



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:39 pm BST

PDB ID : 6IYW
Title : Crystal structure of L,D-transpeptidase LdtMt2 from Mycobacterium tuberculosis in complex with Imipenem adduct
Authors : Li, D.F.; Zhao, F.; Wang, D.C.
Deposited on : 2018-12-17
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

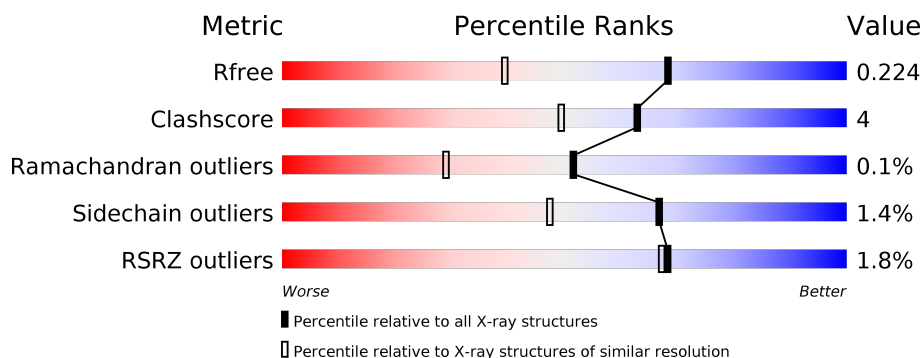
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	272	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>..</div> </div> </div>
1	B	272	<div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	C	272	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	272	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	E	272	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	F	272	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	E	504	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14165 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 L,D-transpeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	3	0
			2055	1294	357	397	7			
1	B	266	Total	C	N	O	S	0	2	0
			2051	1290	358	396	7			
1	C	267	Total	C	N	O	S	0	1	0
			2053	1294	354	398	7			
1	D	264	Total	C	N	O	S	0	1	0
			2032	1279	351	395	7			
1	E	264	Total	C	N	O	S	0	2	0
			2036	1282	353	394	7			
1	F	264	Total	C	N	O	S	0	4	0
			2045	1286	357	395	7			

There are 18 discrepancies between the modelled and reference sequences:

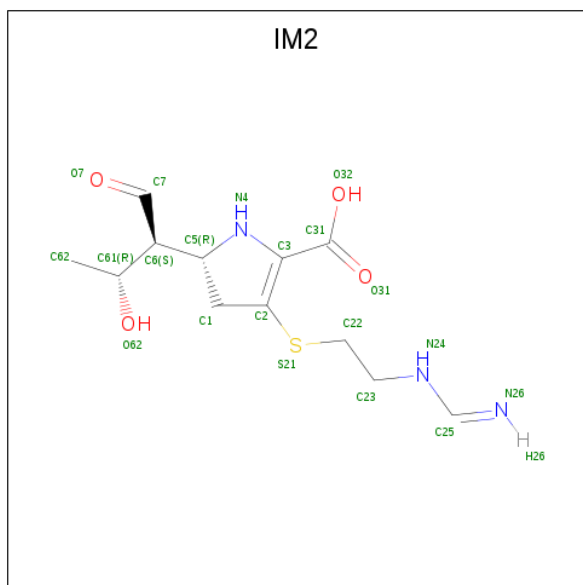
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	-	expression tag	UNP I6Y9J2
A	138	ASN	-	expression tag	UNP I6Y9J2
A	139	ALA	-	expression tag	UNP I6Y9J2
B	137	SER	-	expression tag	UNP I6Y9J2
B	138	ASN	-	expression tag	UNP I6Y9J2
B	139	ALA	-	expression tag	UNP I6Y9J2
C	137	SER	-	expression tag	UNP I6Y9J2
C	138	ASN	-	expression tag	UNP I6Y9J2
C	139	ALA	-	expression tag	UNP I6Y9J2
D	137	SER	-	expression tag	UNP I6Y9J2
D	138	ASN	-	expression tag	UNP I6Y9J2
D	139	ALA	-	expression tag	UNP I6Y9J2
E	137	SER	-	expression tag	UNP I6Y9J2
E	138	ASN	-	expression tag	UNP I6Y9J2
E	139	ALA	-	expression tag	UNP I6Y9J2
F	137	SER	-	expression tag	UNP I6Y9J2
F	138	ASN	-	expression tag	UNP I6Y9J2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	139	ALA	-	expression tag	UNP I6Y9J2

- Molecule 2 is (5R)-5-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-[(2-[(E)-iminomethyl]amino}ethyl)sulfanyl]-4,5-dihydro-1H-pyrrole-2-carboxylic acid (three-letter code: IM2) (formula: C₁₂H₁₉N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			17	10	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			17	11	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			17	11	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			20	12	3	4	1		
2	F	1	Total	C	N	O	S	0	0
			20	12	3	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	303	Total O 303 303	0	0
4	B	314	Total O 314 314	0	0
4	C	229	Total O 229 229	0	0
4	D	222	Total O 222 222	0	0
4	E	307	Total O 307 307	0	0
4	F	267	Total O 267 267	0	0

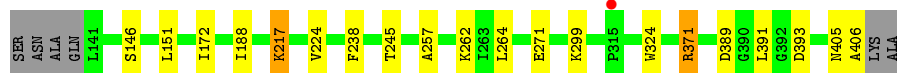
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

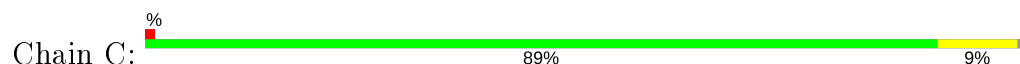
• Molecule 1: L,D-transpeptidase 2



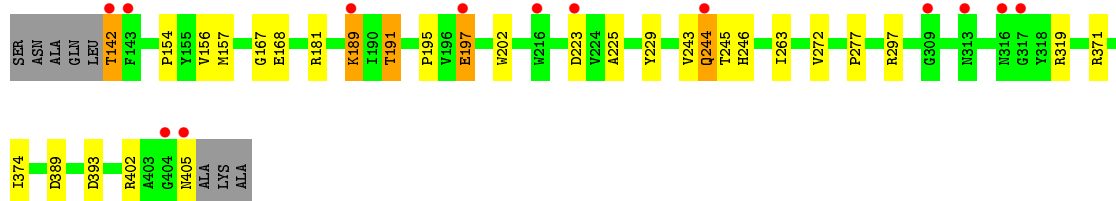
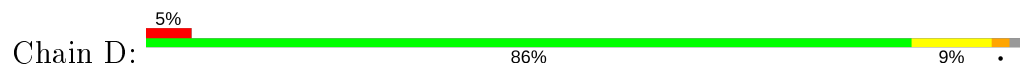
• Molecule 1: L,D-transpeptidase 2



