



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 4U0X / pdb_00004u0x
Title : Structure of ADC-7 beta-lactamase in complex with boronic acid inhibitor S02030
Authors : Powers, R.A.; Wallar, B.J.; Swanson, H.C.
Deposited on : 2014-07-14
Resolution : 2.03 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

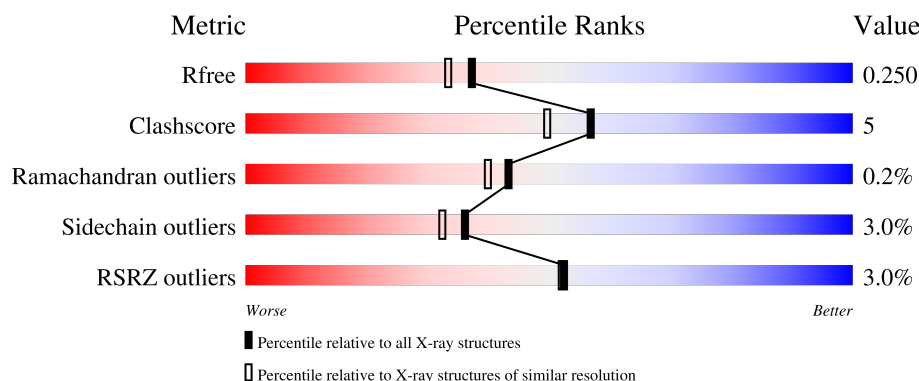
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	360	3% 84% 12% ..
1	B	360	% 90% 10% .
1	C	360	5% 82% 15% ..
1	D	360	3% 86% 10% ..

2 Entry composition [i](#)

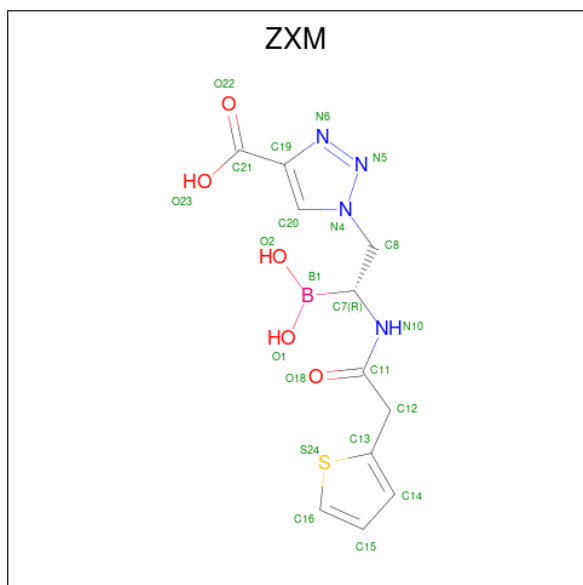
There are 4 unique types of molecules in this entry. The entry contains 12032 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADC-7 beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	358	Total	C	N	O	S	0	8	0
			2876	1850	479	537	10			
1	A	355	Total	C	N	O	S	0	7	0
			2832	1822	466	533	11			
1	C	356	Total	C	N	O	S	0	6	0
			2792	1790	465	527	10			
1	D	352	Total	C	N	O	S	0	5	0
			2757	1771	456	520	10			

- Molecule 2 is 1-{(2R)-2-(dihydroxyboranyl)-2-[(thiophen-2-ylacetyl)amino]ethyl}-1H-1,2,3-tiazole-4-carboxylic acid (CCD ID: ZXM) (formula: C₁₁H₁₃BN₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	B	C	N	O	S	0
			22	1	11	4	5	1	0
2	A	1	Total	B	C	N	O	S	0
			27	1	15	4	5	2	1

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	B	C	N	O	S	0	0
			22	1	11	4	5	1		
2	D	1	Total	B	C	N	O	S	0	0
			22	1	11	4	5	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		

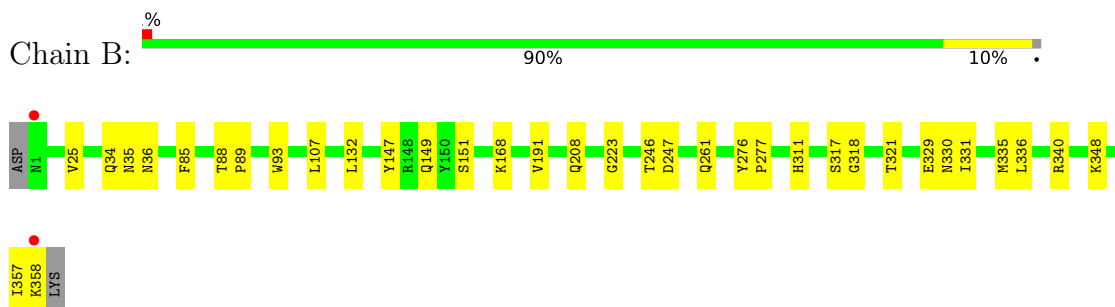
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	279	Total	O	0	4
			283	283		
4	A	152	Total	O	0	1
			153	153		
4	C	131	Total	O	0	2
			133	133		
4	D	106	Total	O	0	2
			108	108		

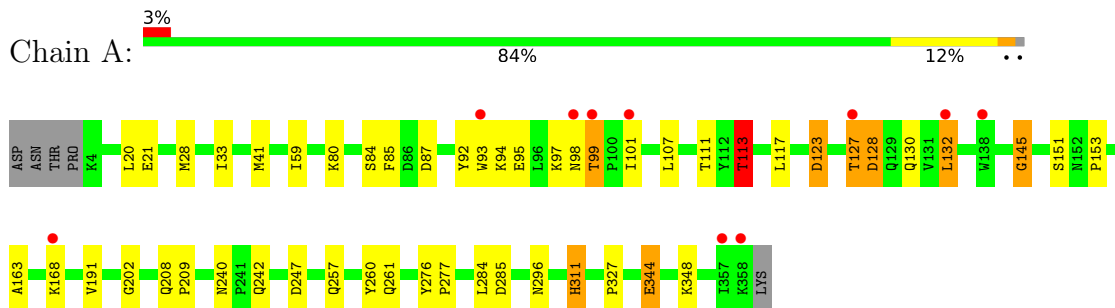
3 Residue-property plots

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.

