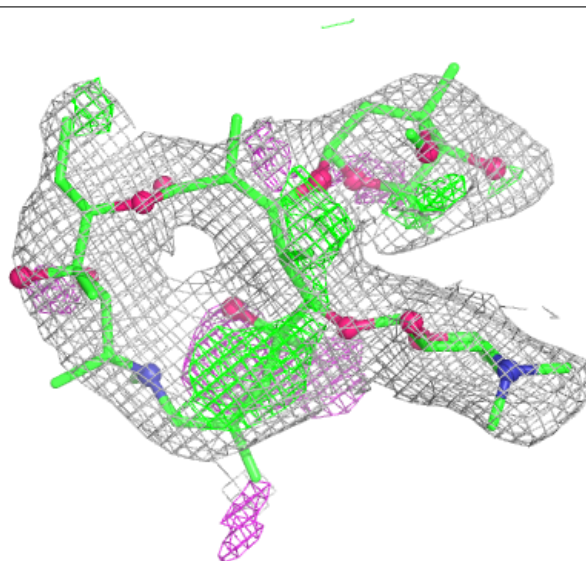
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZIT	B	402	52/52	0.83	0.20	56,75,84,89	0
2	GMP	A	401	20/20	0.93	0.08	38,46,52,53	0
2	GMP	B	401	20/20	0.94	0.08	34,39,52,53	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.

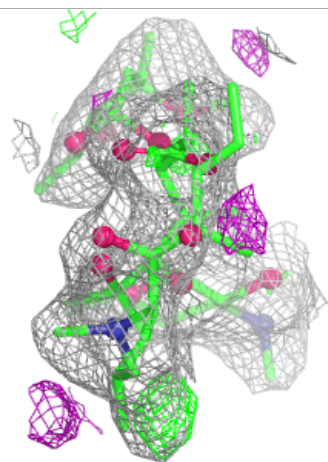
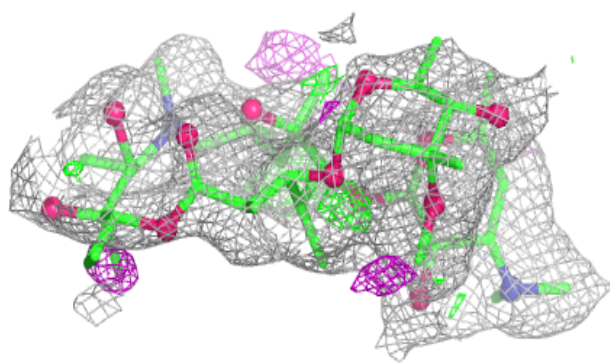
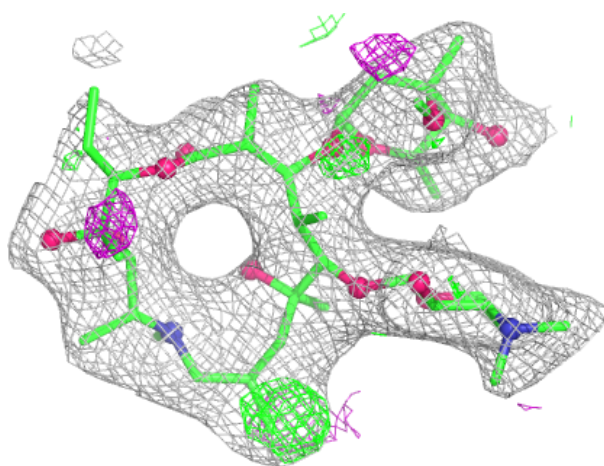
Electron density around ZIT A 402:

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



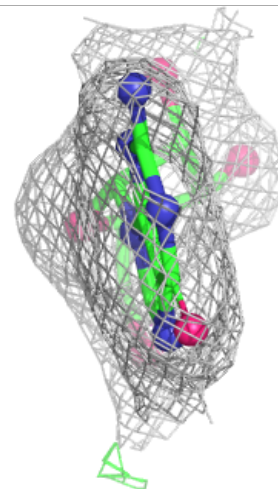
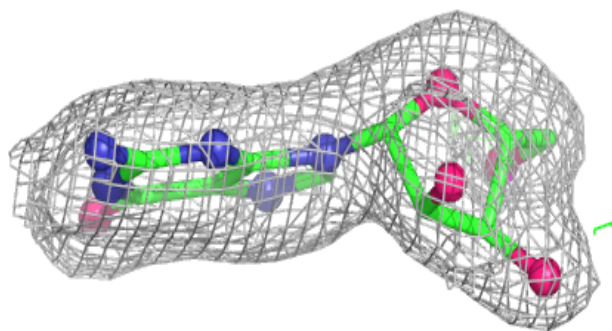
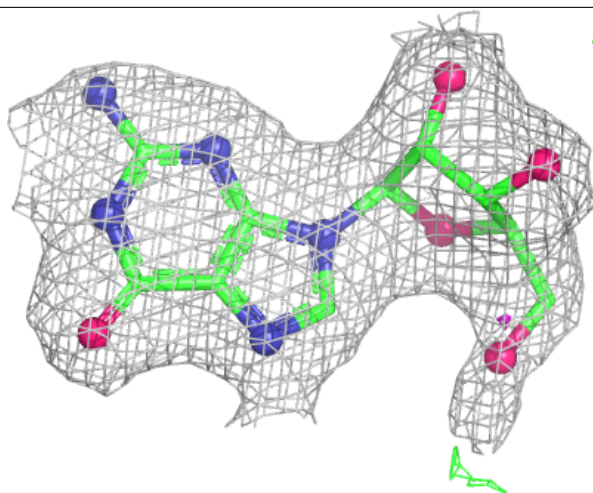
Electron density around ZIT B 402:

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



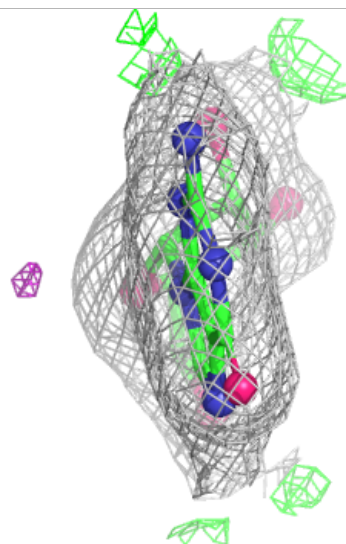
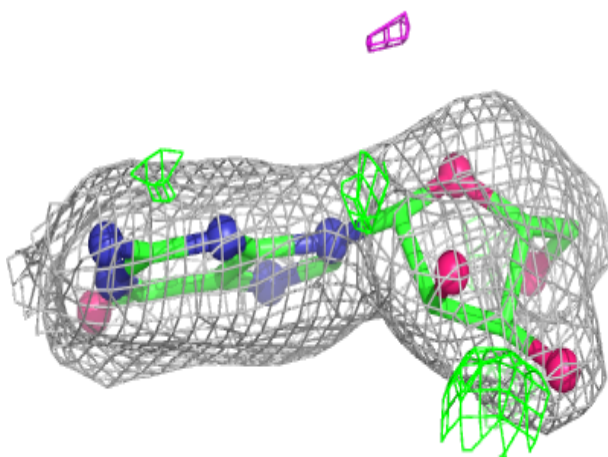
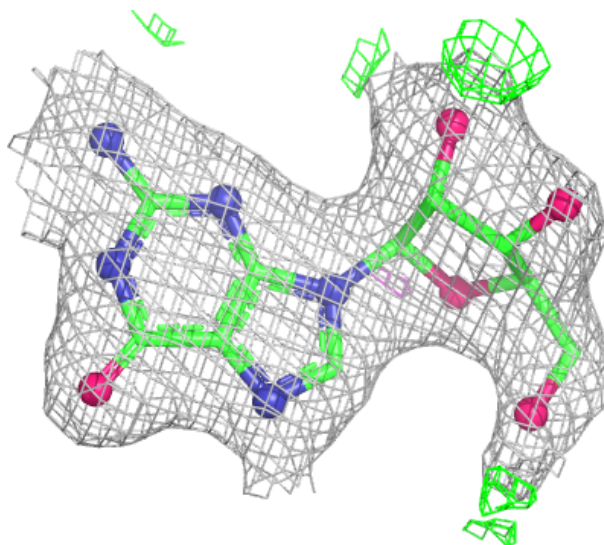
Electron density around GMP A 401:

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



Electron density around GMP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.