



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:25 pm BST

PDB ID : 9GOW / pdb_00009gow
Title : Crystal structure of phosphorylated human IRE1a in complex with IA107
Authors : Liu, Y.; Gasper, R.; Wu, P.
Deposited on : 2024-09-06
Resolution : 3.00 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

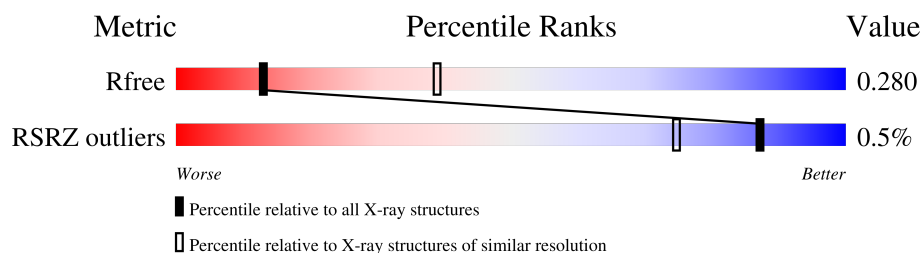
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12419 atoms, of which 60 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.

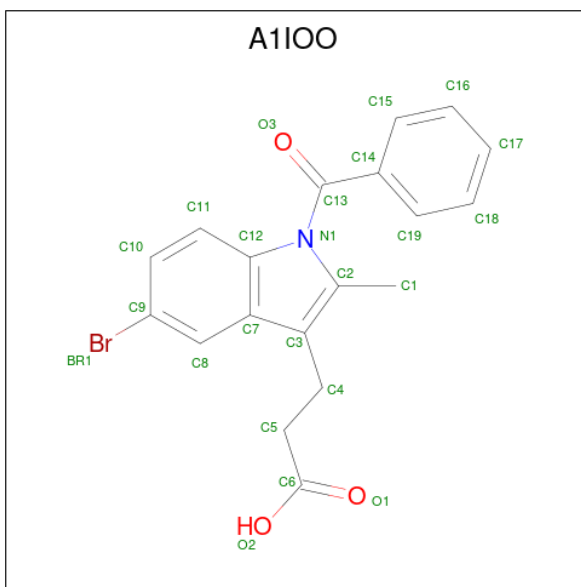
- Molecule 1 is a protein called Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	B	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	C	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	D	303	Total	C	N	O	P	S	0	0	0
			2444	1552	421	452	3	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLY	-	expression tag	UNP O75460
A	545	GLY	-	expression tag	UNP O75460
A	546	SER	-	expression tag	UNP O75460
B	544	GLY	-	expression tag	UNP O75460
B	545	GLY	-	expression tag	UNP O75460
B	546	SER	-	expression tag	UNP O75460
C	544	GLY	-	expression tag	UNP O75460
C	545	GLY	-	expression tag	UNP O75460
C	546	SER	-	expression tag	UNP O75460
D	544	GLY	-	expression tag	UNP O75460
D	545	GLY	-	expression tag	UNP O75460
D	546	SER	-	expression tag	UNP O75460