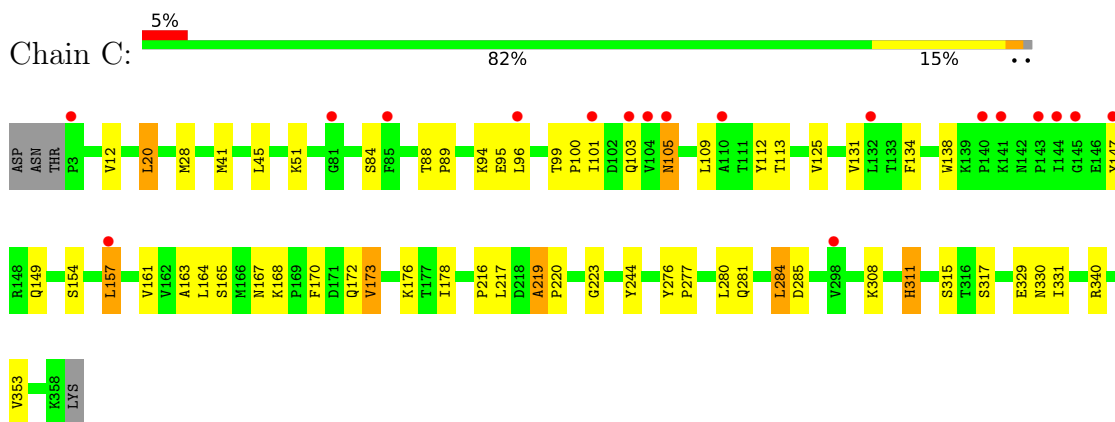
- Molecule 1: ADC-7 beta-lactamase



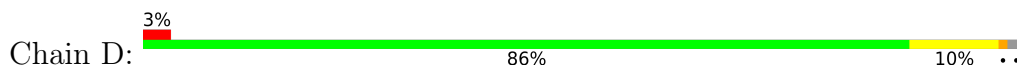
- Molecule 1: ADC-7 beta-lactamase

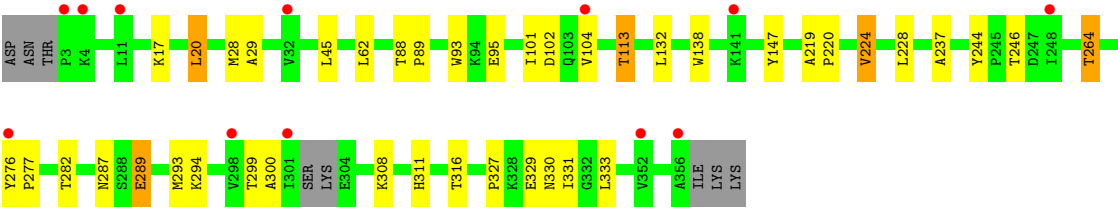


- Molecule 1: ADC-7 beta-lactamase



- Molecule 1: ADC-7 beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.27Å 81.20Å 106.33Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.03 50.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.03) 100.0 (50.00-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.185 , 0.248 0.194 , 0.250	Depositor DCC
R_{free} test set	4563 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12032	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3622e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZXM, PO4

