Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2021 – 10:10 pm GMT

PDB ID	:	7QC1
Title	:	Crystal Structure of Prolyl-tRNA synthetase (ProRS, Proline-tRNA ligase) from Plasmodium falciparum in complex with MAT436
Authors	:	Johansson, C.; Tye, M.; Payne, N.C.; Mazitschek, R.; Oppermann, U.C.T.
Deposited on	:	2021-11-22
Resolution	:	2.51 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 following versions of software and data (see references ⓘ) were used in the production of this report:

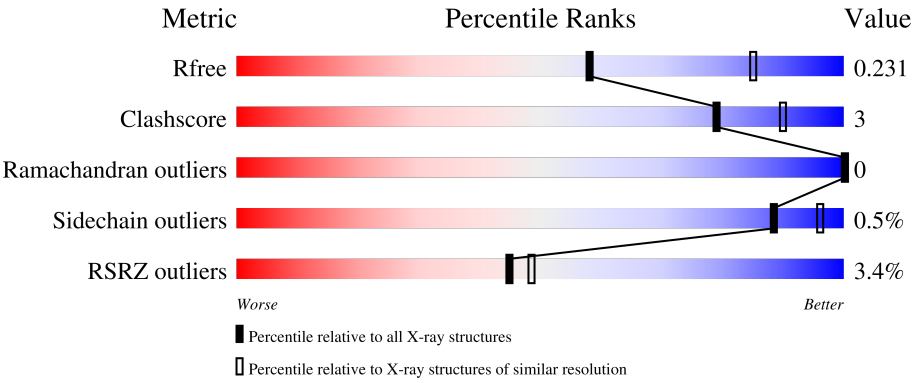
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

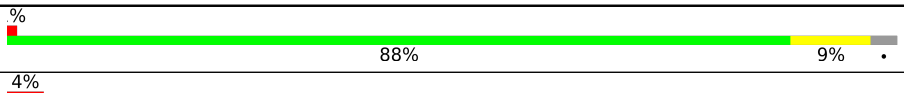
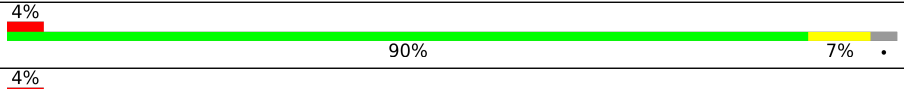
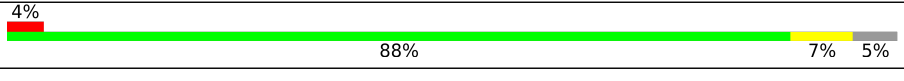
The reported resolution of this entry is 2.51 Å.

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	504	
1	D	504	
1	I	504	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11925 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.

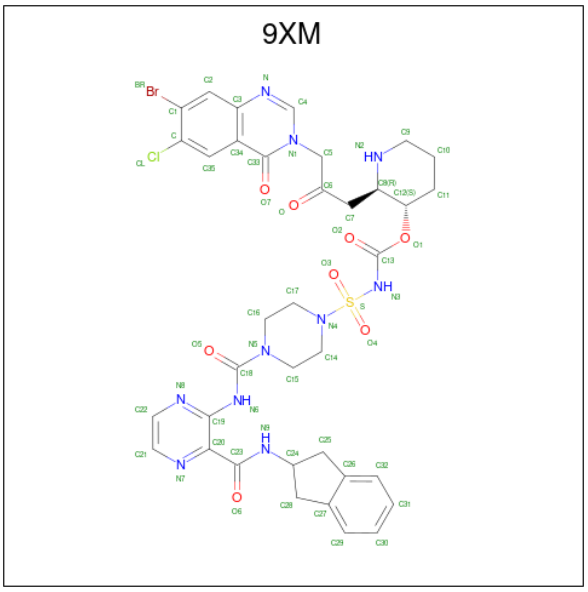
- Molecule 1 is a protein called Proline–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	2	0
			3939	2541	643	734	21			
1	D	489	Total	C	N	O	S	0	0	0
			3882	2502	636	723	21			
1	I	478	Total	C	N	O	S	0	0	0
			3820	2470	628	701	21			

There are 18 discrepancies between the modelled and reference sequences:

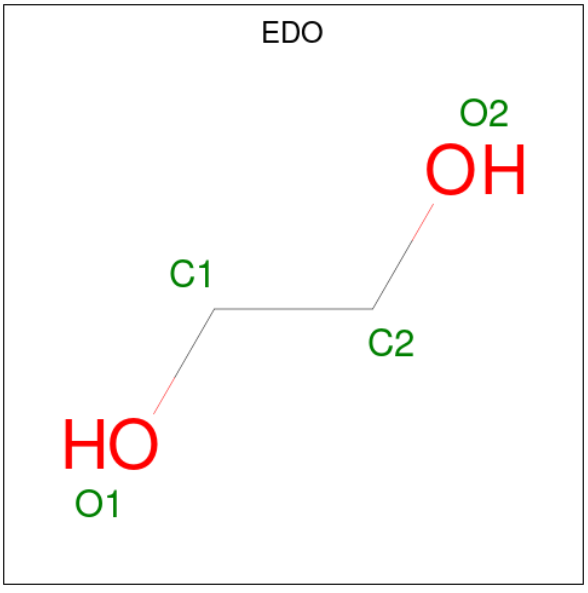
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	SER	-	expression tag	UNP Q8I5R7
A	244	ASP	-	expression tag	UNP Q8I5R7
A	245	ASN	-	expression tag	UNP Q8I5R7
A	246	ALA	-	expression tag	UNP Q8I5R7
A	247	ILE	-	expression tag	UNP Q8I5R7
A	248	ALA	-	expression tag	UNP Q8I5R7
D	243	SER	-	expression tag	UNP Q8I5R7
D	244	ASP	-	expression tag	UNP Q8I5R7
D	245	ASN	-	expression tag	UNP Q8I5R7
D	246	ALA	-	expression tag	UNP Q8I5R7
D	247	ILE	-	expression tag	UNP Q8I5R7
D	248	ALA	-	expression tag	UNP Q8I5R7
I	243	SER	-	expression tag	UNP Q8I5R7
I	244	ASP	-	expression tag	UNP Q8I5R7
I	245	ASN	-	expression tag	UNP Q8I5R7
I	246	ALA	-	expression tag	UNP Q8I5R7
I	247	ILE	-	expression tag	UNP Q8I5R7
I	248	ALA	-	expression tag	UNP Q8I5R7

- Molecule 2 is [(2 {R},3 {S})-2-[3-(7-bromanyl-6-chloranyl-4-oxidanylidene-quinazolin-3-yl)-2-oxidanylidene-propyl]piperidin-3-yl] {N}-[4-[[3-(2,3-dihydro-1 {H}-inden-2-ylcarbamoyl)pyrazin-2-yl]carbamoyl]piperazin-1-yl]sulfonylcarbamate (three-letter code: 9XM) (formula: $C_{36}H_{38}BrClN_{10}O_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	S	0	0
			57	1	36	1	10	8	1		
2	D	1	Total	Br	C	Cl	N	O	S	0	0
			57	1	36	1	10	8	1		
2	I	1	Total	Br	C	Cl	N	O	S	0	0
			57	1	36	1	10	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

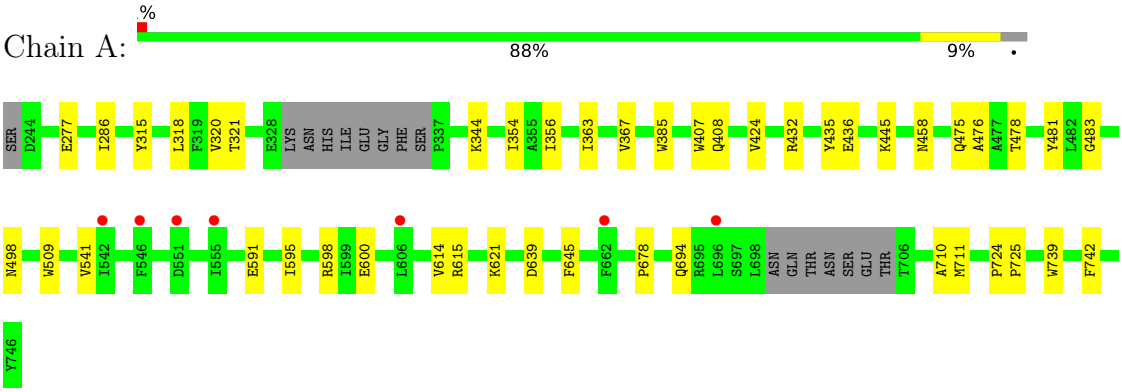
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	31	Total O 31 31	0	0
4	D	23	Total O 23 23	0	0
4	I	19	Total O 19 19	0	0

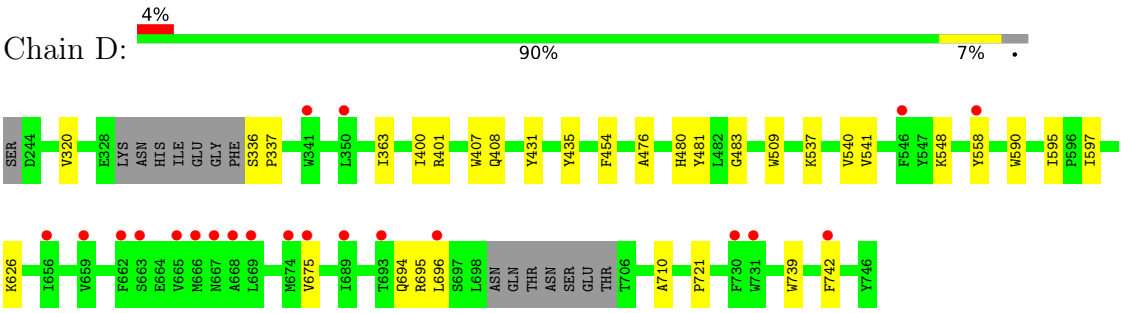
3 Residue-property plots (i)

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.