- Molecule 2 is 3-[5-bromanyl-2-methyl-1-(phenylcarbonyl)indol-3-yl]propanoic acid (CCD ID: A1IOO) (formula: C₁₉H₁₆BrNO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	H	N	O		
2	A	1	Total 39	1	19	15	1	3	0	0
2	B	1	Total 39	1	19	15	1	3	0	0
2	C	1	Total 39	1	19	15	1	3	0	0
2	D	1	Total 39	1	19	15	1	3	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.18Å 77.50Å 141.06Å 74.61° 78.09° 65.63°	Depositor
Resolution (Å)	47.91 – 3.00 47.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (47.91-3.00) 91.9 (47.91-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.231 , 0.281 0.231 , 0.280	Depositor DCC
R_{free} test set	2287 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12419	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	724	1	8,9,10	1.57	1 (12%)	8,12,14	1.32	1 (12%)
1	SEP	D	726	1	8,9,10	1.55	1 (12%)	8,12,14	1.59	2 (25%)
1	SEP	A	726	1	8,9,10	1.58	1 (12%)	8,12,14	1.64	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	D	729	1	8,9,10	1.57	1 (12%)	8,12,14	1.66	2 (25%)
1	SEP	A	729	1	8,9,10	1.55	1 (12%)	8,12,14	1.42	1 (12%)
1	SEP	D	724	1	8,9,10	1.55	1 (12%)	8,12,14	1.56	2 (25%)
1	SEP	B	724	1	8,9,10	1.58	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	C	726	1	8,9,10	1.56	1 (12%)	8,12,14	1.64	2 (25%)
1	SEP	C	729	1	8,9,10	1.57	1 (12%)	8,12,14	1.62	2 (25%)
1	SEP	B	726	1	8,9,10	1.57	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	B	729	1	8,9,10	1.58	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	C	724	1	8,9,10	1.58	1 (12%)	8,12,14	1.44	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	724	1	-	3/5/8/10	-
1	SEP	D	726	1	-	4/5/8/10	-
1	SEP	A	726	1	-	1/5/8/10	-
1	SEP	D	729	1	-	0/5/8/10	-
1	SEP	A	729	1	-	0/5/8/10	-
1	SEP	D	724	1	-	2/5/8/10	-
1	SEP	B	724	1	-	3/5/8/10	-
1	SEP	C	726	1	-	1/5/8/10	-
1	SEP	C	729	1	-	0/5/8/10	-
1	SEP	B	726	1	-	1/5/8/10	-
1	SEP	B	729	1	-	4/5/8/10	-
1	SEP	C	724	1	-	5/5/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	724	SEP	P-O1P	3.47	1.61	1.50
1	B	729	SEP	P-O1P	3.44	1.61	1.50
1	B	726	SEP	P-O1P	3.43	1.61	1.50
1	D	729	SEP	P-O1P	3.43	1.61	1.50
1	C	724	SEP	P-O1P	3.43	1.61	1.50
1	A	724	SEP	P-O1P	3.42	1.61	1.50
1	D	726	SEP	P-O1P	3.41	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	729	SEP	P-O1P	3.40	1.61	1.50
1	A	726	SEP	P-O1P	3.40	1.61	1.50
1	C	726	SEP	P-O1P	3.40	1.61	1.50
1	D	724	SEP	P-O1P	3.39	1.61	1.50
1	A	729	SEP	P-O1P	3.38	1.61	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	SEP	OG-CB-CA	3.38	111.43	108.14
1	B	724	SEP	P-OG-CB	-3.28	109.27	118.30
1	A	726	SEP	OG-CB-CA	3.27	111.33	108.14
1	C	726	SEP	OG-CB-CA	3.18	111.24	108.14
1	D	729	SEP	OG-CB-CA	3.14	111.20	108.14
1	A	729	SEP	P-OG-CB	-3.10	109.75	118.30
1	C	729	SEP	OG-CB-CA	3.02	111.08	108.14
1	D	726	SEP	P-OG-CB	-2.98	110.08	118.30
1	A	724	SEP	P-OG-CB	-2.92	110.25	118.30
1	C	729	SEP	P-OG-CB	-2.88	110.35	118.30
1	C	726	SEP	P-OG-CB	-2.85	110.46	118.30
1	D	726	SEP	OG-CB-CA	2.83	110.90	108.14
1	D	724	SEP	OG-CB-CA	2.82	110.89	108.14
1	B	729	SEP	OG-CB-CA	2.81	110.88	108.14
1	D	729	SEP	P-OG-CB	-2.80	110.57	118.30
1	C	724	SEP	OG-CB-CA	2.80	110.87	108.14
1	B	729	SEP	P-OG-CB	-2.76	110.70	118.30
1	D	724	SEP	P-OG-CB	-2.74	110.74	118.30
1	A	726	SEP	P-OG-CB	-2.71	110.82	118.30
1	B	726	SEP	P-OG-CB	-2.52	111.35	118.30
1	C	724	SEP	P-OG-CB	-2.18	112.29	118.30
1	B	726	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	724	SEP	CB-OG-P-O1P
1	A	724	SEP	CB-OG-P-O2P
1	A	724	SEP	CB-OG-P-O3P
1	B	724	SEP	CB-OG-P-O1P
1	B	724	SEP	CB-OG-P-O3P
1	B	726	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	B	729	SEP	N-CA-CB-OG
1	B	729	SEP	CB-OG-P-O2P
1	B	729	SEP	CB-OG-P-O3P
1	C	724	SEP	CB-OG-P-O2P
1	C	724	SEP	CB-OG-P-O3P
1	D	724	SEP	N-CA-CB-OG
1	D	726	SEP	N-CA-CB-OG
1	D	726	SEP	CB-OG-P-O1P
1	D	726	SEP	CB-OG-P-O2P
1	D	726	SEP	CB-OG-P-O3P
1	C	724	SEP	CB-OG-P-O1P
1	A	726	SEP	CA-CB-OG-P
1	C	724	SEP	CA-CB-OG-P
1	C	726	SEP	CA-CB-OG-P
1	D	724	SEP	CA-CB-OG-P
1	C	724	SEP	N-CA-CB-OG
1	B	724	SEP	CB-OG-P-O2P
1	B	729	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1IOO	B	1001	-	23,26,26	1.04	1 (4%)	27,37,37	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1IOO	D	1001	-	23,26,26	1.04	1 (4%)	27,37,37	0.75	0
2	A1IOO	A	1001	-	23,26,26	1.07	2 (8%)	27,37,37	0.72	0
2	A1IOO	C	1001	-	23,26,26	1.06	2 (8%)	27,37,37	0.81	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
2	A1IOO	B	1001	-	-	4/9/13/13	0/3/3/3
2	A1IOO	D	1001	-	-	4/9/13/13	0/3/3/3
2	A1IOO	A	1001	-	-	2/9/13/13	0/3/3/3
2	A1IOO	C	1001	-	-	4/9/13/13	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	A1IOO	C2-N1	3.62	1.42	1.36
2	B	1001	A1IOO	C2-N1	3.42	1.42	1.36
2	C	1001	A1IOO	C2-N1	3.42	1.42	1.36
2	D	1001	A1IOO	C2-N1	3.40	1.42	1.36
2	C	1001	A1IOO	C12-N1	2.12	1.42	1.39
2	A	1001	A1IOO	C12-N1	2.04	1.42	1.39