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	1.16	3/2902 (0.1%)	1.15	12/3947 (0.3%)
1	B	1.24	4/2952 (0.1%)	1.12	7/4007 (0.2%)
1	C	1.06	0/2860	1.09	6/3896 (0.2%)
1	D	0.98	0/2827	1.06	9/3851 (0.2%)
All	All	1.12	7/11541 (0.1%)	1.11	34/15701 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	GLY	C-O	-6.80	1.19	1.24
1	B	25	VAL	N-CA	6.39	1.51	1.46
1	B	317	SER	C-O	-6.25	1.16	1.24
1	B	335	MET	N-CA	5.89	1.53	1.46
1	A	113	THR	CB-CG2	-5.34	1.34	1.52
1	A	59	ILE	C-O	5.18	1.29	1.24
1	A	153	PRO	C-O	-5.02	1.17	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	GLN	CA-C-N	8.99	129.34	119.90
1	A	208	GLN	C-N-CA	8.99	129.34	119.90
1	A	151	SER	N-CA-C	7.52	121.07	108.13
1	B	168	LYS	CA-C-N	-6.93	113.17	120.03
1	B	168	LYS	C-N-CA	-6.93	113.17	120.03
1	D	17	LYS	CA-C-N	-6.56	113.05	119.87
1	D	17	LYS	C-N-CA	-6.56	113.05	119.87
1	D	45	LEU	CA-C-N	5.97	128.27	120.28
1	D	45	LEU	C-N-CA	5.97	128.27	120.28
1	A	145	GLY	N-CA-C	-5.87	106.43	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	ASN	N-CA-C	5.83	120.20	113.38
1	D	228	LEU	CA-C-N	-5.77	112.64	119.05
1	D	228	LEU	C-N-CA	-5.77	112.64	119.05
1	A	191	VAL	CA-C-N	-5.72	114.36	120.03
1	A	191	VAL	C-N-CA	-5.72	114.36	120.03
1	A	240	ASN	CB-CA-C	-5.71	103.53	111.41
1	D	113	THR	N-CA-C	5.60	119.11	112.72
1	C	45	LEU	CA-C-N	5.60	128.24	120.29
1	C	45	LEU	C-N-CA	5.60	128.24	120.29
1	C	353	VAL	N-CA-C	5.55	116.19	110.36
1	C	178	ILE	N-CA-C	5.50	115.74	110.74
1	B	147	TYR	N-CA-C	5.46	117.80	108.90
1	A	285	ASP	N-CA-C	5.38	117.15	111.28
1	B	191	VAL	N-CA-C	-5.35	104.03	108.63
1	B	151	SER	N-CA-C	5.28	117.21	108.13
1	A	99	THR	N-CA-C	-5.23	103.35	110.36
1	A	33	ILE	CB-CA-C	5.17	118.28	110.63
1	C	219	ALA	CA-C-N	-5.13	114.38	119.56
1	C	219	ALA	C-N-CA	-5.13	114.38	119.56
1	A	240	ASN	N-CA-C	5.13	116.94	109.30
1	A	348	LYS	N-CA-C	5.11	116.54	111.07
1	D	246	THR	N-CA-C	5.07	116.50	111.07
1	B	25	VAL	CB-CA-C	-5.05	105.31	110.71
1	D	316	THR	N-CA-C	-5.03	102.45	109.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2832	0	2788	29	0
1	B	2876	0	2878	17	0
1	C	2792	0	2688	36	0
1	D	2757	0	2660	23	0
2	A	27	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	12	1	0
2	C	22	0	12	0	0
2	D	22	0	12	0	0
3	C	5	0	0	1	0
4	A	153	0	0	5	0
4	B	283	0	0	5	0
4	C	133	0	0	3	0
4	D	108	0	0	1	0
All	All	12032	0	11060	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:HD12	1:D:224:VAL:HG23	1.61	0.81
1:A:20:LEU:HD11	1:A:28[A]:MET:HE2	1.65	0.79
1:B:357:ILE:O	1:B:358[B]:LYS:HB2	1.89	0.71
1:C:96:LEU:O	1:C:99:THR:OG1	2.09	0.70
1:A:113:THR:HG23	1:A:145:GLY:HA2	1.74	0.69
1:C:20:LEU:HD11	1:C:28[B]:MET:HE2	1.74	0.69
1:A:99:THR:OG1	1:A:101:ILE:HG22	1.96	0.66
1:C:113:THR:HA	1:C:147:TYR:O	1.96	0.65
1:A:127:THR:HG23	1:A:130:GLN:H	1.62	0.63
1:C:217:LEU:O	1:C:220:PRO:HD2	2.00	0.62
1:D:287:ASN:HB3	4:D:606:HOH:O	1.99	0.62
1:C:170:PHE:HA	1:C:173:VAL:HG13	1.82	0.62
1:D:62:LEU:HD12	1:D:224:VAL:CG2	2.31	0.61
1:A:344[A]:GLU:H	1:A:344[A]:GLU:CD	2.08	0.61
1:D:20:LEU:HD11	1:D:28[A]:MET:HE2	1.84	0.60
1:D:276:TYR:CD1	1:D:277:PRO:HA	2.35	0.60
1:A:127:THR:HG21	4:A:650:HOH:O	2.01	0.60
1:D:299:THR:HG22	1:D:300:ALA:O	2.02	0.60
1:C:12:VAL:HG21	1:C:41:MET:HE3	1.83	0.60
1:A:80:LYS:NZ	1:A:247:ASP:OD1	2.34	0.59
1:A:127:THR:HG23	1:A:130:GLN:CB	2.32	0.59
1:C:163:ALA:HB1	1:C:168:LYS:O	2.03	0.57
1:C:317[A]:SER:HB2	4:C:625:HOH:O	2.04	0.57
1:D:264:THR:HB	1:D:282:THR:HG23	1.88	0.56
1:C:317[B]:SER:HB3	4:C:625:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TYR:HB3	1:C:149:GLN:O	2.08	0.54
1:C:20:LEU:CD1	1:C:28[B]:MET:HE2	2.38	0.53
1:A:128:ASP:OD1	1:A:128:ASP:N	2.40	0.53
1:D:88:THR:HG21	1:D:102:ASP:O	2.09	0.52
1:C:105[A]:ASN:OD1	1:C:105[A]:ASN:N	2.28	0.52
1:D:88:THR:HG22	1:D:104:VAL:O	2.10	0.52
1:C:281:GLN:NE2	1:C:285:ASP:OD1	2.42	0.52
1:A:123:ASP:N	1:A:123:ASP:OD1	2.40	0.51
1:C:101:ILE:HA	1:C:138:TRP:CZ3	2.45	0.51
1:C:100:PRO:HB2	1:C:138:TRP:O	2.10	0.50
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.46	0.50
1:A:163:ALA:HB1	1:A:168[C]:LYS:O	2.11	0.50
1:D:294:LYS:HE2	1:D:294:LYS:HA	1.94	0.50
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.46	0.50
1:D:28[B]:MET:HG2	1:D:29:ALA:N	2.27	0.50
1:A:163:ALA:HB1	1:A:168[A]:LYS:O	2.12	0.49
1:C:95:GLU:N	1:C:95:GLU:OE2	2.44	0.49
1:A:20:LEU:HD11	1:A:28[A]:MET:CE	2.41	0.49
1:A:261:GLN:NE2	4:A:640:HOH:O	2.30	0.49
1:C:96:LEU:C	1:C:99:THR:HG1	2.18	0.49
1:D:219:ALA:HB3	1:D:220:PRO:HD3	1.96	0.48
1:A:111:THR:O	1:A:260:TYR:OH	2.23	0.48
1:C:101:ILE:HA	1:C:138:TRP:CE3	2.49	0.48
1:B:261:GLN:CD	4:B:728:HOH:O	2.57	0.48
1:C:164:LEU:O	1:C:167:ASN:N	2.32	0.48
1:C:131:VAL:O	1:C:134:PHE:HB3	2.13	0.47
1:C:276:TYR:HA	1:C:277:PRO:C	2.39	0.47
1:C:315:SER:HB3	1:C:340:ARG:HD3	1.95	0.47
1:A:93:TRP:CZ2	1:A:132:LEU:HG	2.50	0.47
1:A:113:THR:HG21	4:A:532:HOH:O	2.14	0.46
1:B:93:TRP:CE2	1:B:132:LEU:HD13	2.50	0.46
1:C:219:ALA:HA	1:C:223:GLY:HA3	1.98	0.46
1:D:88:THR:HB	1:D:89:PRO:HD2	1.96	0.46
1:D:333:LEU:C	1:D:333:LEU:HD23	2.41	0.46
1:A:163:ALA:HB1	1:A:168[B]:LYS:O	2.15	0.46
1:B:261:GLN:CG	4:B:728:HOH:O	2.64	0.45
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.97	0.45
1:B:88:THR:HB	1:B:89:PRO:HD2	1.98	0.45
1:B:208[A]:GLN:OE1	1:C:51:LYS:HA	2.16	0.45
1:B:247:ASP:HB2	4:B:516:HOH:O	2.16	0.45
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASN:HA	1:B:330:ASN:ND2	2.33	0.44
1:A:311:HIS:CD2	1:A:311:HIS:C	2.95	0.44
1:D:93:TRP:CZ2	1:D:132:LEU:HD13	2.52	0.44
1:C:109:LEU:O	1:C:154:SER:OG	2.32	0.44
1:A:85:PHE:HB3	1:A:107:LEU:HB2	2.00	0.44
1:D:329:GLU:HB2	1:D:331:ILE:HG22	1.99	0.44
1:B:321:THR:HG23	1:B:336:LEU:HD23	1.99	0.44
1:B:223:GLY:HA2	4:B:746:HOH:O	2.17	0.44
1:B:276:TYR:CD1	1:B:277:PRO:HA	2.52	0.44
1:D:101:ILE:HD13	1:D:138:TRP:CD2	2.54	0.43
1:B:340:ARG:NH2	4:B:760[B]:HOH:O	2.52	0.43
1:A:117:LEU:N	4:A:599:HOH:O	2.48	0.43
1:C:280:LEU:HG	1:C:284:LEU:CD2	2.48	0.42
1:B:340:ARG:NH2	2:B:401:ZXM:N6	2.67	0.42
1:D:289[A]:GLU:OE1	1:D:293:MET:HB2	2.19	0.42
1:B:34:GLN:O	1:B:35:ASN:C	2.62	0.42
1:B:329:GLU:HB2	1:B:331:ILE:HG22	2.01	0.42
1:A:21:GLU:HG3	4:A:568:HOH:O	2.19	0.42
1:A:127:THR:HG23	1:A:130:GLN:N	2.32	0.42
1:A:284:LEU:HD22	1:A:344[A]:GLU:HB3	2.01	0.42
1:C:172:GLN:HB3	1:C:176:LYS:HD2	2.00	0.42
1:C:157:LEU:O	1:C:161:VAL:HG23	2.20	0.42
1:B:358[A]:LYS:HB3	1:B:358[A]:LYS:HE3	1.85	0.42
1:A:202:GLY:O	1:A:209:PRO:HA	2.20	0.42
1:C:94:LYS:CB	4:C:626:HOH:O	2.68	0.42
1:C:244:TYR:OH	3:C:402:PO4:O1	2.38	0.42
1:D:289[A]:GLU:OE1	1:D:289[A]:GLU:C	2.63	0.41
1:D:308:LYS:O	1:D:327:PRO:HD2	2.20	0.41
1:D:237:ALA:HA	1:D:244:TYR:CE1	2.55	0.41
1:A:113:THR:CG2	1:A:145:GLY:HA2	2.48	0.41
1:C:88:THR:HB	1:C:89:PRO:HD2	2.01	0.41
1:C:329:GLU:HB2	1:C:331:ILE:HG22	2.03	0.41
1:D:289[A]:GLU:OE1	1:D:289[A]:GLU:O	2.38	0.41
1:A:93:TRP:O	1:A:94:LYS:C	2.64	0.41
1:C:125:VAL:O	1:C:216:PRO:HG3	2.21	0.40
1:D:113:THR:HA	1:D:147:TYR:O	2.21	0.40
1:C:311:HIS:CD2	1:C:311:HIS:C	2.98	0.40
1:C:99:THR:CG2	1:C:100:PRO:HD2	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	361/360 (100%)	342 (95%)	16 (4%)	3 (1%)	16	8
1	B	362/360 (101%)	352 (97%)	10 (3%)	0	100	100
1	C	360/360 (100%)	345 (96%)	15 (4%)	0	100	100
1	D	353/360 (98%)	344 (98%)	9 (2%)	0	100	100
All	All	1436/1440 (100%)	1383 (96%)	50 (4%)	3 (0%)	43	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	98	ASN
1	A	97	LYS