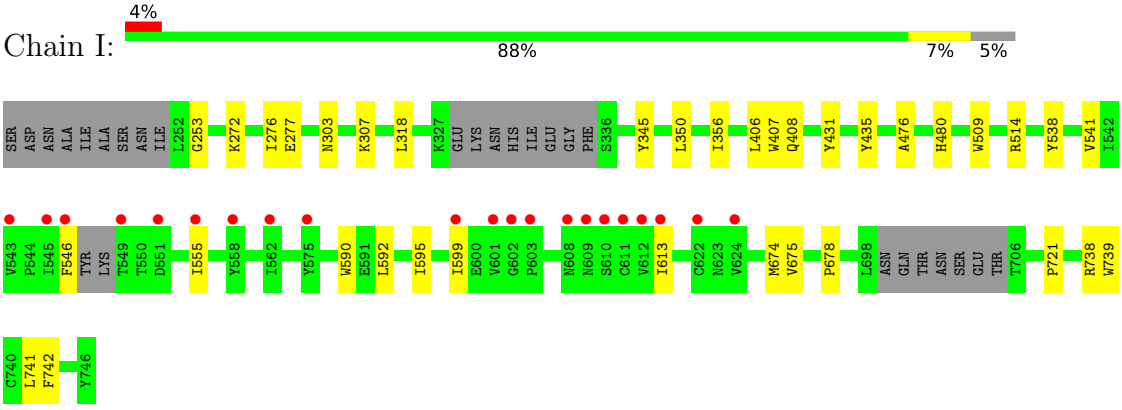
• Molecule 1: Proline–tRNA ligase



• Molecule 1: Proline–tRNA ligase



• Molecule 1: Proline–tRNA ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	207.21Å 207.21Å 115.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.53 – 2.51 65.53 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.53-2.51) 100.0 (65.53-2.51)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.191 , 0.233 0.189 , 0.231	Depositor DCC
R_{free} test set	4289 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11925	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 9XM

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	0.31	0/4037	0.51	0/5477
1	D	0.30	0/3979	0.51	0/5410
1	I	0.30	0/3917	0.50	0/5318
All	All	0.30	0/11933	0.51	0/16205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3939	0	3814	29	0
1	D	3882	0	3709	19	0
1	I	3820	0	3689	22	0
2	A	57	0	0	0	0
2	D	57	0	0	0	0
2	I	57	0	0	1	0
3	A	20	0	30	1	0
3	D	8	0	12	1	0
3	I	12	0	18	1	0
4	A	31	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	23	0	0	0	0
4	I	19	0	0	1	0
All	All	11925	0	11272	65	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 3.

All (65) 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:541:VAL:HG23	1:A:595:ILE:HG21	1.58	0.85
1:D:541:VAL:HG23	1:D:595:ILE:HG21	1.61	0.83
1:D:320:VAL:HG22	1:D:363:ILE:HD11	1.64	0.78
1:A:432:ARG:O	1:A:436[B]:GLU:HG2	1.84	0.76
1:A:598:ARG:NH1	1:A:600:GLU:OE2	2.21	0.74
1:I:514:ARG:HH12	3:I:803:EDO:H21	1.57	0.69
1:D:435:TYR:CZ	1:D:476:ALA:HB1	2.34	0.62
1:A:435:TYR:CZ	1:A:476:ALA:HB1	2.38	0.59
1:I:303:ASN:O	1:I:307:LYS:HG2	2.03	0.59
1:A:432:ARG:NH1	1:A:436[A]:GLU:OE1	2.36	0.58
1:I:253:GLY:O	1:I:272:LYS:NZ	2.31	0.57
1:I:738:ARG:NH1	4:I:901:HOH:O	2.33	0.56
1:D:537:LYS:H	3:D:803:EDO:H12	1.71	0.54
1:D:400:ILE:HG22	1:D:401:ARG:HG3	1.89	0.54
1:A:320:VAL:HG22	1:A:363:ILE:HD11	1.90	0.54
1:I:345:TYR:HD1	1:I:350:LEU:HD12	1.73	0.53
1:I:408:GLN:NE2	1:I:431:TYR:OH	2.39	0.53
1:A:385:TRP:O	3:A:806:EDO:O1	2.23	0.51
1:A:315:TYR:CD2	1:I:406:LEU:HD11	2.46	0.51