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	A1IOO	N1-C13-C14-C19
2	C	1001	A1IOO	N1-C13-C14-C15
2	D	1001	A1IOO	N1-C13-C14-C15
2	D	1001	A1IOO	N1-C13-C14-C19
2	C	1001	A1IOO	N1-C13-C14-C19
2	B	1001	A1IOO	C4-C5-C6-O1
2	C	1001	A1IOO	C4-C5-C6-O1
2	D	1001	A1IOO	C4-C5-C6-O2
2	D	1001	A1IOO	C4-C5-C6-O1

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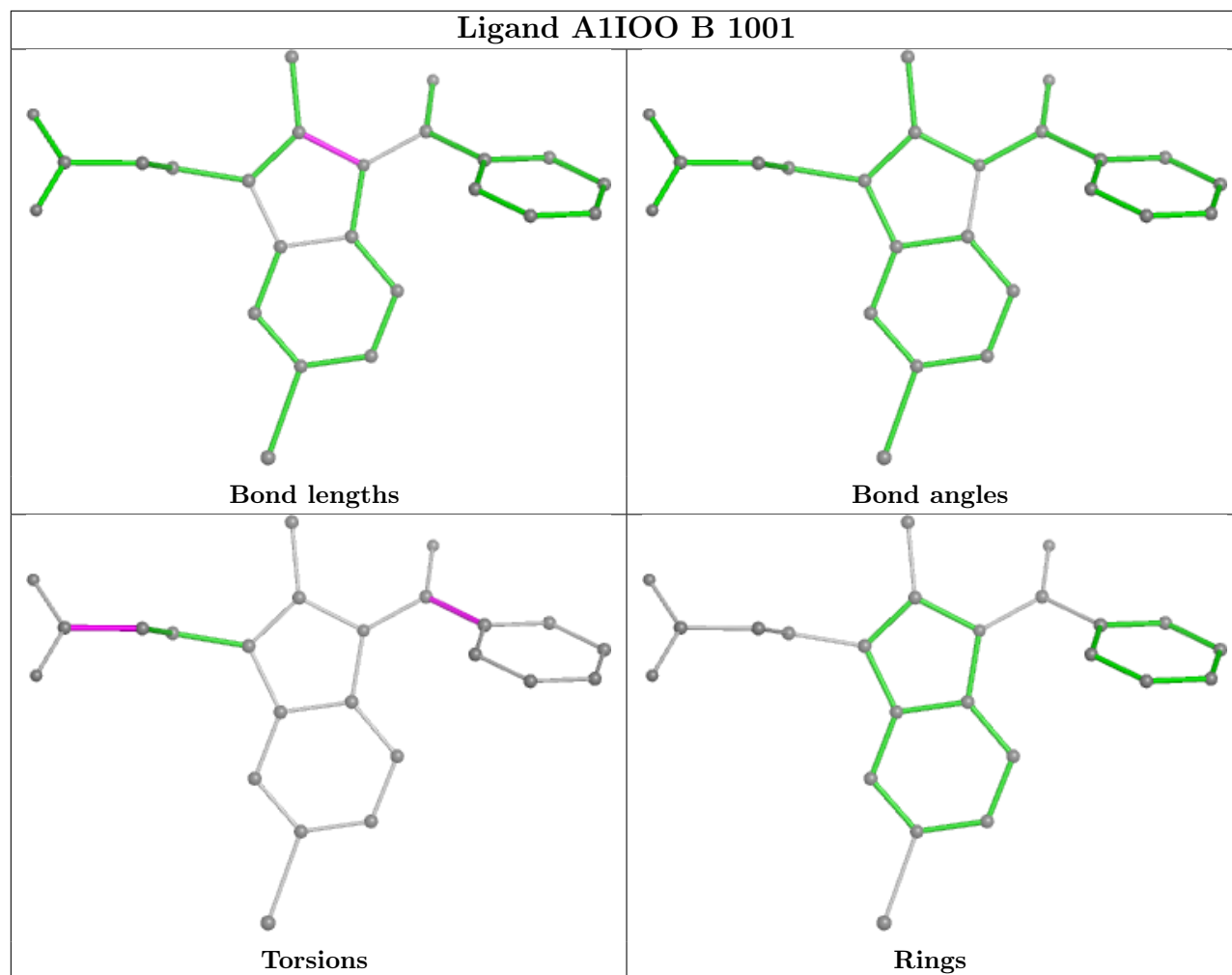
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Mol	Chain	Res	Type	Atoms
2	B	1001	A1IOO	C4-C5-C6-O2
2	A	1001	A1IOO	C4-C5-C6-O2
2	C	1001	A1IOO	C4-C5-C6-O2
2	A	1001	A1IOO	C4-C5-C6-O1
2	B	1001	A1IOO	N1-C13-C14-C15