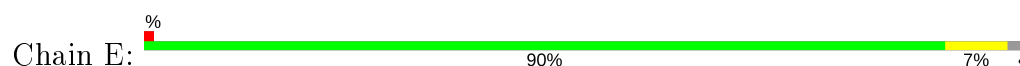
• Molecule 1: L,D-transpeptidase 2



• Molecule 1: L,D-transpeptidase 2

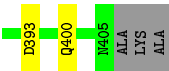
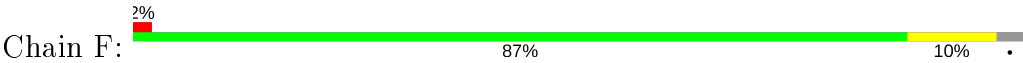


• Molecule 1: L,D-transpeptidase 2





● Molecule 1: L,D-transpeptidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 103.70Å 103.81Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	46.41 – 1.60 46.41 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.41-1.60) 93.8 (46.41-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.186 , 0.224 0.186 , 0.224	Depositor DCC
R_{free} test set	1990 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.238 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14165	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 57.83 % 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 2.2341e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, IM2

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	0.39	0/2129	0.67	4/2912 (0.1%)
1	B	0.41	0/2122	0.66	3/2903 (0.1%)
1	C	0.38	0/2116	0.62	2/2896 (0.1%)
1	D	0.42	1/2095 (0.0%)	0.70	5/2868 (0.2%)
1	E	0.41	0/2105	0.61	1/2881 (0.0%)
1	F	0.39	0/2124	0.62	0/2906
All	All	0.40	1/12691 (0.0%)	0.65	15/17366 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	LYS	CE-NZ	6.45	1.65	1.49

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	LYS	CB-CG-CD	-9.95	85.72	111.60
1	A	244	GLN	CA-CB-CG	7.09	129.00	113.40
1	A	315	PRO	C-N-CA	6.97	139.12	121.70
1	D	197	GLU	CA-CB-CG	6.92	128.62	113.40
1	B	271	GLU	CA-CB-CG	-6.33	99.47	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	244	GLN	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	2055	0	1948	14	1
1	B	2051	0	1936	14	0
1	C	2053	0	1946	15	0
1	D	2032	0	1916	25	1
1	E	2036	0	1924	15	0
1	F	2045	0	1935	20	0
2	A	16	0	10	1	0
2	B	17	0	10	1	0
2	C	17	0	12	0	0
2	D	17	0	12	0	0
2	E	20	0	16	1	0
2	F	20	0	15	1	0
3	A	30	0	40	5	0
3	B	36	0	48	3	0
3	C	12	0	16	0	0
3	D	6	0	8	0	0
3	E	36	0	48	8	0
3	F	24	0	32	7	0
4	A	303	0	0	4	3
4	B	314	0	0	2	3
4	C	229	0	0	6	1
4	D	222	0	0	5	1
4	E	307	0	0	2	3
4	F	267	0	0	4	1
All	All	14165	0	11872	105	7

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 4.

The worst 5 of 105 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:225:ALA:HA	1:D:244:GLN:HE22	1.18	1.07
1:D:197:GLU:OE1	4:D:601:HOH:O	1.76	1.03
1:D:225:ALA:HA	1:D:244:GLN:NE2	1.82	0.94
1:D:244:GLN:HA	1:D:244:GLN:HE21	1.31	0.91
1:A:225:ALA:HA	1:A:244:GLN:OE1	1.75	0.87

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:OE1	1:D:189:LYS:NZ[1_455]	1.84	0.36
4:B:655:HOH:O	4:E:878:HOH:O[2_1046]	2.09	0.11
4:A:644:HOH:O	4:E:792:HOH:O[1_554]	2.14	0.06
4:C:797:HOH:O	4:D:766:HOH:O[2_1056]	2.15	0.05
4:A:757:HOH:O	4:F:834:HOH:O[2_1056]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/272 (98%)	260 (97%)	6 (2%)	1 (0%)	34	15
1	B	266/272 (98%)	261 (98%)	5 (2%)	0	100	100
1	C	266/272 (98%)	262 (98%)	4 (2%)	0	100	100
1	D	263/272 (97%)	259 (98%)	4 (2%)	0	100	100
1	E	264/272 (97%)	259 (98%)	5 (2%)	0	100	100
1	F	266/272 (98%)	262 (98%)	4 (2%)	0	100	100
All	All	1592/1632 (98%)	1563 (98%)	28 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/223 (100%)	220 (99%)	2 (1%)	78	65
1	B	221/223 (99%)	217 (98%)	4 (2%)	59	36
1	C	221/223 (99%)	218 (99%)	3 (1%)	67	47
1	D	219/223 (98%)	215 (98%)	4 (2%)	59	36
1	E	220/223 (99%)	217 (99%)	3 (1%)	67	47
1	F	222/223 (100%)	217 (98%)	5 (2%)	50	25
All	All	1325/1338 (99%)	1304 (98%)	21 (2%)	67	41