1:I:435:TYR:CZ	1:I:476:ALA:HB1	2.45	0.51
1:A:424:VAL:HG21	1:A:481:TYR:HB2	1.93	0.49
1:A:694:GLN:HB2	1:A:710:ALA:HB2	1.93	0.49
1:I:480:HIS:HE2	2:I:801:9XM:C13	2.25	0.49
1:A:436[A]:GLU:HG3	1:A:645:PHE:CE1	2.49	0.48
1:I:678:PRO:HD3	1:I:739:TRP:CZ3	2.49	0.48
1:I:272:LYS:HB3	1:I:592:LEU:HD21	1.95	0.48
1:I:546:PHE:HB3	1:I:555:ILE:HD12	1.94	0.48
1:A:614:VAL:HG22	1:A:621:LYS:HG2	1.96	0.47
1:A:344:LYS:NZ	4:A:903:HOH:O	2.48	0.47
1:A:318:LEU:HD21	1:I:318:LEU:HD21	1.95	0.47
1:D:675:VAL:HG23	1:D:742:PHE:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:OE2	1:A:598:ARG:NH2	2.48	0.47
1:A:354:ILE:HD13	1:A:354:ILE:HA	1.79	0.47
1:A:367:VAL:HG11	1:I:277:GLU:HG2	1.98	0.46
1:I:541:VAL:HG21	1:I:590:TRP:CD1	2.50	0.46
1:A:321:THR:HA	1:A:354:ILE:HD13	1.98	0.46
1:A:498:ASN:OD1	1:D:548:LYS:HA	2.16	0.46
1:D:694:GLN:HB2	1:D:710:ALA:HB2	1.97	0.46
1:I:674:MET:HE1	1:I:741:LEU:HD22	1.97	0.45
1:I:538:TYR:HB2	1:I:595:ILE:HD12	1.99	0.45
1:D:540:VAL:HG22	1:D:597:ILE:HB	1.99	0.45
1:A:475:GLN:NE2	1:A:478:THR:HB	2.32	0.44
1:D:408:GLN:NE2	1:D:431:TYR:OH	2.48	0.44
1:D:695:ARG:HH21	1:D:696:LEU:HD21	1.82	0.43
1:A:615:ARG:NH1	1:A:639[A]:ASP:OD2	2.49	0.43
1:I:276:ILE:HD13	1:I:276:ILE:HA	1.89	0.43
1:I:721:PRO:HD2	1:I:739:TRP:CD1	2.54	0.43
1:A:458:ASN:ND2	1:A:483:GLY:HA3	2.34	0.42
1:A:711:MET:HG2	1:A:742:PHE:HB3	2.01	0.42
1:D:454:PHE:HB2	1:D:480:HIS:CE1	2.54	0.42
1:A:432:ARG:HD3	1:A:445:LYS:HE3	2.00	0.42
1:I:675:VAL:HG23	1:I:742:PHE:HB2	2.01	0.42
1:A:724:PRO:HA	1:A:725:PRO:HD3	1.89	0.42
1:D:481:TYR:CZ	1:D:483:GLY:HA2	2.54	0.42
1:D:320:VAL:CG2	1:D:363:ILE:HD11	2.44	0.42
1:D:541:VAL:HG11	1:D:590:TRP:CD1	2.55	0.42
1:I:599:ILE:HG12	1:I:613:ILE:HG12	2.03	0.41
1:D:336:SER:HB2	1:D:337:PRO:HD3	2.02	0.41
1:A:277:GLU:HB3	1:A:286:ILE:HB	2.02	0.41
1:A:356:ILE:HD11	1:I:356:ILE:HD11	2.03	0.41
1:D:320:VAL:HG13	1:D:363:ILE:HD11	2.02	0.41
1:A:385:TRP:CE3	1:A:408:GLN:HB3	2.55	0.41
1:A:678:PRO:HD3	1:A:739:TRP:CZ3	2.55	0.41
1:D:721:PRO:HD2	1:D:739:TRP:CD1	2.56	0.41
1:D:558:TYR:CE2	1:D:626:LYS:HD2	2.55	0.41