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	307/318 (96%)	292 (95%)	15 (5%)	22	15
1	B	316/318 (99%)	312 (99%)	4 (1%)	61	63
1	C	295/318 (93%)	283 (96%)	12 (4%)	27	20
1	D	292/318 (92%)	284 (97%)	8 (3%)	39	37
All	All	1210/1272 (95%)	1171 (97%)	39 (3%)	36	30

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	149	GLN
1	B	246	THR
1	B	311	HIS
1	B	348	LYS
1	A	41[A]	MET
1	A	41[B]	MET
1	A	84	SER
1	A	113	THR
1	A	123	ASP
1	A	127	THR
1	A	128	ASP
1	A	132	LEU
1	A	242	GLN
1	A	257	GLN
1	A	296	ASN
1	A	311	HIS
1	A	327	PRO
1	A	344[A]	GLU
1	A	344[B]	GLU
1	C	20	LEU
1	C	84	SER
1	C	103	GLN
1	C	105[A]	ASN
1	C	105[B]	ASN
1	C	157	LEU
1	C	165	SER
1	C	173	VAL
1	C	284	LEU
1	C	308	LYS
1	C	311	HIS
1	C	330	ASN
1	D	20	LEU
1	D	95	GLU
1	D	224	VAL
1	D	264	THR
1	D	289[A]	GLU
1	D	289[B]	GLU
1	D	311	HIS
1	D	330	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	ASN
1	B	186	HIS
1	B	198	ASN
1	B	238	ASN
1	B	330	ASN
1	A	36	ASN
1	A	126	GLN
1	A	186	HIS
1	A	195	GLN
1	A	198	ASN
1	A	240	ASN
1	A	242	GLN
1	A	249	GLN
1	A	253	ASN
1	A	287	ASN
1	A	343	ASN
1	C	149	GLN
1	C	195	GLN
1	C	198	ASN
1	C	205	GLN
1	C	281	GLN
1	D	103	GLN
1	D	261	GLN
1	D	287	ASN
1	D	290	GLN
1	D	296	ASN
1	D	330	ASN

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

6 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	ZXM	A	401[A]	-	20,23,23	1.99	4 (20%)	24,31,31	2.38	10 (41%)
2	ZXM	A	401[B]	-	20,23,23	1.95	4 (20%)	24,31,31	2.51	10 (41%)
2	ZXM	B	401	1	20,23,23	1.85	4 (20%)	24,31,31	1.88	8 (33%)
2	ZXM	C	401	1	20,23,23	1.71	3 (15%)	24,31,31	2.15	10 (41%)
3	PO4	C	402	-	4,4,4	0.62	0	6,6,6	0.84	0
2	ZXM	D	401	1	20,23,23	1.86	2 (10%)	24,31,31	1.61	4 (16%)

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	ZXM	A	401[A]	-	-	0/14/20/20	0/2/2/2
2	ZXM	A	401[B]	-	-	2/14/20/20	0/2/2/2
2	ZXM	B	401	1	-	5/14/20/20	0/2/2/2
2	ZXM	C	401	1	-	6/14/20/20	0/2/2/2
2	ZXM	D	401	1	-	5/14/20/20	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ZXM	N6-N5	6.01	1.41	1.32
2	B	401	ZXM	N6-N5	5.68	1.41	1.32
2	C	401	ZXM	N6-N5	5.63	1.41	1.32
2	A	401[A]	ZXM	N6-N5	5.13	1.40	1.32
2	A	401[B]	ZXM	N6-N5	5.13	1.40	1.32
2	D	401	ZXM	N4-N5	4.17	1.41	1.34
2	A	401[A]	ZXM	C19-C21	3.95	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	ZXM	C19-C21	3.95	1.52	1.48
2	A	401[A]	ZXM	C20-C19	3.73	1.41	1.37
2	A	401[B]	ZXM	C20-C19	3.73	1.41	1.37
2	C	401	ZXM	N4-N5	3.39	1.40	1.34
2	B	401	ZXM	N4-N5	2.95	1.39	1.34
2	A	401[A]	ZXM	N4-N5	2.64	1.39	1.34
2	A	401[B]	ZXM	N4-N5	2.64	1.39	1.34
2	C	401	ZXM	O23-C21	-2.15	1.24	1.30
2	B	401	ZXM	C8-N4	-2.05	1.42	1.46
2	B	401	ZXM	O22-C21	2.05	1.27	1.22

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	ZXM	O23-C21-C19	5.15	121.66	113.40
2	A	401[B]	ZXM	O23-C21-C19	5.15	121.66	113.40
2	A	401[B]	ZXM	C12-C13-S24	-4.93	111.67	122.11
2	C	401	ZXM	O23-C21-C19	4.81	121.12	113.40
2	A	401[A]	ZXM	C8-N4-N5	-4.55	111.48	120.28
2	A	401[B]	ZXM	C8-N4-N5	-4.55	111.48	120.28
2	A	401[A]	ZXM	C8-N4-C20	4.43	138.59	129.27
2	A	401[B]	ZXM	C8-N4-C20	4.43	138.59	129.27
2	C	401	ZXM	O22-C21-C19	-4.26	115.29	122.02
2	D	401	ZXM	C21-C19-N6	4.25	129.74	122.64
2	A	401[A]	ZXM	C11-C12-C13	-4.20	100.09	111.92
2	B	401	ZXM	N4-N5-N6	-3.99	103.43	107.02
2	D	401	ZXM	C20-C19-C21	-3.74	120.74	128.20
2	A	401[B]	ZXM	C11-C12-C13	3.56	121.95	111.92
2	A	401[B]	ZXM	C12-C13-C14	3.41	136.50	126.56
2	B	401	ZXM	O18-C11-C12	-3.14	116.45	121.40
2	D	401	ZXM	N4-N5-N6	-3.13	104.20	107.02
2	A	401[A]	ZXM	O22-C21-C19	-3.01	117.27	122.02
2	A	401[B]	ZXM	O22-C21-C19	-3.01	117.27	122.02
2	C	401	ZXM	C20-C19-C21	-3.01	122.20	128.20
2	A	401[A]	ZXM	O18-C11-C12	-2.99	116.69	121.40
2	A	401[B]	ZXM	O18-C11-C12	-2.99	116.69	121.40
2	B	401	ZXM	C20-N4-N5	2.98	113.66	110.75
2	C	401	ZXM	O18-C11-C12	-2.83	116.93	121.40
2	C	401	ZXM	C12-C13-S24	-2.73	116.32	122.11
2	C	401	ZXM	C20-C19-N6	2.68	111.01	108.33
2	B	401	ZXM	C21-C19-N6	2.66	127.08	122.64
2	B	401	ZXM	C20-C19-C21	-2.66	122.90	128.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ZXM	C12-C13-C14	2.64	134.26	126.56
2	B	401	ZXM	O18-C11-N10	2.64	127.42	122.95
2	A	401[A]	ZXM	C12-C13-C14	2.59	134.11	126.56
2	C	401	ZXM	C19-N6-N5	-2.59	106.64	108.84
2	A	401[A]	ZXM	C12-C13-S24	-2.52	116.78	122.11
2	C	401	ZXM	N4-N5-N6	-2.49	104.78	107.02
2	D	401	ZXM	C19-C20-N4	2.46	107.41	104.95
2	C	401	ZXM	C21-C19-N6	2.45	126.73	122.64
2	B	401	ZXM	O22-C21-C19	-2.37	118.28	122.02
2	A	401[A]	ZXM	O18-C11-N10	2.25	126.77	122.95
2	A	401[B]	ZXM	O18-C11-N10	2.25	126.77	122.95
2	B	401	ZXM	C8-N4-N5	-2.23	115.98	120.28
2	A	401[A]	ZXM	C19-C20-N4	2.22	107.17	104.95
2	A	401[B]	ZXM	C19-C20-N4	2.22	107.17	104.95

There are no chirality outliers.