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	297	ARG
1	D	389	ASP
1	F	319[A]	ARG
1	C	393	ASP
1	F	319[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	D	193	ASN
1	D	227	ASN
1	D	244	GLN
1	D	246	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	F	503	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	E	503	-	5,5,5	0.36	0	5,5,5	0.97	0
3	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.33	0
2	IM2	E	501	1	13,20,20	3.38	5 (38%)	7,26,26	2.39	2 (28%)
2	IM2	D	501	1	11,17,20	3.41	4 (36%)	7,23,26	1.91	2 (28%)
2	IM2	C	501	1	11,17,20	3.23	4 (36%)	7,23,26	1.78	2 (28%)
3	GOL	F	504	-	5,5,5	0.38	0	5,5,5	0.50	0
3	GOL	A	506	-	5,5,5	0.34	0	5,5,5	0.51	0
3	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	B	506	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	D	502	-	5,5,5	0.39	0	5,5,5	0.34	0
3	GOL	E	505	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	A	505	-	5,5,5	0.35	0	5,5,5	0.25	0
3	GOL	E	502	-	5,5,5	0.39	0	5,5,5	0.36	0
3	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.61	0
3	GOL	B	504	-	5,5,5	0.35	0	5,5,5	0.46	0
3	GOL	C	503	-	5,5,5	0.39	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	507	-	5,5,5	0.43	0	5,5,5	0.30	0
3	GOL	F	502	-	5,5,5	0.41	0	5,5,5	0.47	0
3	GOL	B	505	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	A	502	-	5,5,5	0.51	0	5,5,5	0.43	0
3	GOL	B	507	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	E	504	-	5,5,5	0.31	0	5,5,5	0.26	0
3	GOL	B	502	-	5,5,5	0.41	0	5,5,5	0.22	0
2	IM2	B	501	1	10,16,20	3.46	4 (40%)	5,22,26	1.65	1 (20%)
2	IM2	A	501	1	10,16,20	3.52	4 (40%)	5,22,26	2.29	3 (60%)
3	GOL	F	505	-	5,5,5	0.34	0	5,5,5	0.32	0
2	IM2	F	501	1	13,20,20	3.38	5 (38%)	7,26,26	1.85	2 (28%)
3	GOL	C	502	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	E	506	-	5,5,5	0.37	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	503	-	-	2/4/4/4	-
3	GOL	E	503	-	-	2/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
2	IM2	E	501	1	-	0/13/32/32	0/1/1/1
2	IM2	D	501	1	-	2/11/29/32	0/1/1/1
2	IM2	C	501	1	-	4/11/29/32	0/1/1/1
3	GOL	F	504	-	-	4/4/4/4	-
3	GOL	A	506	-	-	4/4/4/4	-
3	GOL	A	503	-	-	1/4/4/4	-
3	GOL	B	506	-	-	0/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	E	505	-	-	2/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	E	502	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	E	507	-	-	4/4/4/4	-
3	GOL	F	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	E	504	-	-	2/4/4/4	-
3	GOL	B	502	-	-	0/4/4/4	-
2	IM2	B	501	1	-	2/9/28/32	0/1/1/1
2	IM2	A	501	1	-	2/9/28/32	0/1/1/1
3	GOL	F	505	-	-	2/4/4/4	-
2	IM2	F	501	1	-	3/13/32/32	0/1/1/1
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	E	506	-	-	2/4/4/4	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IM2	C5-N4	7.90	1.58	1.46
2	B	501	IM2	C5-N4	7.76	1.57	1.46
2	D	501	IM2	C5-N4	7.65	1.57	1.46
2	C	501	IM2	C5-N4	7.60	1.57	1.46
2	F	501	IM2	C5-N4	7.44	1.57	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	IM2	C22-S21-C2	4.78	111.77	103.94
2	D	501	IM2	C22-S21-C2	3.62	110.33	104.19
2	E	501	IM2	C2-C3-N4	3.43	116.84	108.37
2	F	501	IM2	C22-S21-C2	3.39	109.50	103.94
2	D	501	IM2	C2-C3-N4	3.37	116.70	108.37

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	503	GOL	C1-C2-C3-O3
3	E	503	GOL	O1-C1-C2-C3
3	A	504	GOL	O1-C1-C2-C3
2	D	501	IM2	C61-C6-C7-O7
2	C	501	IM2	C61-C6-C7-O7

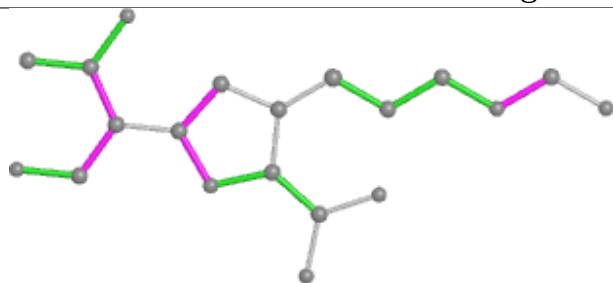
There are no ring outliers.

16 monomers are involved in 27 short contacts:

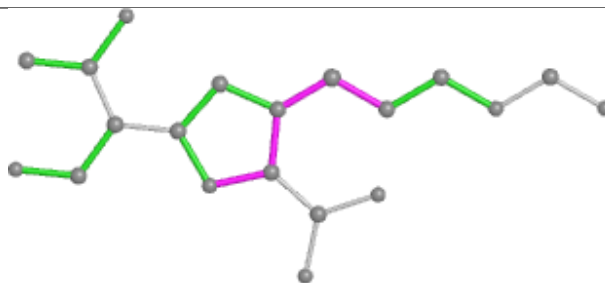
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	GOL	1	0
2	E	501	IM2	1	0
3	F	504	GOL	1	0
3	A	506	GOL	2	0
3	A	503	GOL	2	0
3	B	506	GOL	1	0
3	E	505	GOL	1	0
3	B	503	GOL	2	0
3	E	507	GOL	1	0
3	F	502	GOL	3	0
3	E	504	GOL	5	0
2	B	501	IM2	1	0
2	A	501	IM2	1	0
3	F	505	GOL	3	0
2	F	501	IM2	1	0
3	E	506	GOL	1	0

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.