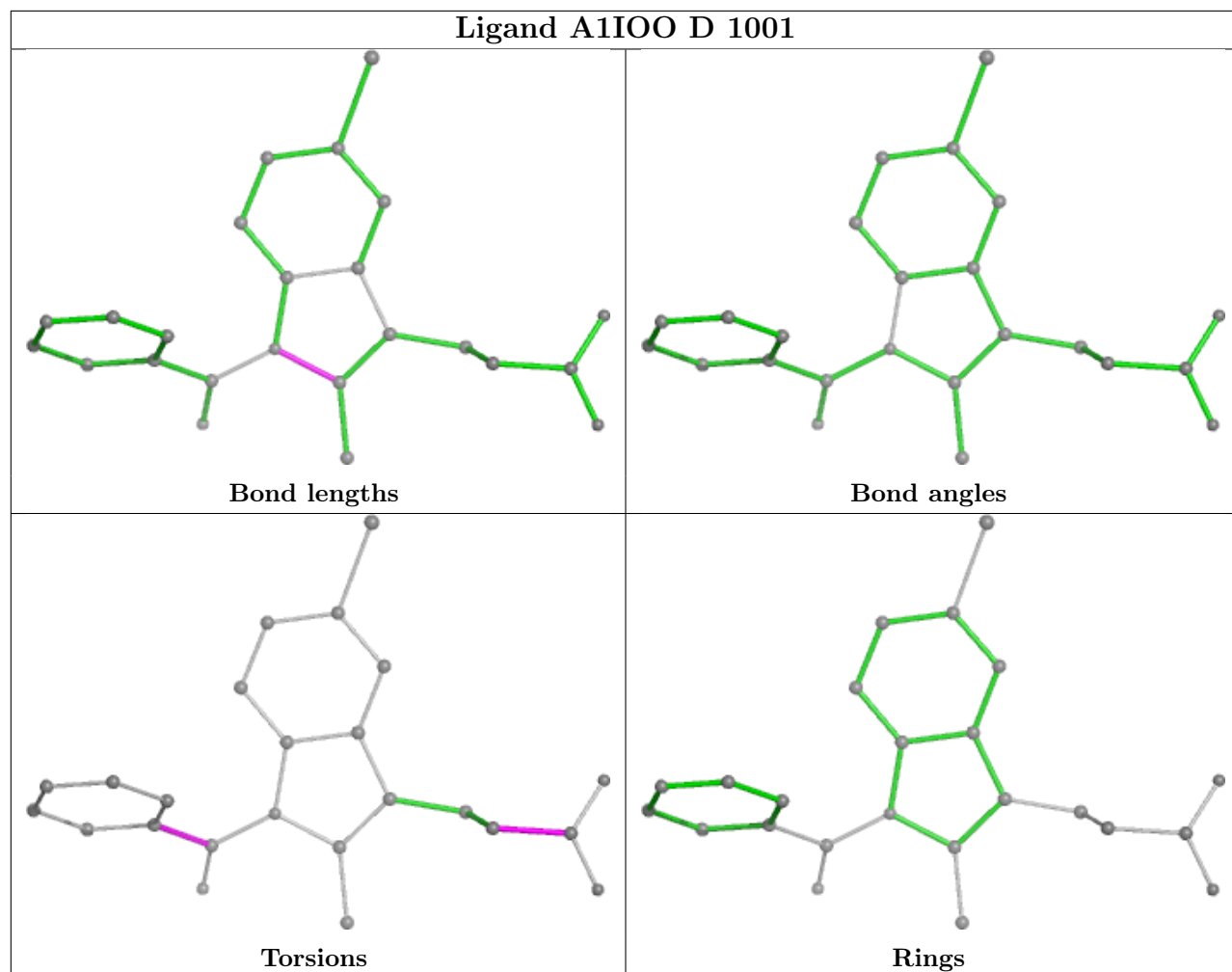
There are no ring outliers.