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	484/504 (96%)	473 (98%)	11 (2%)	0	100	100
1	D	483/504 (96%)	473 (98%)	10 (2%)	0	100	100
1	I	470/504 (93%)	460 (98%)	10 (2%)	0	100	100
All	All	1437/1512 (95%)	1406 (98%)	31 (2%)	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	420/457 (92%)	418 (100%)	2 (0%)	88	96
1	D	407/457 (89%)	405 (100%)	2 (0%)	88	96
1	I	404/457 (88%)	402 (100%)	2 (0%)	88	96
All	All	1231/1371 (90%)	1225 (100%)	6 (0%)	88	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	TRP
1	A	509	TRP
1	D	407	TRP
1	D	509	TRP
1	I	407	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	509	TRP

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

Mol	Chain	Res	Type
1	A	299	GLN
1	A	408	GLN
1	A	458	ASN
1	D	408	GLN
1	D	485	ASN
1	I	408	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

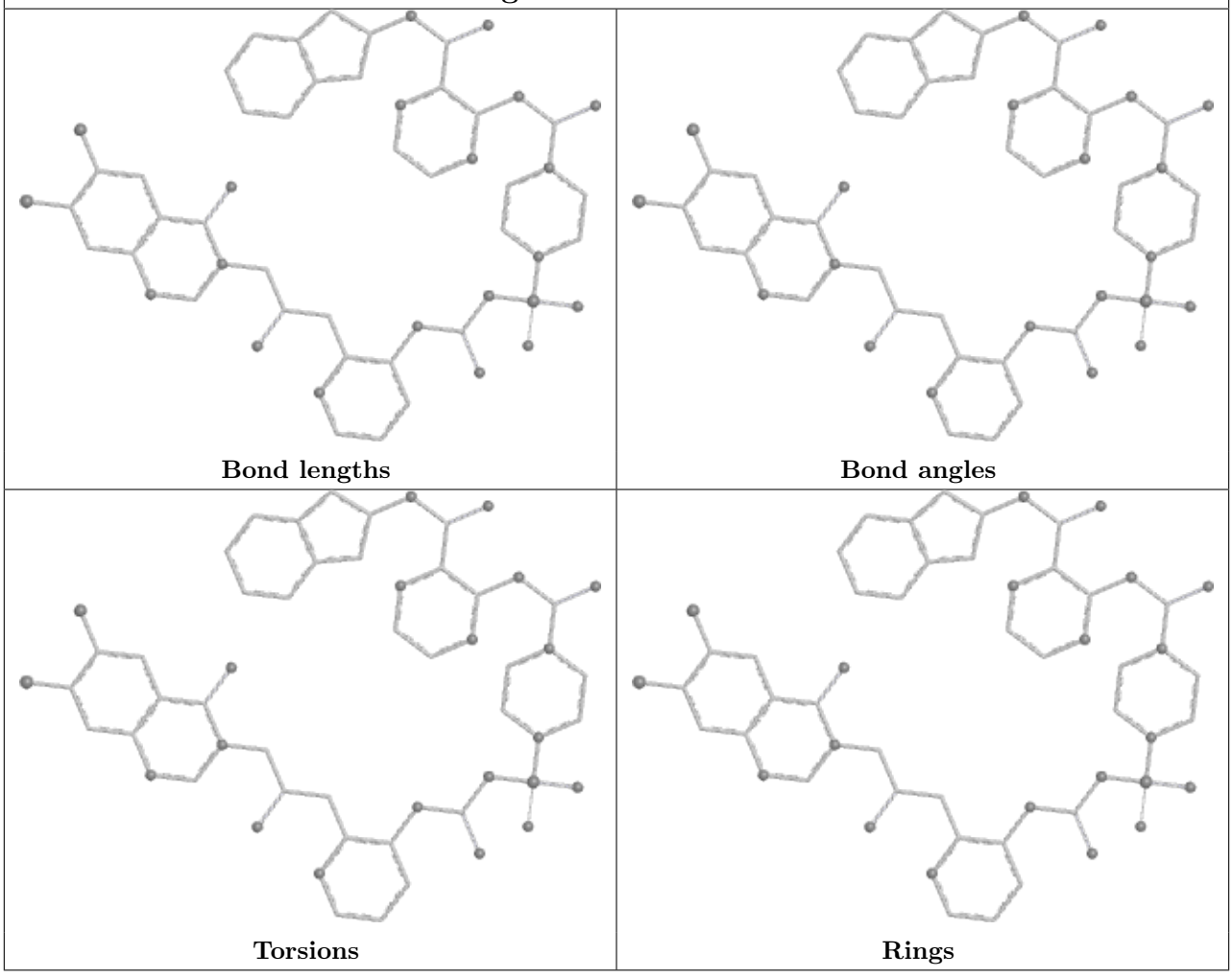
There are no ring outliers.

No monomer is involved in short contacts.

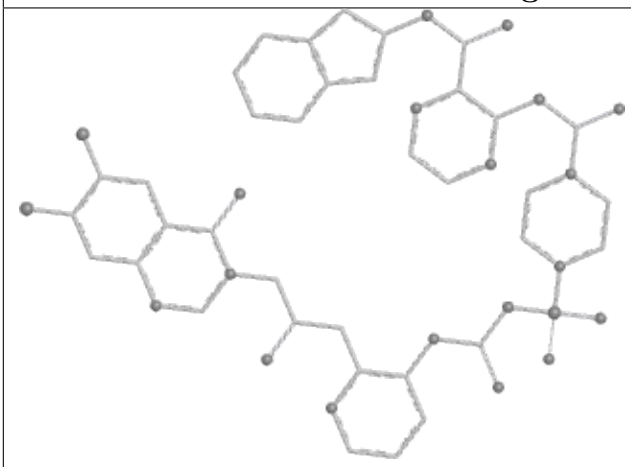
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