All (18) torsion outliers are listed below:

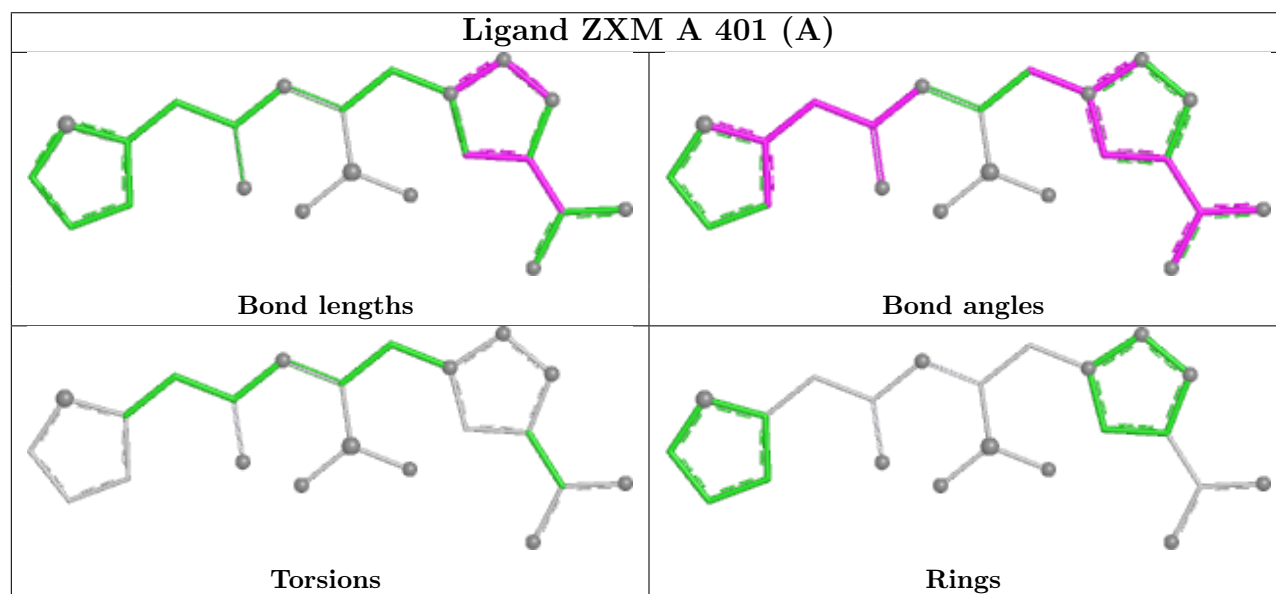
Mol	Chain	Res	Type	Atoms
2	B	401	ZXM	N10-C7-C8-N4
2	B	401	ZXM	N6-C19-C21-O23
2	A	401[B]	ZXM	C11-C12-C13-S24
2	C	401	ZXM	N10-C7-C8-N4
2	C	401	ZXM	N6-C19-C21-O22
2	C	401	ZXM	N6-C19-C21-O23
2	C	401	ZXM	C20-C19-C21-O22
2	C	401	ZXM	C20-C19-C21-O23
2	D	401	ZXM	N6-C19-C21-O22
2	D	401	ZXM	N6-C19-C21-O23
2	D	401	ZXM	C20-C19-C21-O22
2	D	401	ZXM	C20-C19-C21-O23
2	B	401	ZXM	N6-C19-C21-O22
2	A	401[B]	ZXM	C11-C12-C13-C14
2	D	401	ZXM	C8-C7-N10-C11
2	B	401	ZXM	C20-C19-C21-O23
2	C	401	ZXM	O18-C11-C12-C13
2	B	401	ZXM	C20-C19-C21-O22

