Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:35 am BST

PDB ID	:	5HL9
Title	:	E. coli PBP1b in complex with acyl-ampicillin and moenomycin
Authors	:	King, D.T.; Strynadka, N.C.J.
Deposited on	:	2016-01-14
Resolution	:	2.70 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:

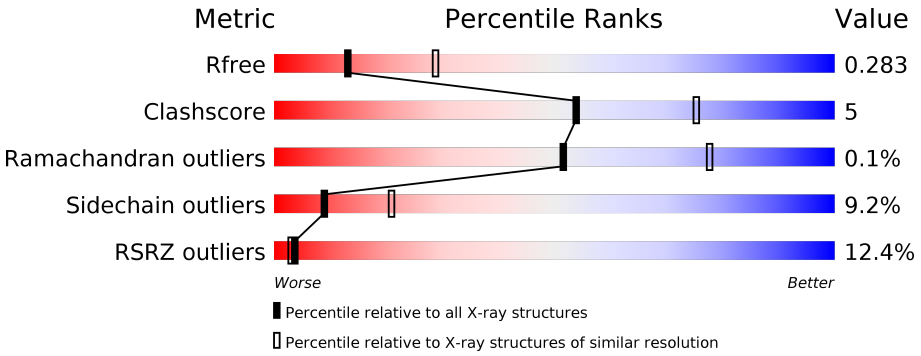
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	747	12% 78% 14% • 7%

2 Entry composition

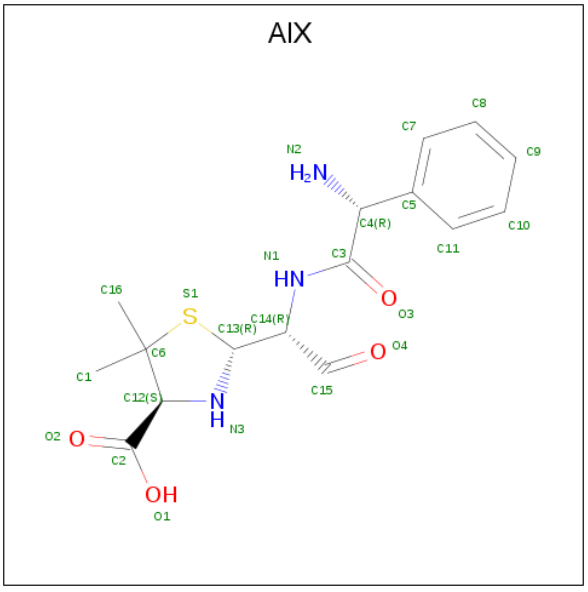
There are 4 unique types of molecules in this entry. The entry contains 5689 atoms, of which 19 are hydrogens and 0 are deuteriums.

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 Penicillin-binding protein 1B.

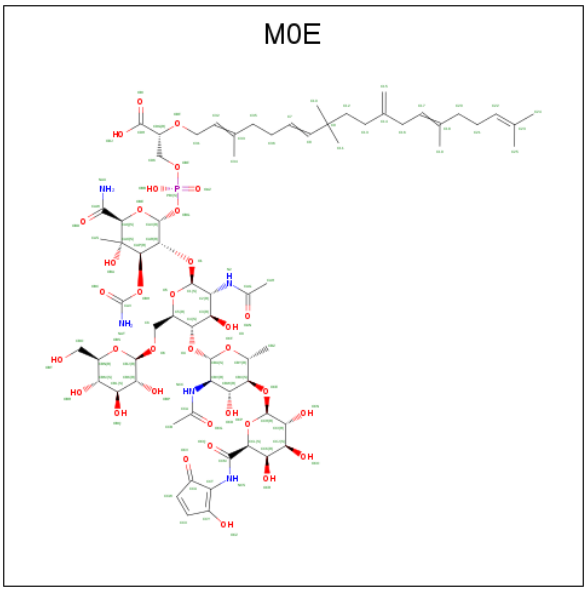
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5462	3468	962	1007	25			

- Molecule 2 is (2R,4S)-2-[(1R)-1-{[(2R)-2-amino-2-phenylacetyl]amino}-2-oxoethyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: AIX) (formula: $C_{16}H_{21}N_3O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			43	16	19	3	4	1		

- Molecule 3 is MOENOMYCIN (three-letter code: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			77	39	5	32	1		

- Molecule 4 is water.