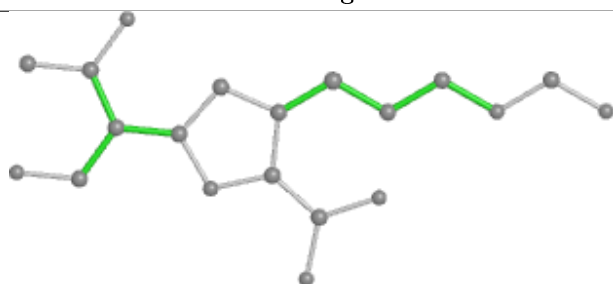
Ligand IM2 E 501



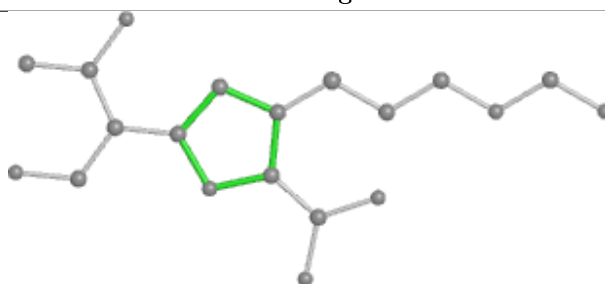
Bond lengths



Bond angles

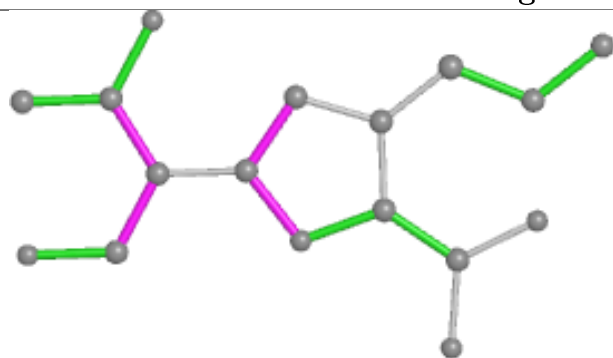


Torsions

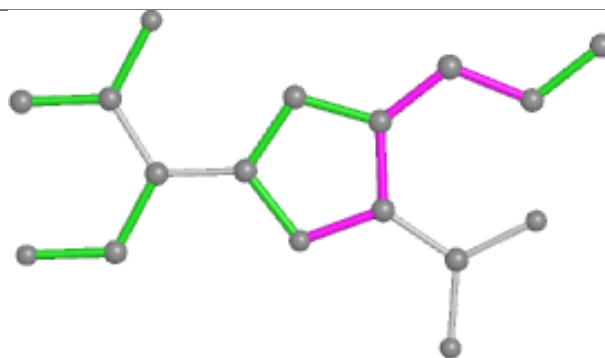