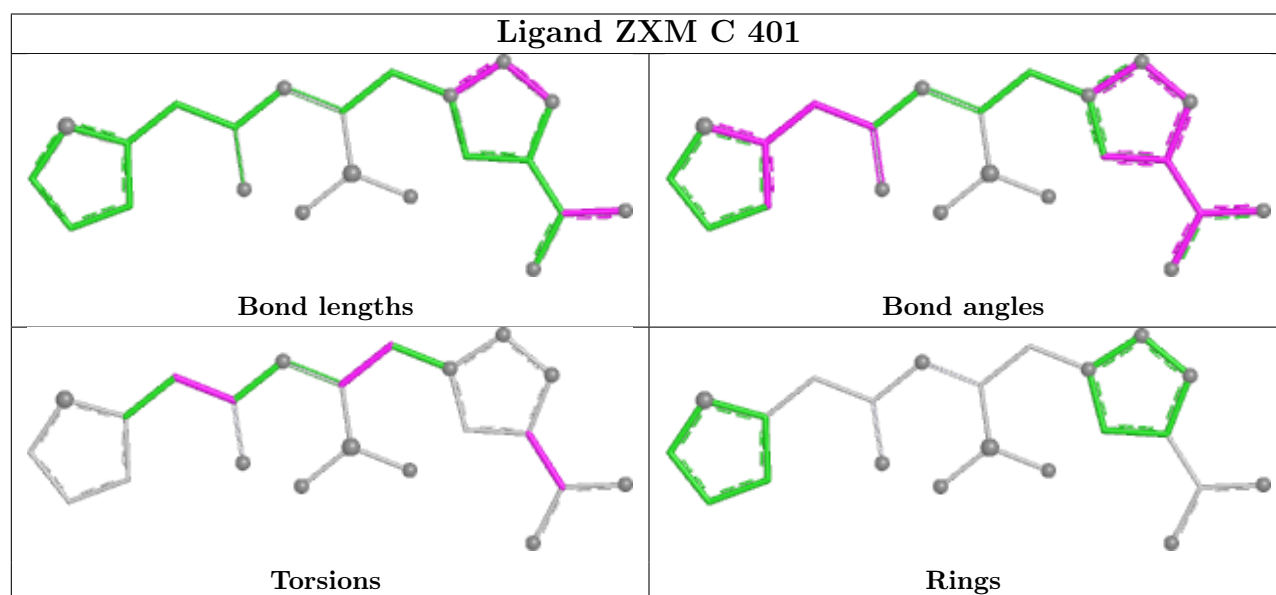
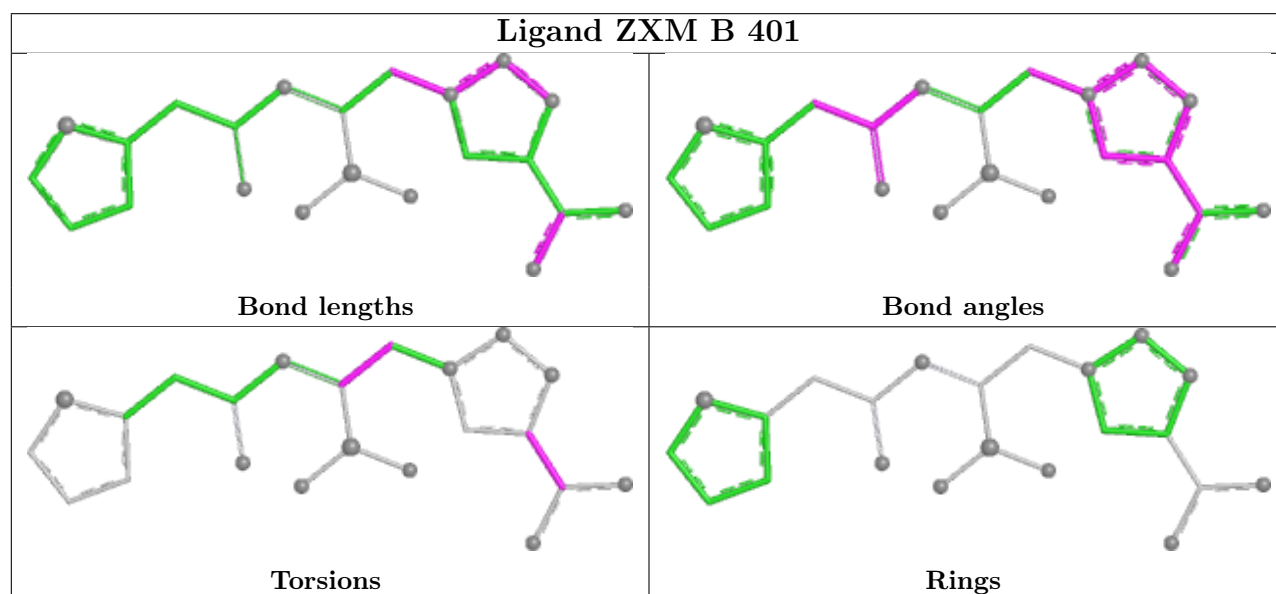
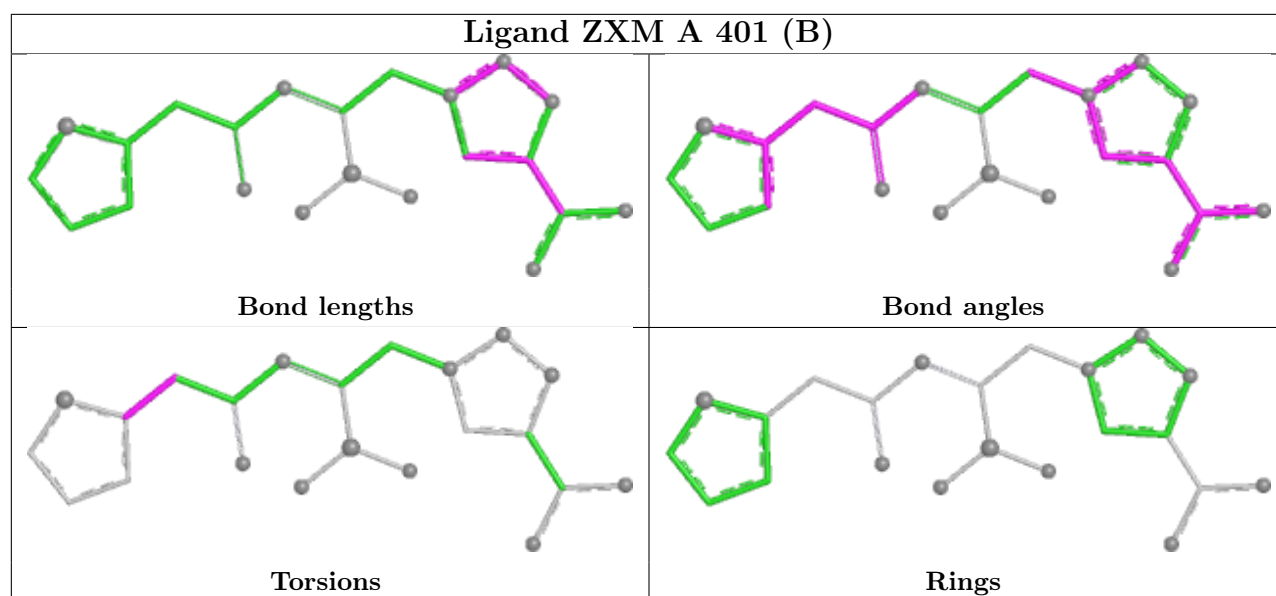
There are no ring outliers.

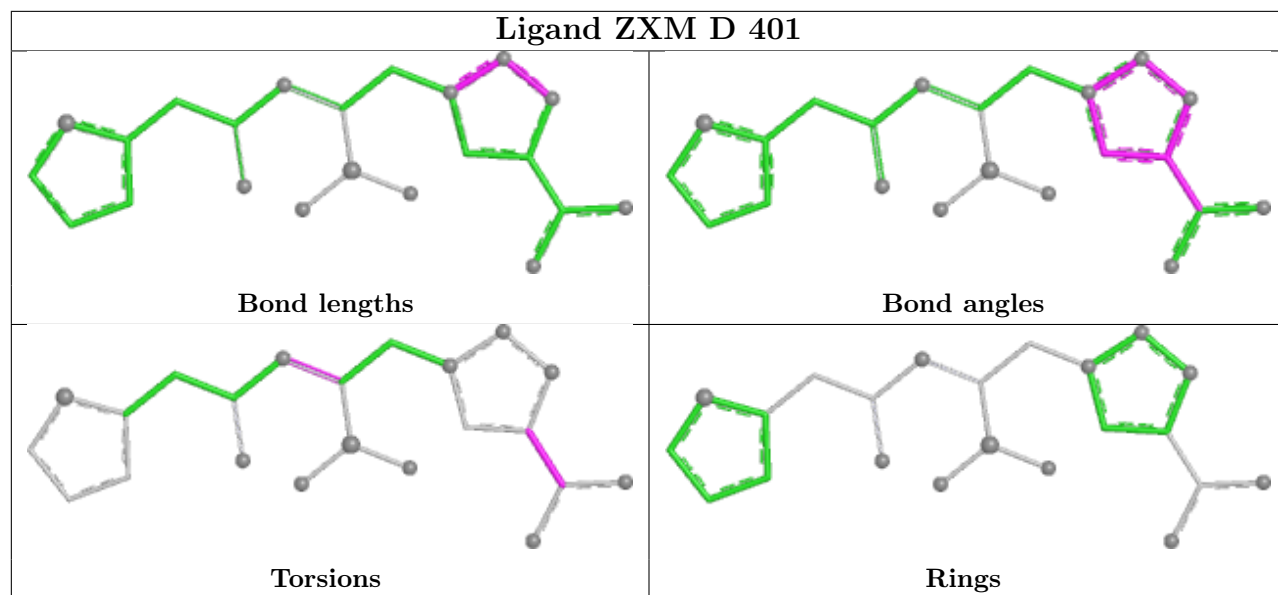
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ZXM	1	0
3	C	402	PO4	1	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	355/360 (98%)	0.06	10 (2%) 55 54	12, 29, 52, 64	7 (1%)
1	B	358/360 (99%)	-0.50	2 (0%) 85 86	10, 22, 35, 46	8 (2%)
1	C	356/360 (98%)	0.39	18 (5%) 33 33	10, 37, 63, 75	6 (1%)
1	D	352/360 (97%)	0.43	12 (3%) 48 47	13, 41, 58, 83	5 (1%)
All	All	1421/1440 (98%)	0.09	42 (2%) 52 52	10, 31, 57, 83	26 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	301	ILE	4.6
1	B	1[A]	ASN	4.5
1	C	3	PRO	3.7
1	C	145	GLY	3.2
1	C	144	ILE	3.2
1	C	140	PRO	3.1
1	C	101	ILE	3.1
1	A	168[A]	LYS	2.8
1	A	358	LYS	2.8
1	B	358[A]	LYS	2.8
1	A	132	LEU	2.8
1	D	3	PRO	2.7
1	A	101	ILE	2.6
1	A	357	ILE	2.6
1	D	141[A]	LYS	2.6
1	C	104	VAL	2.6
1	C	132	LEU	2.5
1	D	352	VAL	2.5
1	C	85	PHE	2.4
1	C	105[A]	ASN	2.4
1	D	32	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	248	ILE	2.3
1	D	298	VAL	2.3
1	A	98	ASN	2.3
1	C	96	LEU	2.3
1	A	127	THR	2.3
1	C	298	VAL	2.3
1	D	11	LEU	2.3
1	D	356	ALA	2.2
1	A	93	TRP	2.2
1	C	103	GLN	2.2
1	C	81	GLY	2.2
1	C	141	LYS	2.2
1	C	157	LEU	2.1
1	C	110	ALA	2.1
1	A	99	THR	2.0
1	D	4	LYS	2.0
1	D	104	VAL	2.0
1	A	138	TRP	2.0
1	C	143	PRO	2.0
1	C	147	TYR	2.0
1	D	276	TYR	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($\text{\AA}^2$)	Q<0.9
3	PO4	C	402	5/5	0.78	0.11	49,68,74,74	0
2	ZXM	A	401[B]	22/22	0.88	0.12	27,45,60,61	5