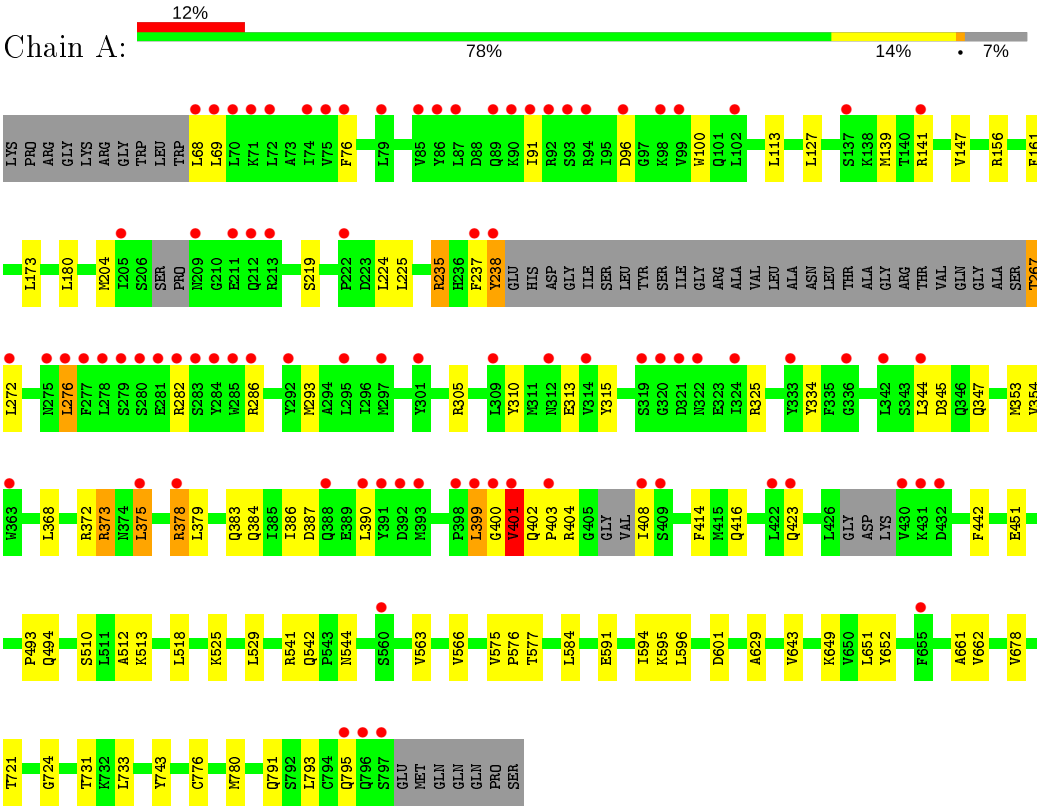
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		

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 (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: Penicillin-binding protein 1B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.44Å 63.80Å 299.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.34 – 2.70 62.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.34-2.70) 99.7 (62.40-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.240 , 0.265 0.257 , 0.283	Depositor DCC
R_{free} test set	1717 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5689	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: M0E, AIX