No monomer is involved in short contacts.

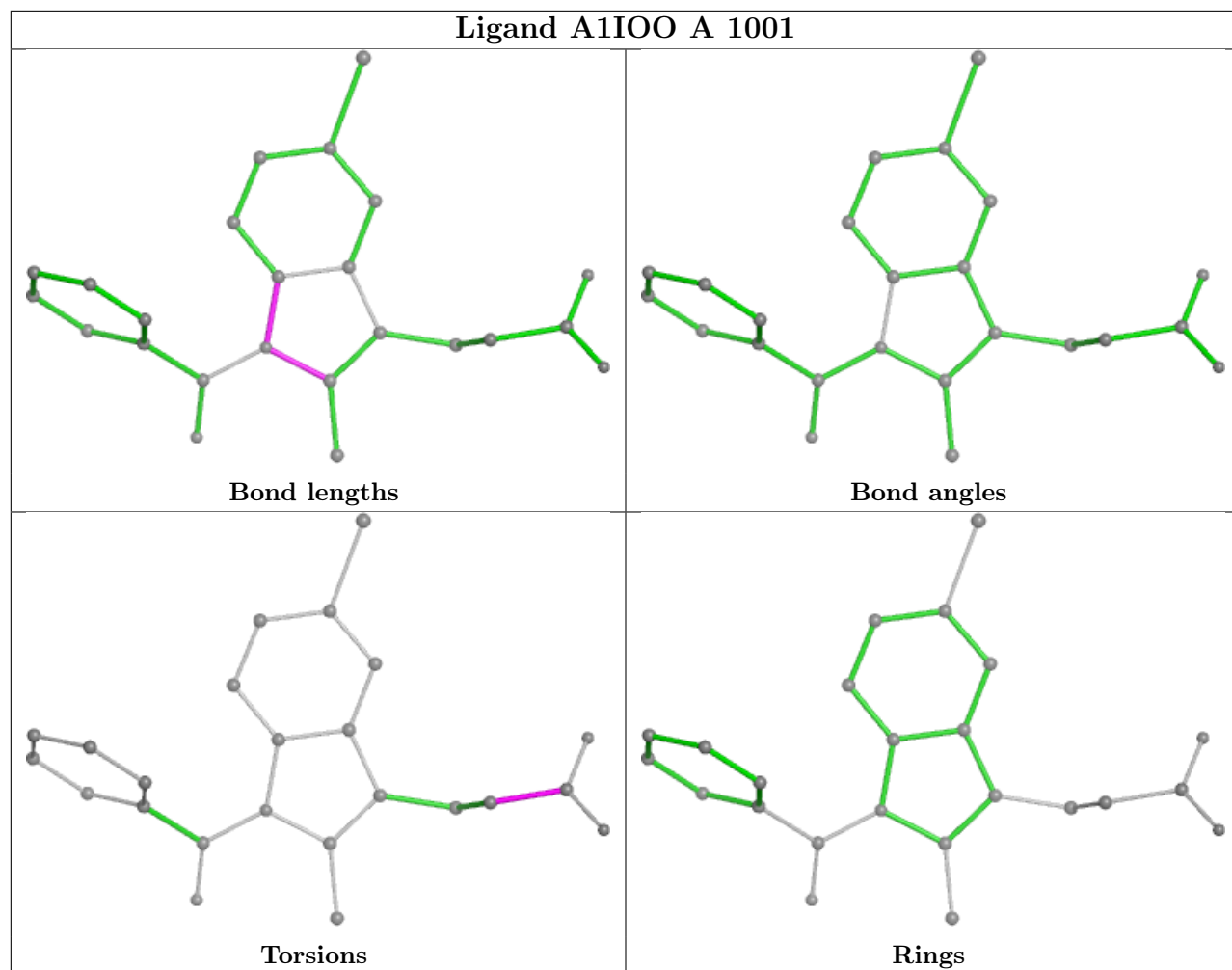
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