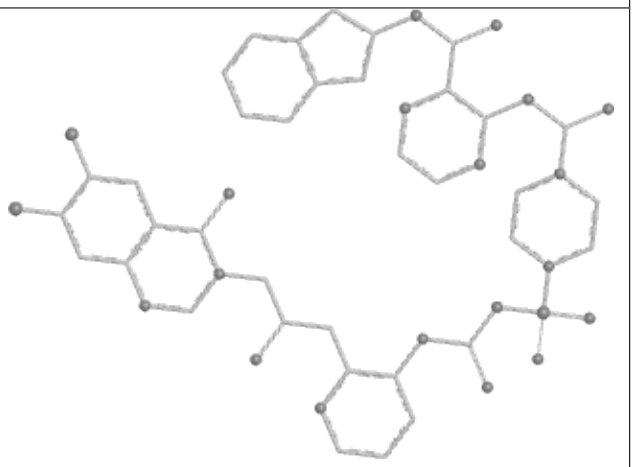
Ligand 9XM A 801



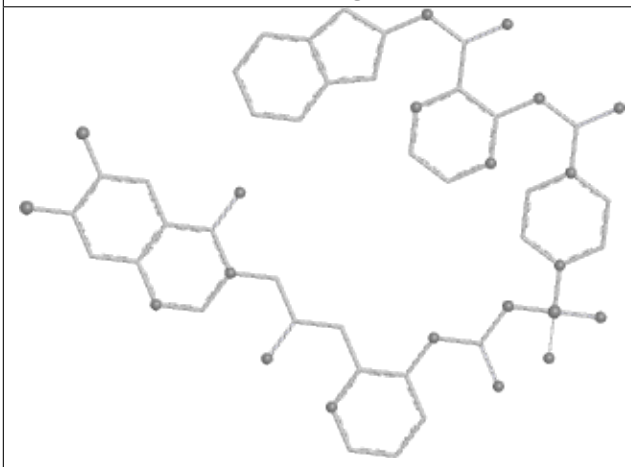
Ligand 9XM D 801



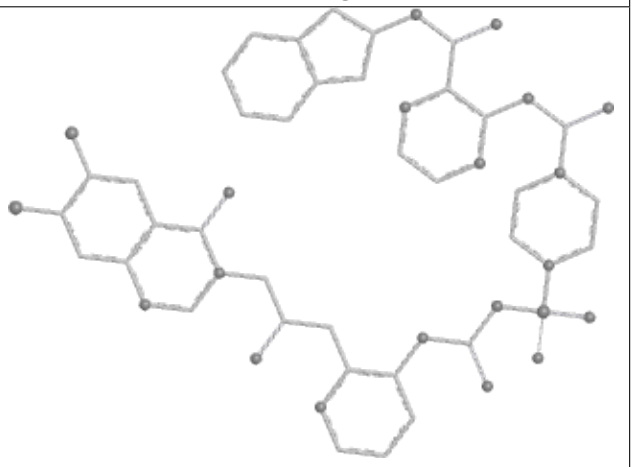
Bond lengths



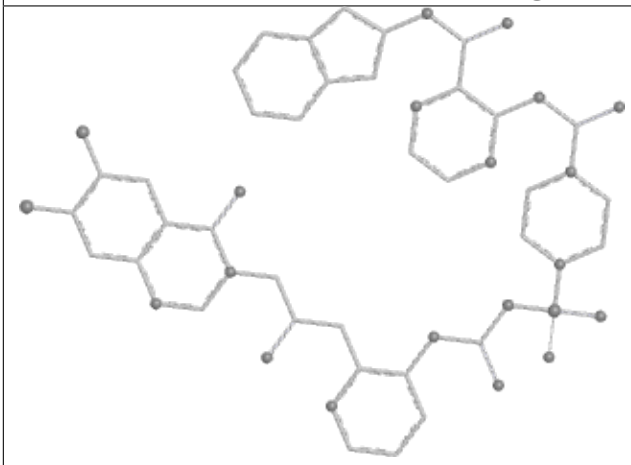
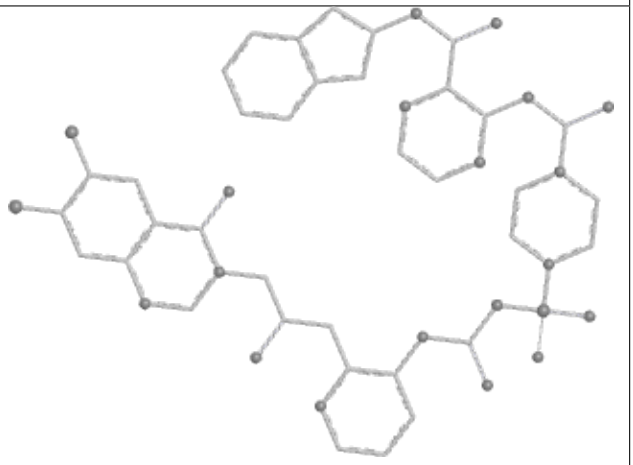
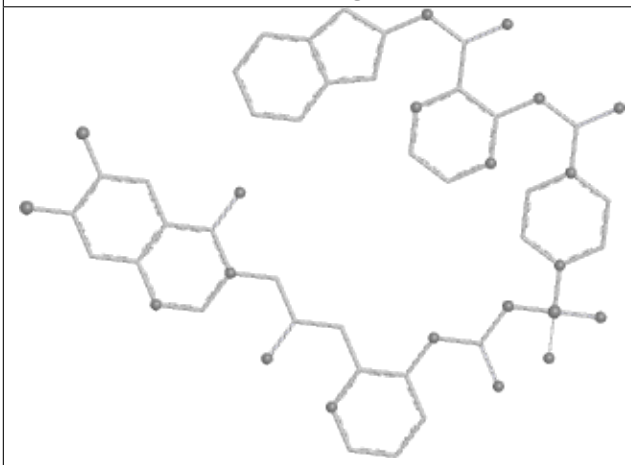
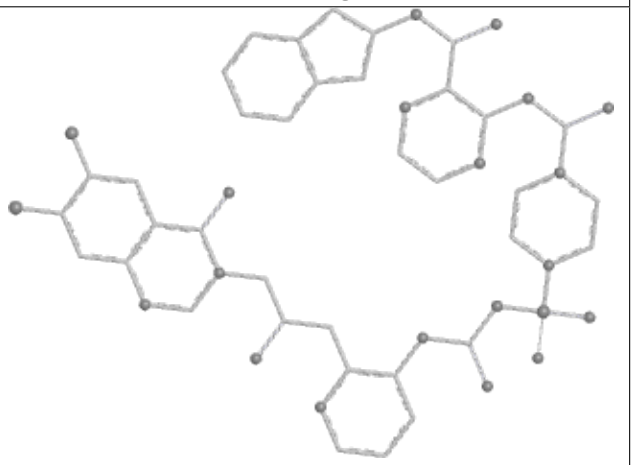
Bond angles