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	0.43	0/5569	0.68	0/7554

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	5462	0	5519	49	0
2	A	24	19	19	0	0
3	A	77	0	58	14	0
4	A	107	0	0	0	0
All	All	5670	19	5596	59	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 (59) 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)
3:A:902:M0E:O1	3:A:902:M0E:CAR	1.65	1.45
3:A:902:M0E:OBG	3:A:902:M0E:CAX	1.67	1.43
3:A:902:M0E:C1	3:A:902:M0E:CAR	2.27	1.13
1:A:271:GLN:HG2	3:A:902:M0E:HAT2	1.08	1.11
1:A:235:ARG:HB3	1:A:237:PHE:CE2	2.06	0.89
1:A:271:GLN:HG2	3:A:902:M0E:NAT	1.90	0.84
1:A:399:LEU:HD13	1:A:399:LEU:H	1.51	0.75
3:A:902:M0E:O1	3:A:902:M0E:CAP	2.37	0.72
1:A:643:VAL:HG22	1:A:652:TYR:HB3	1.75	0.68
1:A:678:VAL:O	1:A:684:ARG:HA	2.04	0.58
1:A:378:ARG:HG3	1:A:379:LEU:N	2.19	0.57
3:A:902:M0E:HAS2	3:A:902:M0E:OBD	2.04	0.57
3:A:902:M0E:HCB2	3:A:902:M0E:HBJ	1.87	0.56
1:A:356:GLY:HA2	3:A:902:M0E:OCG	2.06	0.56
3:A:902:M0E:PBI	3:A:902:M0E:CAX	2.93	0.56
1:A:776:CYS:HA	1:A:793:LEU:HD22	1.87	0.55
1:A:235:ARG:HB3	1:A:237:PHE:CZ	2.42	0.54
1:A:91:ILE:HD11	1:A:293:MET:HG2	1.92	0.52
1:A:345:ASP:HB2	1:A:373:ARG:HH21	1.74	0.52
3:A:902:M0E:OCD	3:A:902:M0E:OCP	2.18	0.52
1:A:386:ILE:HG13	1:A:390:LEU:HD12	1.92	0.51
3:A:902:M0E:H1	3:A:902:M0E:CAR	2.32	0.51
1:A:595:LYS:HB3	1:A:661:ALA:HB1	1.94	0.50
1:A:315:TYR:HA	1:A:325:ARG:HB3	1.92	0.50
1:A:362:PRO:HG2	1:A:402:GLN:HE21	1.77	0.50
1:A:235:ARG:CB	1:A:237:PHE:CE2	2.89	0.50
1:A:235:ARG:O	1:A:237:PHE:CE1	2.65	0.49
1:A:267:THR:O	1:A:271:GLN:OE1	2.31	0.49
1:A:225:LEU:HD13	1:A:347:GLN:HG2	1.95	0.49
1:A:276:LEU:HD12	1:A:313:GLU:HG2	1.95	0.49
3:A:902:M0E:OBG	3:A:902:M0E:CAR	2.55	0.49
1:A:399:LEU:CD1	1:A:399:LEU:H	2.23	0.47
1:A:113:LEU:HD13	1:A:173:LEU:HD21	1.96	0.47
1:A:529:LEU:HB3	1:A:566:VAL:HB	1.95	0.47
1:A:591:GLU:HA	1:A:594:ILE:HD12	1.97	0.47
1:A:224:LEU:HD21	1:A:344:LEU:HD13	1.96	0.47
1:A:272:LEU:HD12	1:A:310:TYR:HB2	1.96	0.46
1:A:518:LEU:HD21	1:A:662:VAL:HG21	1.97	0.46
1:A:414:PHE:CE2	1:A:442:PHE:HB2	2.51	0.46
1:A:354:VAL:HG22	3:A:902:M0E:HAH3	1.98	0.46
1:A:479:ARG:HG3	1:A:629:ALA:HB1	1.97	0.46
1:A:643:VAL:HG23	1:A:651:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:HG22	1:A:270:GLN:HB2	1.98	0.45
1:A:451:GLU:HG3	1:A:493:PRO:HG2	1.99	0.45
1:A:510:SER:C	1:A:512:ALA:H	2.20	0.44
1:A:575:VAL:HB	1:A:576:PRO:HD3	2.00	0.44
1:A:373:ARG:HB3	1:A:373:ARG:HE	1.70	0.44
1:A:375:LEU:O	1:A:379:LEU:HD13	2.18	0.43
1:A:721:THR:HG21	1:A:743:TYR:HB2	1.99	0.43
1:A:238:TYR:CD2	1:A:238:TYR:N	2.86	0.43
1:A:513:LYS:HG2	1:A:577:THR:HG21	2.00	0.43
1:A:334:TYR:O	1:A:403:PRO:HD3	2.19	0.42
1:A:400:GLY:HA2	1:A:401:VAL:HG12	2.02	0.42
1:A:510:SER:C	1:A:512:ALA:N	2.72	0.42
1:A:156:ARG:HH22	1:A:166:GLU:HB3	1.84	0.42
1:A:724:GLY:HA2	1:A:731:THR:HG21	2.01	0.41
1:A:235:ARG:HG3	1:A:237:PHE:CZ	2.56	0.41
1:A:235:ARG:HG3	1:A:237:PHE:CE2	2.56	0.41
1:A:161:PHE:HB2	1:A:164:SER:O	2.21	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	685/747 (92%)	647 (94%)	37 (5%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	VAL