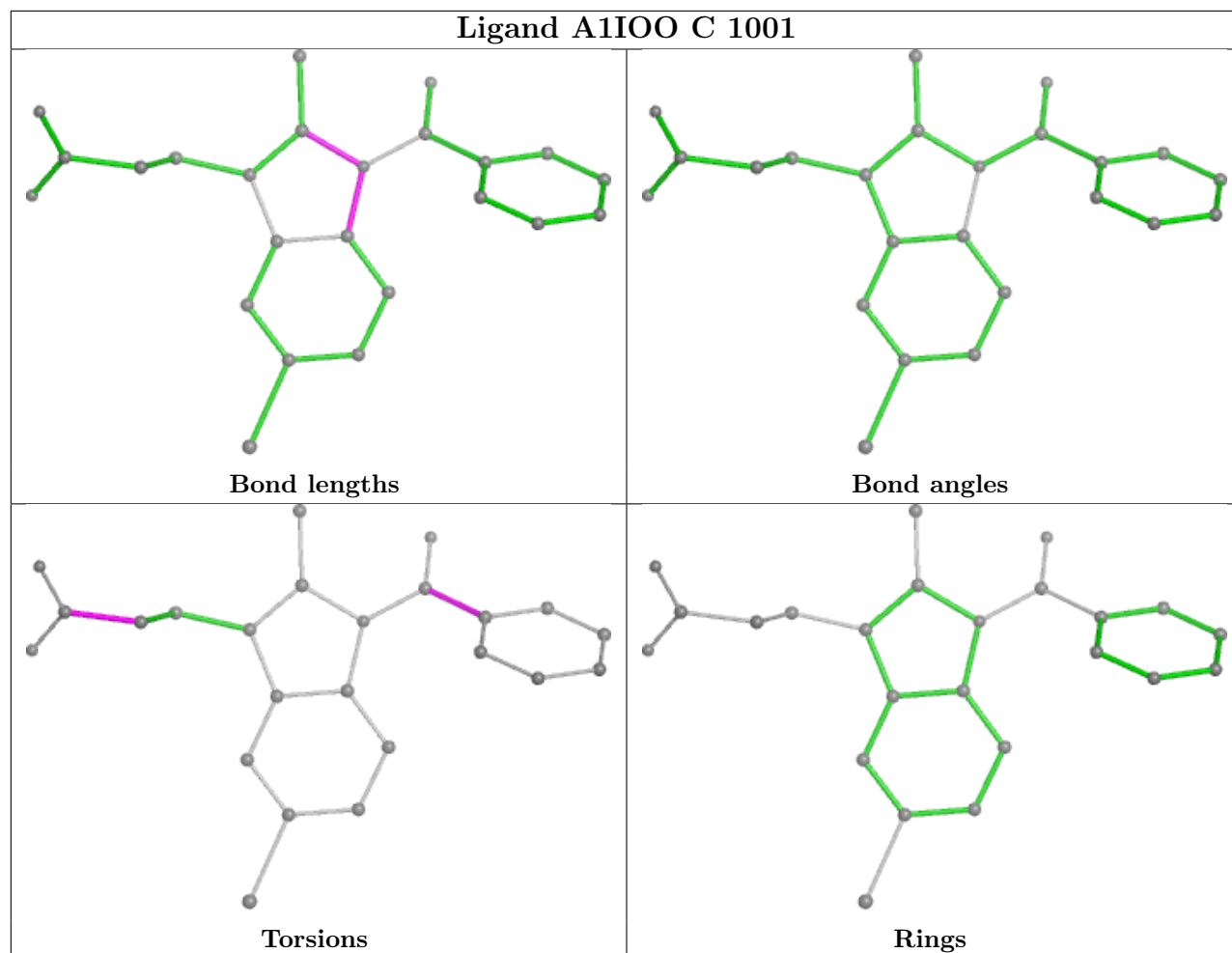


Ligand A1IOO D 1001



Ligand A1IOO A 1001





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	400/434 (92%)	-0.20	2 (0%) 87 75	52, 77, 114, 139	0
1	B	400/434 (92%)	-0.29	1 (0%) 90 81	51, 72, 100, 122	0
1	C	400/434 (92%)	-0.03	1 (0%) 90 81	58, 91, 122, 180	0
1	D	300/434 (69%)	0.11	3 (1%) 79 60	62, 93, 131, 154	0
All	All	1500/1736 (86%)	-0.12	7 (0%) 87 75	51, 82, 121, 180	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	VAL	3.2
1	D	731	VAL	2.7
1	B	891	THR	2.4
1	D	841	PHE	2.3
1	A	645	CYS	2.3
1	D	842	PHE	2.3
1	C	906	ASN	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	C	726	10/11	0.71	0.10	126,137,148,148	0
1	SEP	D	724	10/11	0.73	0.10	127,130,132,135	0
1	SEP	C	729	10/11	0.77	0.10	124,140,147,147	0
1	SEP	D	726	10/11	0.78	0.10	120,127,129,130	0
1	SEP	B	726	10/11	0.80	0.13	97,108,120,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	D	729	10/11	0.83	0.09	112,118,123,127	0
1	SEP	C	724	10/11	0.86	0.08	113,122,129,133	0
1	SEP	B	729	10/11	0.88	0.10	93,103,110,111	0
1	SEP	A	726	10/11	0.89	0.09	83,92,104,108	0
1	SEP	B	724	10/11	0.91	0.07	83,88,104,106	0
1	SEP	A	724	10/11	0.92	0.07	85,90,106,109	0
1	SEP	A	729	10/11	0.94	0.07	75,80,87,95	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