Torsions



Rings

Ligand 9XM I 801	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	488/504 (96%)	0.04	7 (1%)	75	77	50, 68, 108, 150	0
1	D	489/504 (97%)	0.12	21 (4%)	35	38	54, 73, 109, 148	0
1	I	478/504 (94%)	0.19	21 (4%)	34	37	53, 73, 116, 156	0
All	All	1455/1512 (96%)	0.12	49 (3%)	45	48	50, 72, 111, 156	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	601	VAL	6.4
1	I	546	PHE	5.2
1	I	545	ILE	4.0
1	D	669	LEU	4.0
1	I	549	THR	3.8
1	I	613	ILE	3.6
1	I	611	CYS	3.3
1	I	555	ILE	3.2
1	A	555	ILE	3.1
1	D	665	VAL	3.1
1	I	612	VAL	3.1
1	D	674	MET	3.0
1	A	546	PHE	3.0
1	I	543	VAL	3.0
1	I	602	GLY	2.9
1	I	624	VAL	2.8
1	D	667	ASN	2.7
1	D	730	PHE	2.7
1	A	606	LEU	2.7
1	I	558	TYR	2.7
1	D	656	ILE	2.7
1	D	546	PHE	2.6
1	I	599	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	731	TRP	2.6
1	D	668	ALA	2.6
1	D	666	MET	2.6
1	D	696	LEU	2.5
1	D	675	VAL	2.5
1	D	742	PHE	2.4
1	I	603	PRO	2.4
1	I	610	SER	2.4
1	D	662	PHE	2.3
1	D	341	TRP	2.3
1	D	689	ILE	2.3
1	D	663	SER	2.2
1	I	575	TYR	2.2
1	I	608	ASN	2.2
1	D	558	TYR	2.2
1	I	609	ASN	2.2
1	I	562	ILE	2.2
1	I	551	ASP	2.1
1	A	662	PHE	2.1
1	D	659	VAL	2.1
1	A	696	LEU	2.1
1	A	551	ASP	2.1
1	D	693	THR	2.1
1	D	350	LEU	2.1
1	A	542	ILE	2.1
1	I	622	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

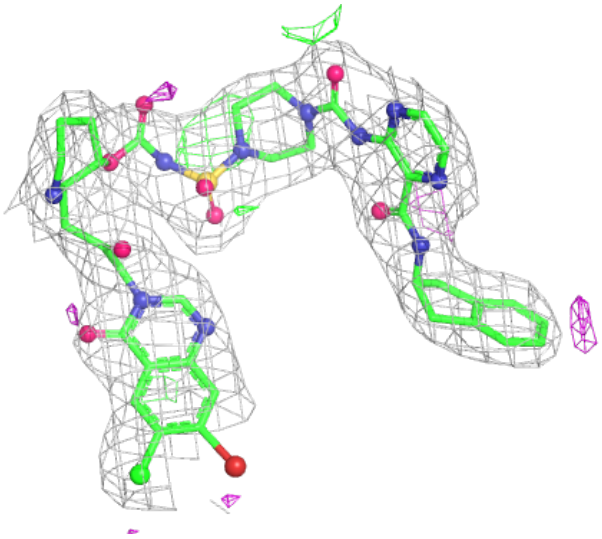
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

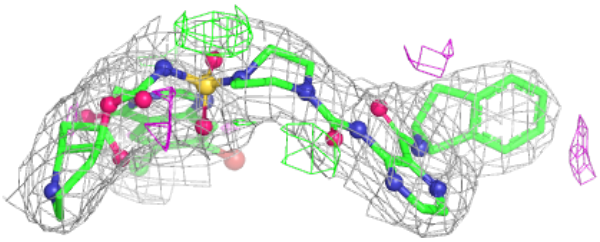
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	805	4/4	0.80	0.26	56,60,65,71	0
3	EDO	D	802	4/4	0.84	0.27	82,84,84,84	0
3	EDO	D	803	4/4	0.84	0.20	60,68,70,77	0
3	EDO	A	804	4/4	0.87	0.16	83,86,92,93	0
3	EDO	I	803	4/4	0.88	0.16	70,72,77,81	0
3	EDO	I	804	4/4	0.88	0.18	74,83,85,89	0
3	EDO	A	803	4/4	0.89	0.16	72,76,82,82	0
3	EDO	I	802	4/4	0.92	0.16	64,68,74,82	0
3	EDO	A	806	4/4	0.93	0.19	68,68,69,70	0
3	EDO	A	802	4/4	0.93	0.21	68,72,74,81	0
2	9XM	D	801	57/57	0.97	0.14	58,70,85,106	0
2	9XM	I	801	57/57	0.97	0.17	55,63,76,89	0
2	9XM	A	801	57/57	0.97	0.15	51,58,70,83	0

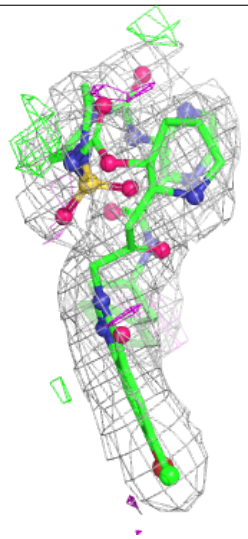
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9XM D 801:

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

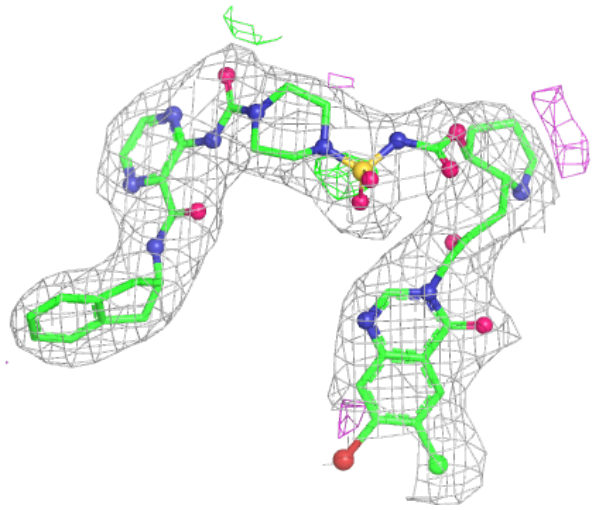


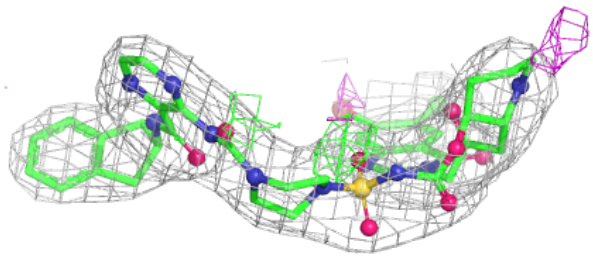


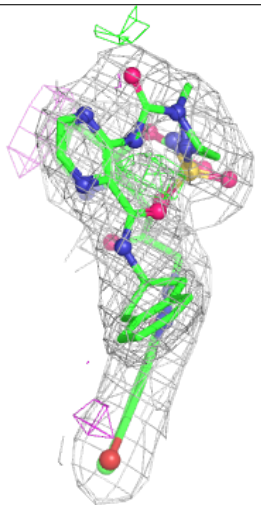


Electron density around 9XM I 801:

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

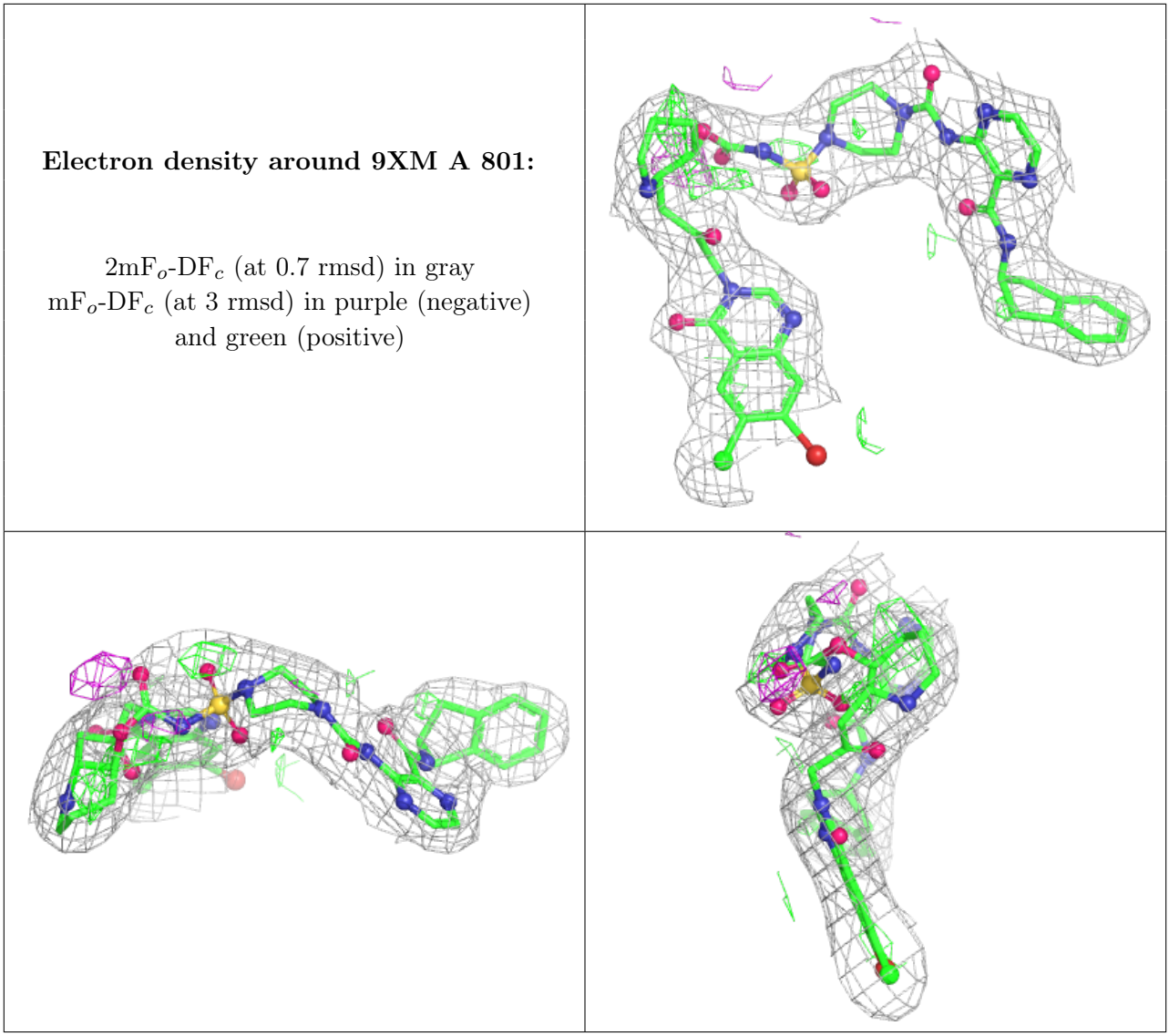






Electron density around 9XM A 801:

$2mF_o$-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.