Rings

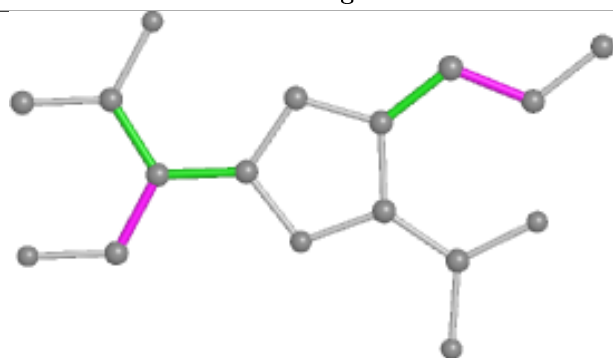
Ligand IM2 D 501



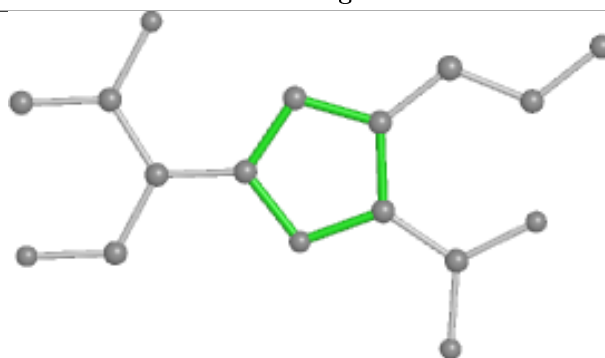
Bond lengths



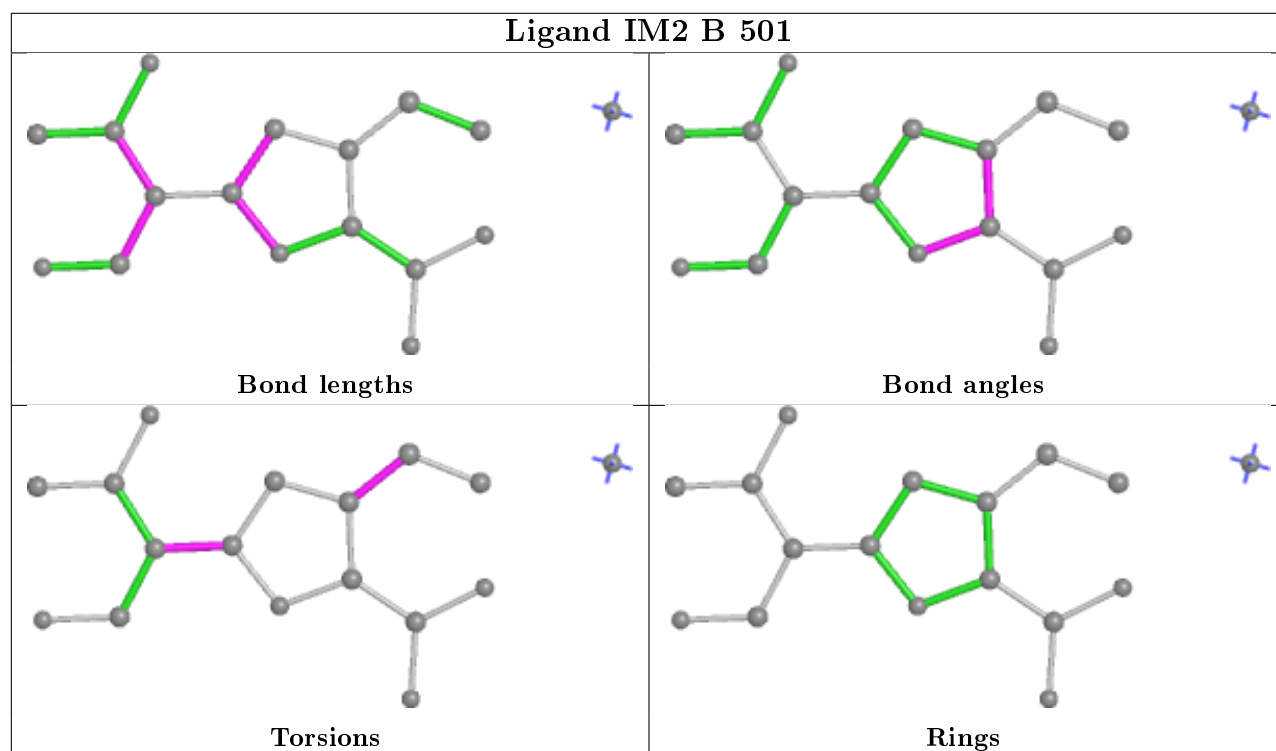
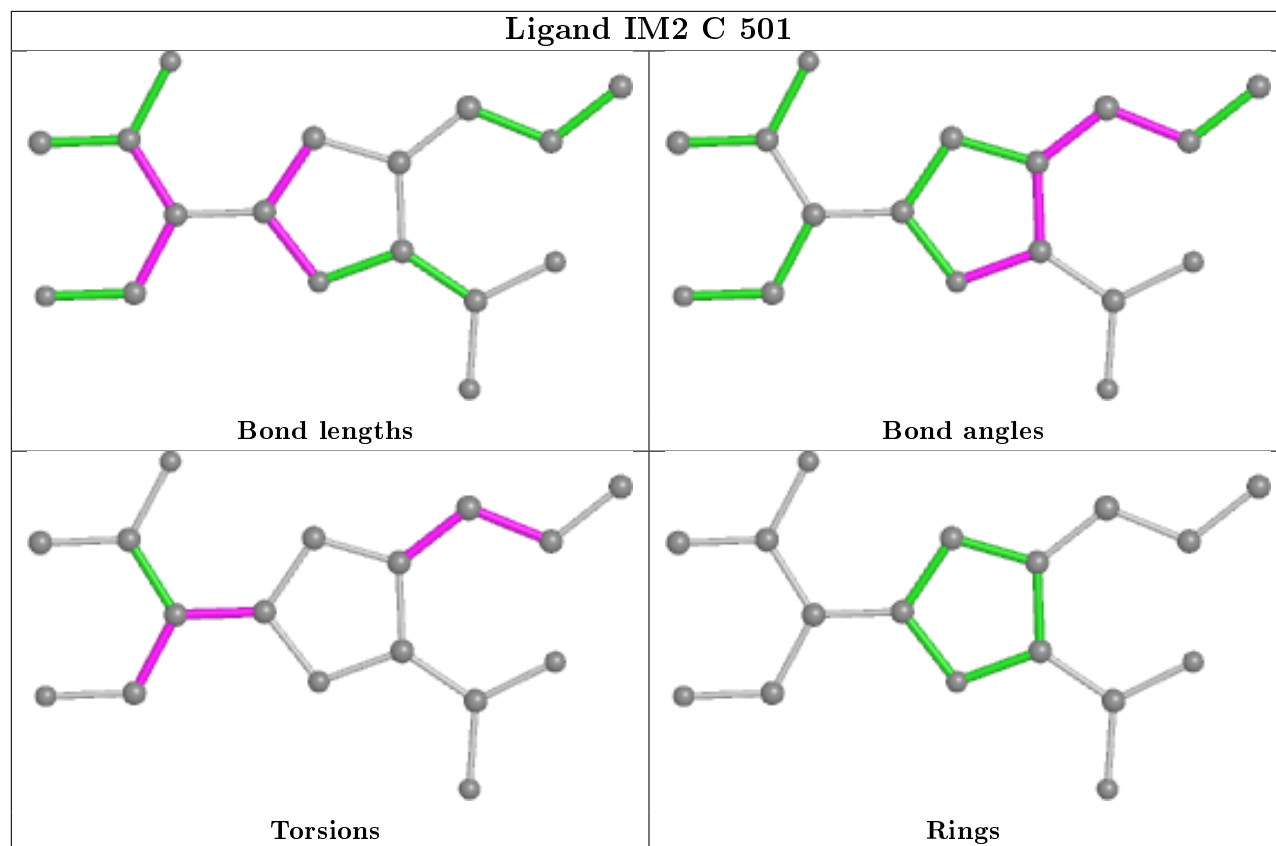
Bond angles