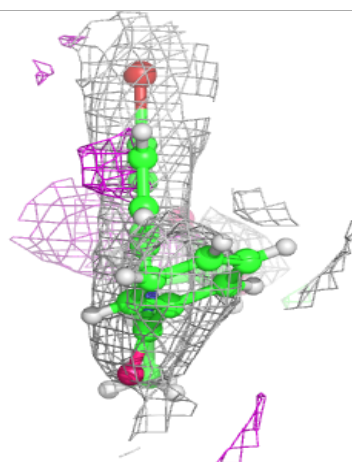
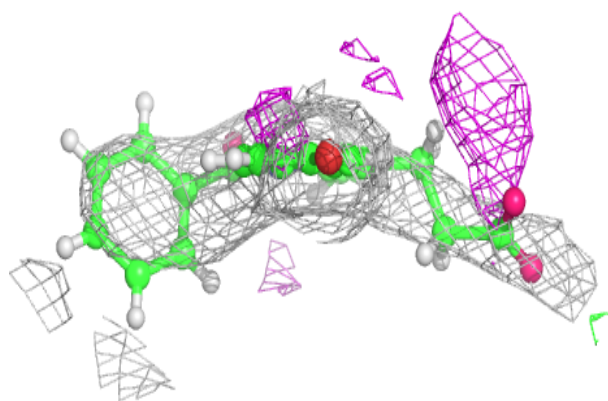
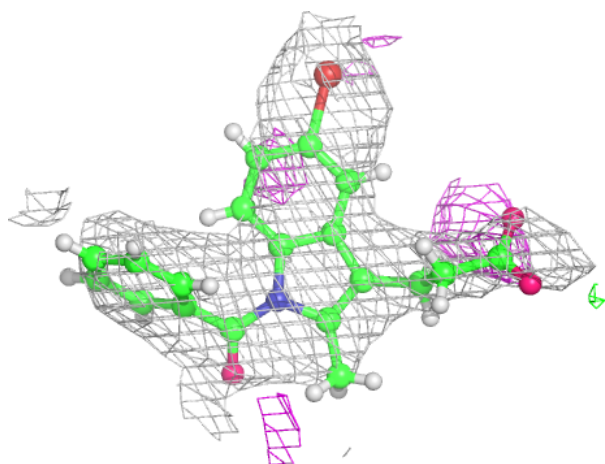
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1IOO	A	1001	24/24	0.84	0.12	79,96,128,165	0
2	A1IOO	C	1001	24/24	0.88	0.11	77,93,116,147	0
2	A1IOO	D	1001	24/24	0.94	0.09	73,80,97,113	0
2	A1IOO	B	1001	24/24	0.95	0.08	64,77,93,117	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.

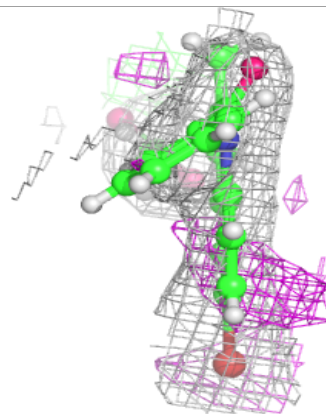
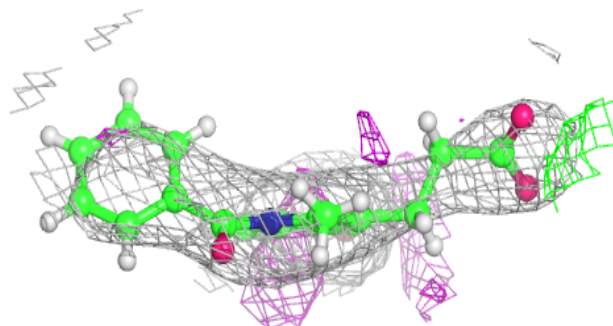
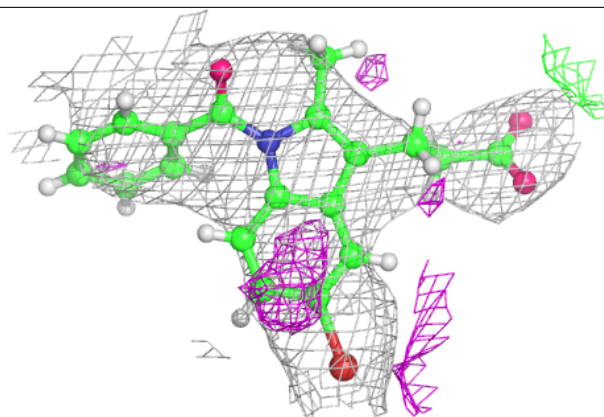
Electron density around A1IOO A 1001:

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



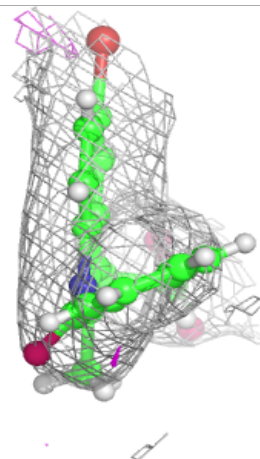
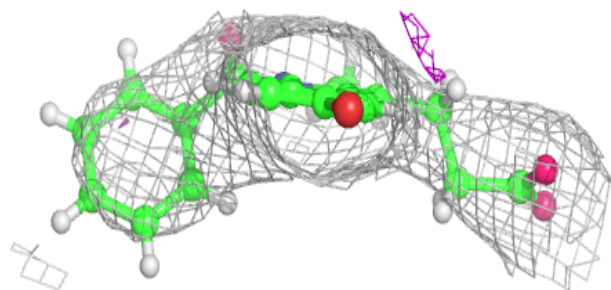
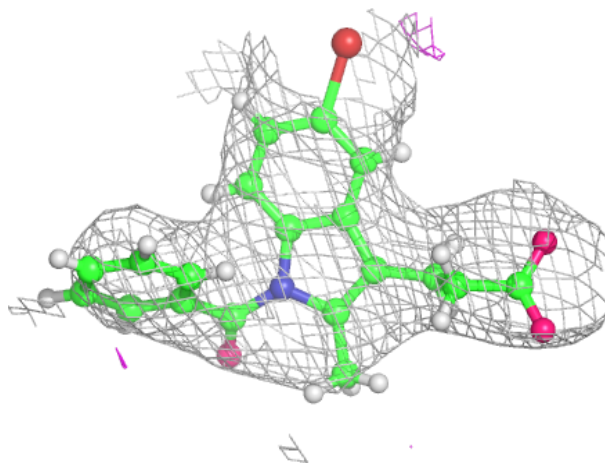
Electron density around A1IOO C 1001:

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



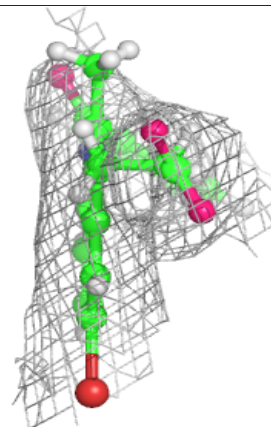
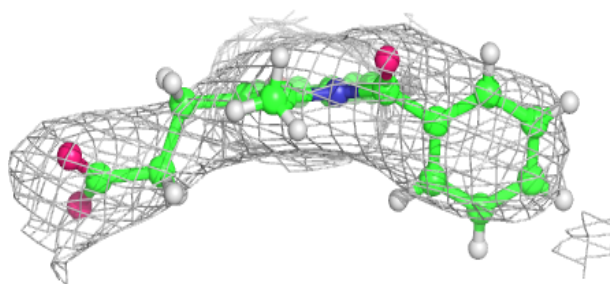
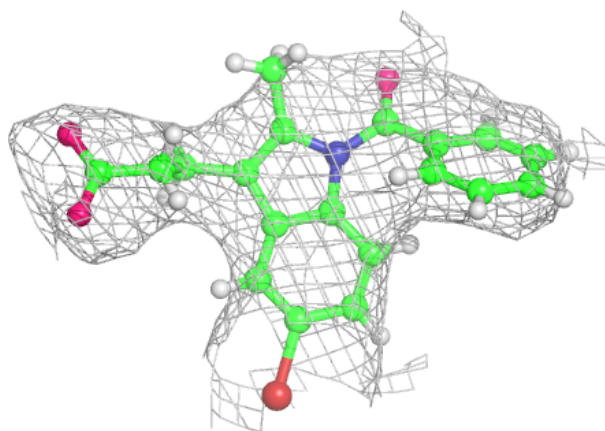
Electron density around A1IOO D 1001:

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



Electron density around A1IOO B 1001:

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



5.5 Other polymers ⓘ

There are no such residues in this entry.