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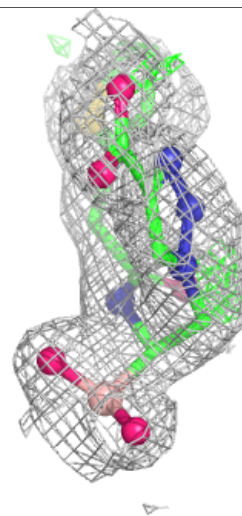
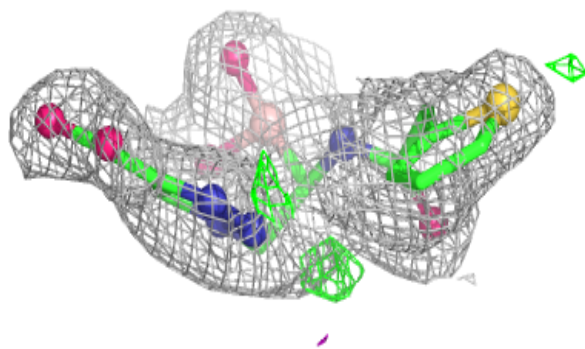
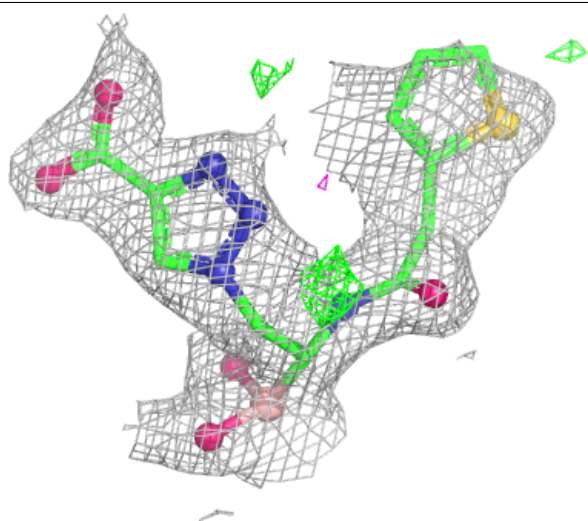
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZXM	D	401	22/22	0.88	0.11	34,47,71,77	0
2	ZXM	A	401[A]	22/22	0.88	0.12	27,39,60,61	5
2	ZXM	B	401	22/22	0.91	0.10	18,37,55,60	0
2	ZXM	C	401	22/22	0.91	0.09	35,43,64,72	0

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.

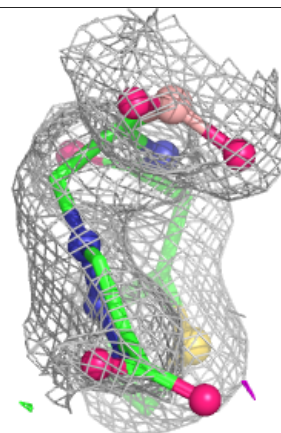
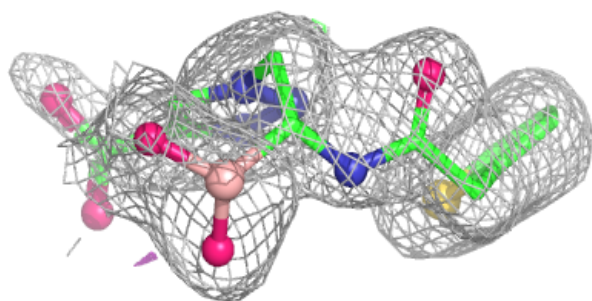
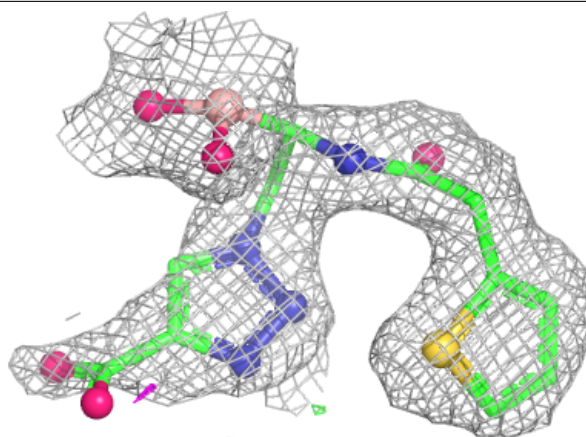
Electron density around ZXM A 401 (B):

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



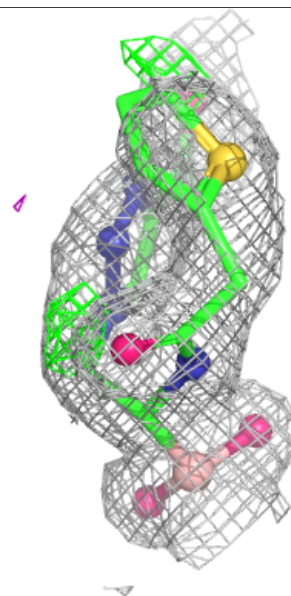
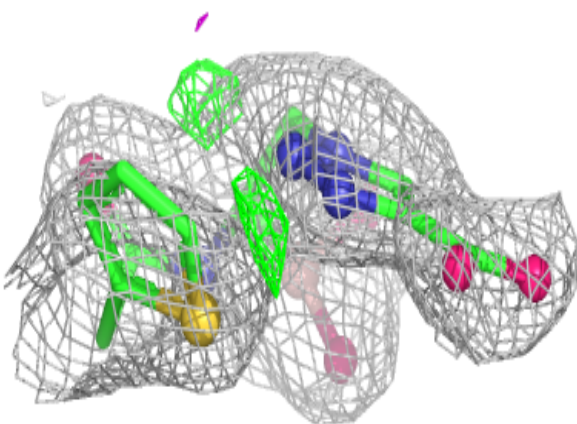
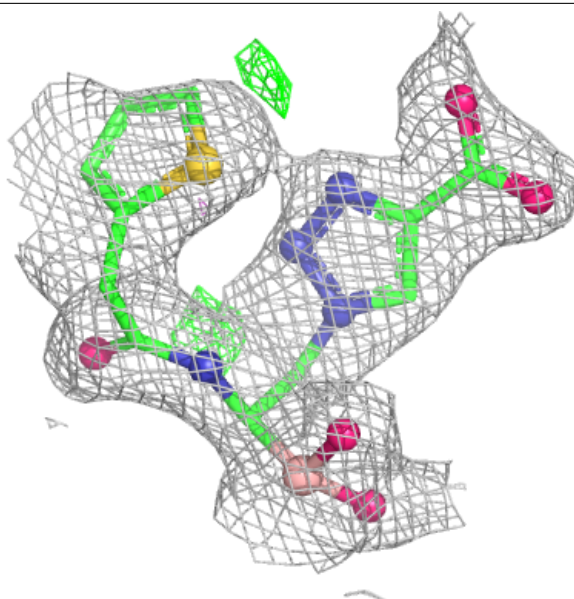
Electron density around ZXM D 401:

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



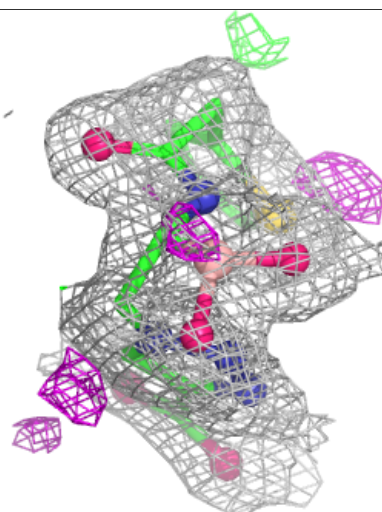
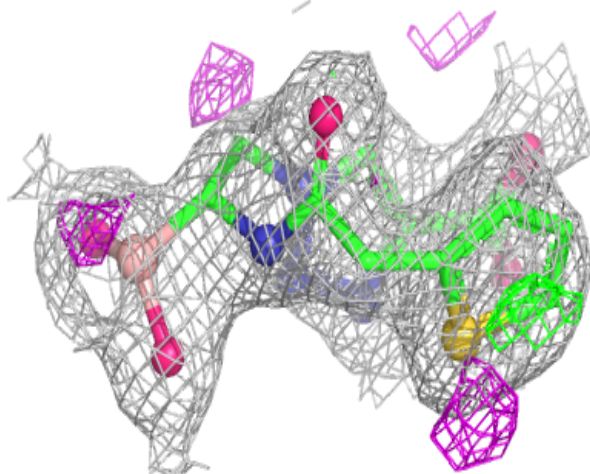
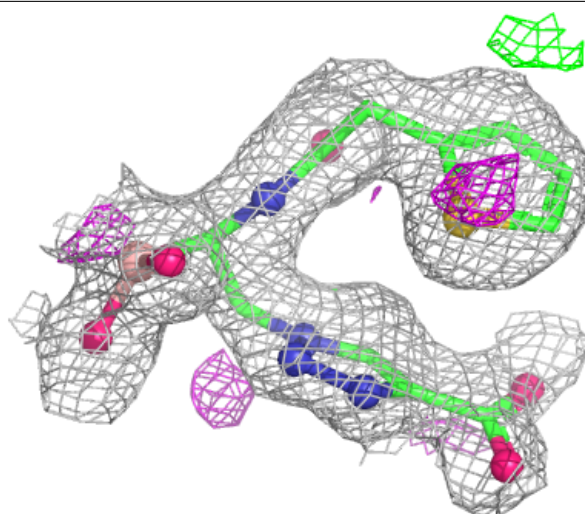
Electron density around ZXM A 401 (A):

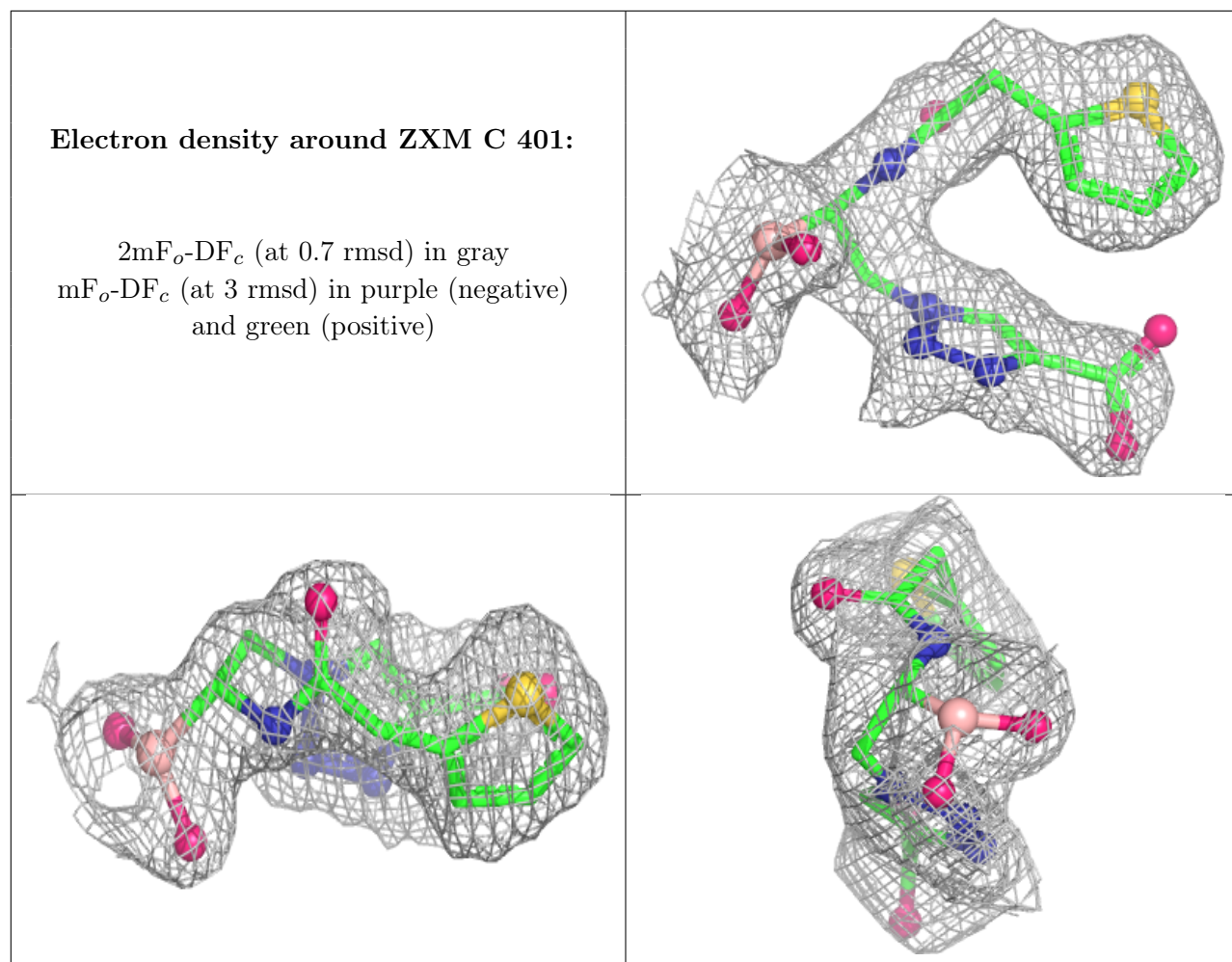
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZXM 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 [i](#)

There are no such residues in this entry.