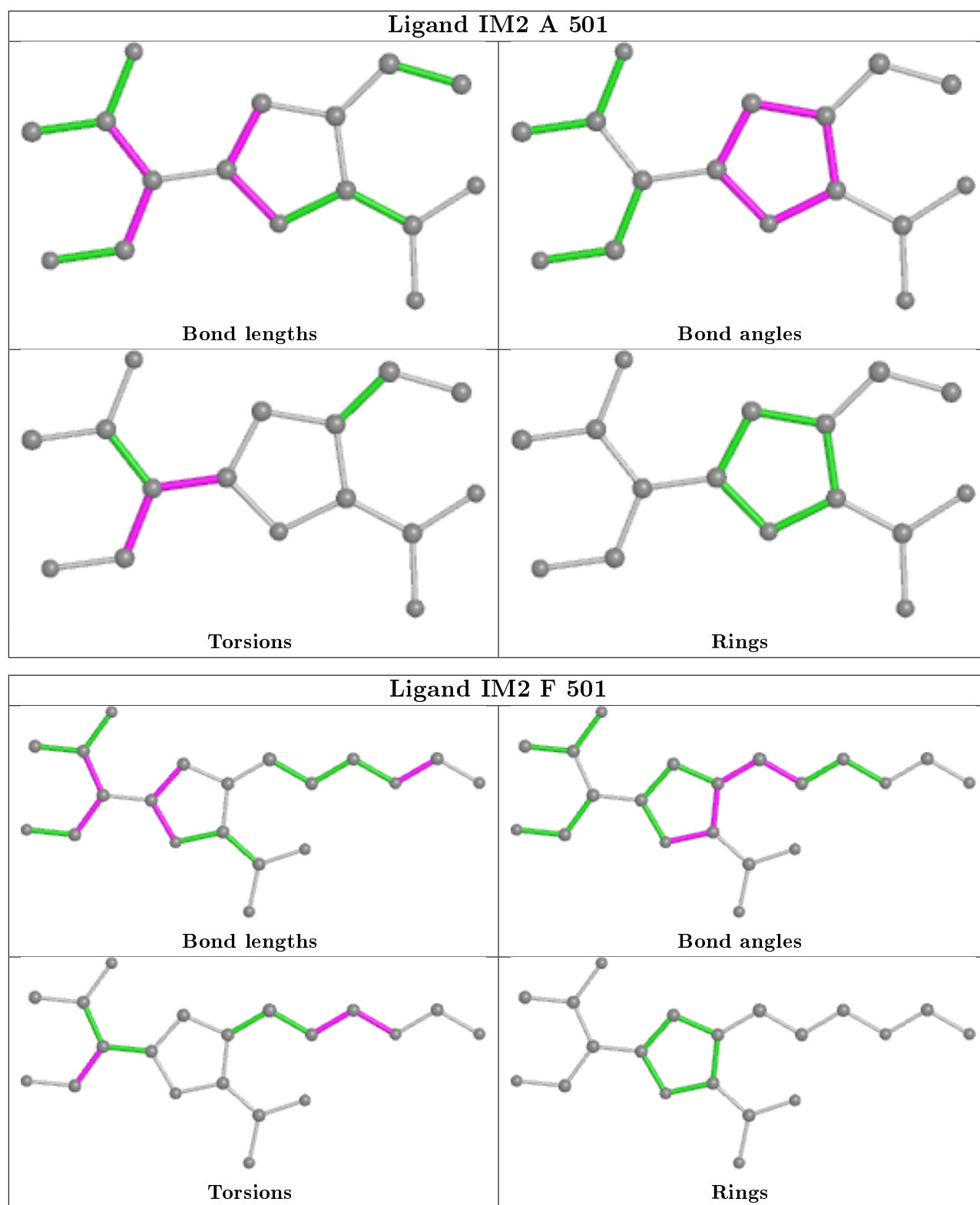


Torsions



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	266/272 (97%)	-0.31	3 (1%) 80 80	13, 20, 33, 62	0
1	B	266/272 (97%)	-0.36	1 (0%) 92 92	12, 20, 34, 62	0
1	C	267/272 (98%)	-0.10	3 (1%) 80 80	16, 26, 42, 61	0
1	D	264/272 (97%)	0.14	13 (4%) 29 27	15, 28, 44, 58	0
1	E	264/272 (97%)	-0.34	3 (1%) 80 80	13, 21, 33, 51	0
1	F	264/272 (97%)	-0.24	5 (1%) 66 65	13, 23, 37, 52	0
All	All	1591/1632 (97%)	-0.20	28 (1%) 68 67	12, 22, 39, 62	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	PRO	5.3
1	E	316	ASN	4.6
1	F	316	ASN	4.2
1	D	244	GLN	4.1
1	E	404	GLY	3.7

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 carbohydrates in this entry.

6.4 Ligands ⓘ

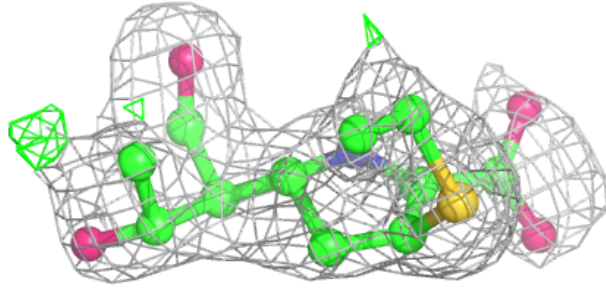
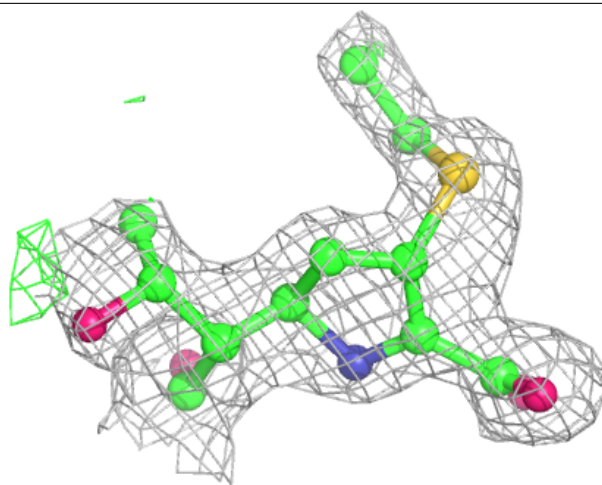
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	506	6/6	0.71	0.37	33,37,47,48	0
3	GOL	D	502	6/6	0.74	0.29	36,41,51,53	0
3	GOL	B	503	6/6	0.74	0.21	27,33,38,40	0
3	GOL	E	504	6/6	0.74	0.29	20,36,45,54	0
3	GOL	B	507	6/6	0.75	0.29	37,47,50,54	0
3	GOL	B	504	6/6	0.76	0.25	36,39,42,43	0
3	GOL	F	505	6/6	0.76	0.21	36,46,52,56	0
3	GOL	E	507	6/6	0.77	0.15	34,35,38,38	0
3	GOL	F	502	6/6	0.78	0.22	25,33,38,49	0
3	GOL	A	505	6/6	0.80	0.19	39,42,42,48	0
3	GOL	B	506	6/6	0.81	0.23	29,34,38,41	0
3	GOL	E	506	6/6	0.81	0.29	28,36,41,44	0
3	GOL	E	505	6/6	0.82	0.31	32,37,39,42	0
3	GOL	F	503	6/6	0.82	0.26	27,29,40,51	0
3	GOL	C	503	6/6	0.83	0.33	27,36,49,54	0
3	GOL	A	504	6/6	0.84	0.23	31,39,43,43	0
3	GOL	A	503	6/6	0.85	0.20	15,33,39,43	0
3	GOL	F	504	6/6	0.85	0.16	26,31,47,48	0
3	GOL	B	505	6/6	0.86	0.18	30,35,38,39	0
3	GOL	A	502	6/6	0.86	0.24	28,35,38,43	0
2	IM2	C	501	17/20	0.86	0.14	27,40,51,67	0
3	GOL	C	502	6/6	0.89	0.13	23,38,42,42	0
2	IM2	B	501	17/20	0.89	0.11	20,27,44,52	0
2	IM2	A	501	16/20	0.91	0.10	22,30,42,55	0
3	GOL	E	503	6/6	0.91	0.17	24,32,34,44	0
2	IM2	D	501	17/20	0.92	0.08	19,24,33,34	0
3	GOL	B	502	6/6	0.93	0.14	19,26,35,38	0
2	IM2	F	501	20/20	0.93	0.09	18,21,50,51	0
2	IM2	E	501	20/20	0.95	0.10	17,20,64,71	0
3	GOL	E	502	6/6	0.95	0.10	18,28,35,40	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.

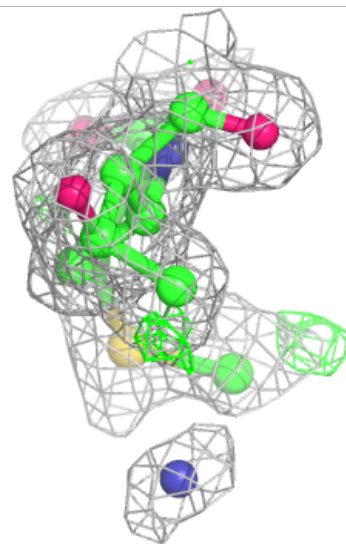
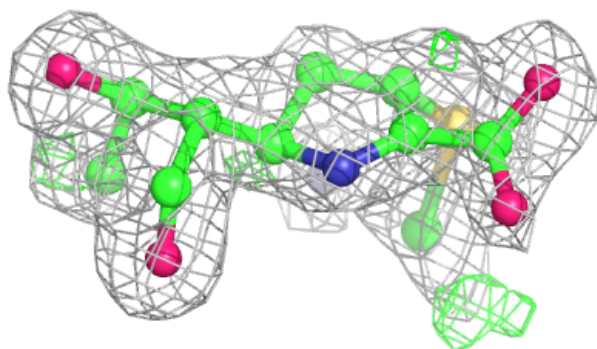
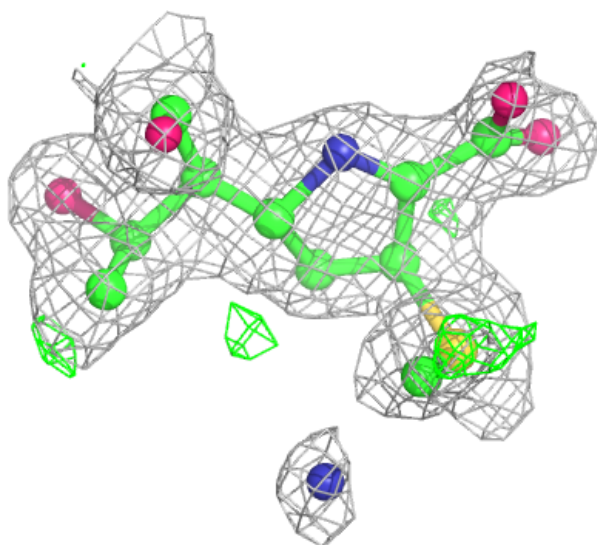
Electron density around IM2 C 501:

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



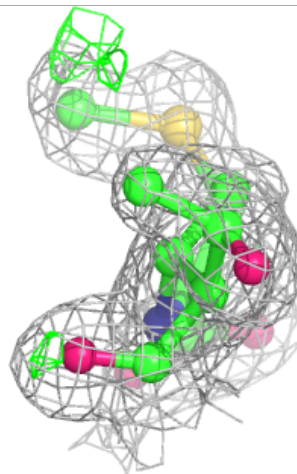
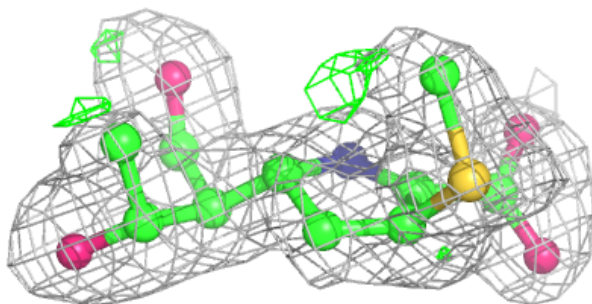
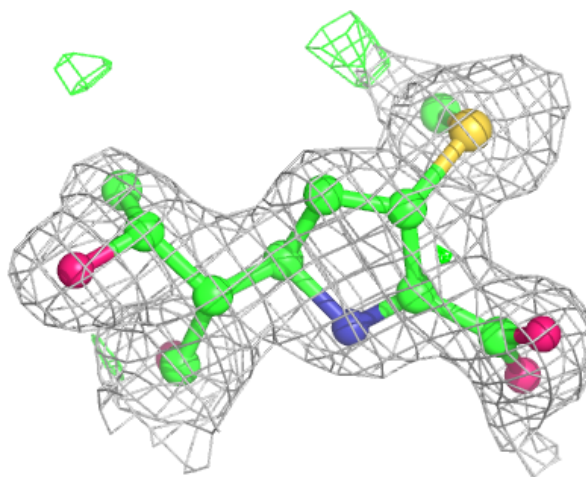
Electron density around IM2 B 501:

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



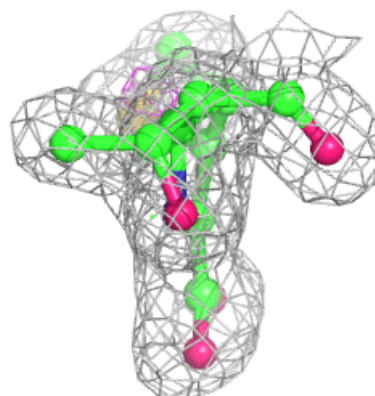
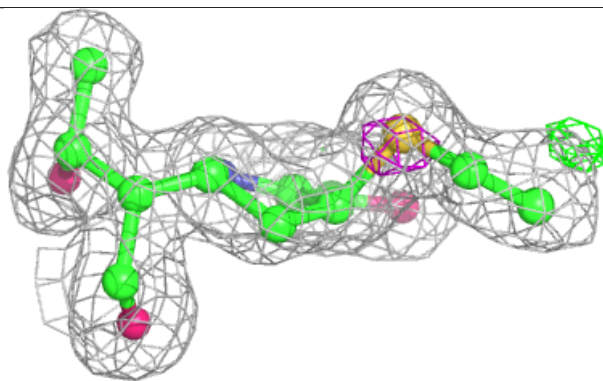
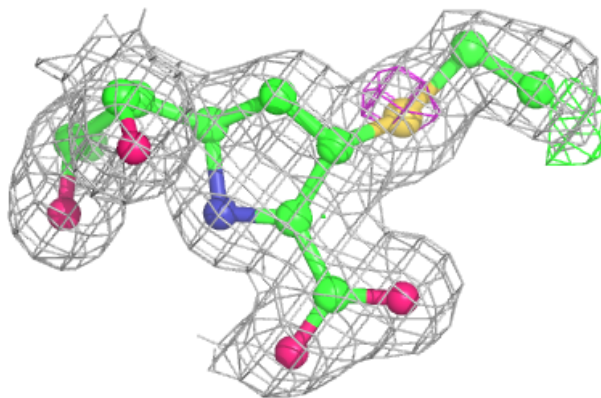
Electron density around IM2 A 501:

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

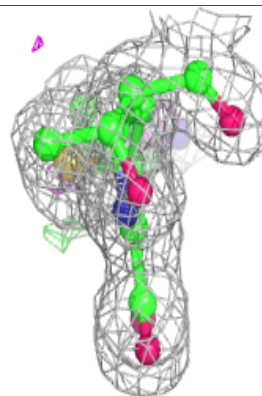
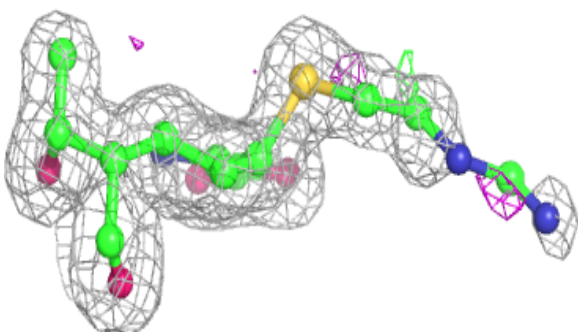
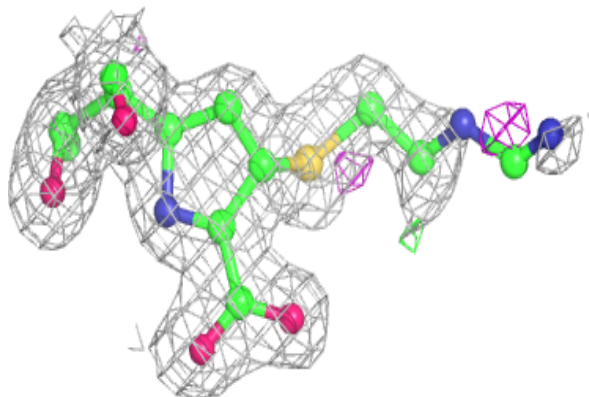


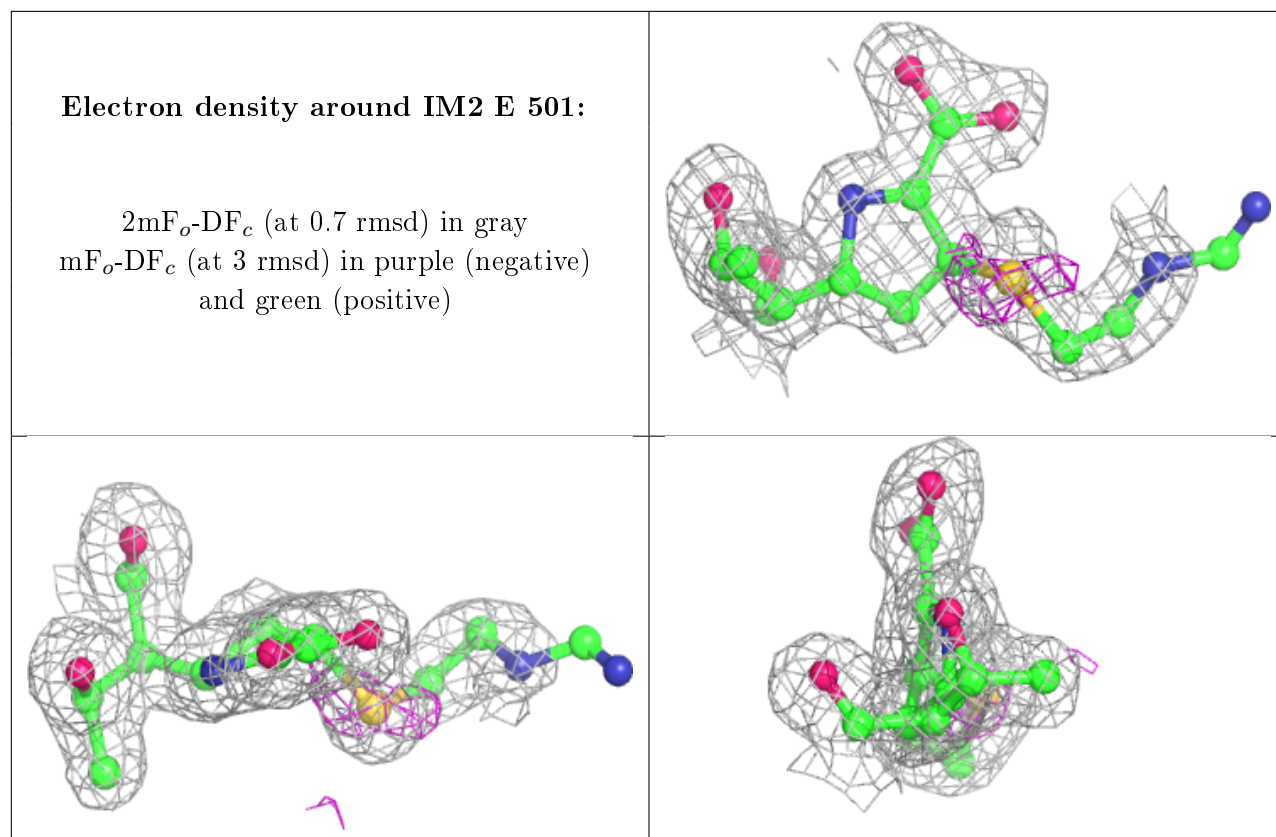
Electron density around IM2 D 501:

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

**Electron density around IM2 F 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.