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	587/627 (94%)	533 (91%)	54 (9%)	9 21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	69	LEU
1	A	76	PHE
1	A	96	ASP
1	A	100	TRP
1	A	127	LEU
1	A	139	MET
1	A	141	ARG
1	A	147	VAL
1	A	165	LYS
1	A	180	LEU
1	A	204	MET
1	A	219	SER
1	A	235	ARG
1	A	238	TYR
1	A	267	THR
1	A	268	LEU
1	A	276	LEU
1	A	282	ARG
1	A	286	ARG
1	A	305	ARG
1	A	353	MET
1	A	355	LYS
1	A	368	LEU
1	A	372	ARG
1	A	373	ARG
1	A	375	LEU
1	A	378	ARG
1	A	383	GLN
1	A	384	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	387	ASP
1	A	399	LEU
1	A	401	VAL
1	A	404	ARG
1	A	408	ILE
1	A	416	GLN
1	A	423	GLN
1	A	465	ARG
1	A	466	LYS
1	A	494	GLN
1	A	525	LYS
1	A	541	ARG
1	A	542	GLN
1	A	544	ASN
1	A	563	VAL
1	A	584	LEU
1	A	596	LEU
1	A	601	ASP
1	A	649	LYS
1	A	686	LEU
1	A	733	LEU
1	A	780	MET
1	A	791	GLN
1	A	795	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	M0E	A	902	-	76,81,114	3.91	39 (51%)	110,122,166	2.99	20 (18%)
2	AIX	A	901	1	16,25,25	3.01	6 (37%)	20,36,36	1.52	4 (20%)

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	M0E	A	902	-	-	15/47/158/206	0/5/5/6
2	AIX	A	901	1	-	0/12/37/37	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	M0E	OBH-CAV	12.17	1.63	1.35
3	A	902	M0E	O1-C1	-10.55	1.12	1.41
3	A	902	M0E	CAW-NAU	10.50	1.59	1.32
3	A	902	M0E	ODF-CDG	-8.59	1.23	1.42
3	A	902	M0E	O1-CAR	8.34	1.65	1.43
3	A	902	M0E	CCL-CCM	-7.70	1.41	1.52
3	A	902	M0E	CAV-NAT	7.50	1.47	1.33
3	A	902	M0E	OCD-CBW	7.37	1.60	1.43
2	A	901	AIX	C5-C4	-6.90	1.44	1.52
3	A	902	M0E	CAH-CAG	6.64	1.64	1.50
3	A	902	M0E	OBR-CBM	-6.45	1.27	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	AIX	C6-S1	-5.60	1.73	1.85
3	A	902	M0E	CBV-NCC	5.54	1.54	1.45
3	A	902	M0E	CAR-CAP	-5.30	1.41	1.52
3	A	902	M0E	O6-C6	4.91	1.52	1.43
3	A	902	M0E	OCP-CCL	4.79	1.51	1.43
2	A	901	AIX	C13-S1	-4.67	1.73	1.84
3	A	902	M0E	CCA-NCC	4.63	1.50	1.34
3	A	902	M0E	PBI-OBG	4.21	1.71	1.60
2	A	901	AIX	C12-N3	-4.06	1.40	1.46
3	A	902	M0E	CBZ-CBY	4.06	1.61	1.51
3	A	902	M0E	CBK-CBL	-3.96	1.42	1.52
3	A	902	M0E	OBH-CAP	3.88	1.52	1.45
3	A	902	M0E	CDK-CDG	-3.84	1.37	1.50
3	A	902	M0E	CCK-CCL	3.61	1.59	1.53
3	A	902	M0E	O6-CBJ	3.51	1.46	1.40
3	A	902	M0E	O5-C5	3.34	1.52	1.44
3	A	902	M0E	CAG-N2	3.16	1.45	1.34
3	A	902	M0E	CAO-CAP	-2.99	1.49	1.54
3	A	902	M0E	CCK-CCJ	-2.87	1.45	1.52
3	A	902	M0E	OCE-CBX	2.68	1.50	1.43
3	A	902	M0E	CBJ-CBK	2.61	1.60	1.52
2	A	901	AIX	C14-N1	-2.58	1.43	1.46
3	A	902	M0E	OCO-CCJ	2.52	1.48	1.43
3	A	902	M0E	C6-C5	-2.52	1.43	1.51
2	A	901	AIX	O3-C3	-2.46	1.18	1.23
3	A	902	M0E	CBW-CBV	-2.44	1.48	1.53
3	A	902	M0E	OBD-CAW	2.41	1.28	1.23
3	A	902	M0E	OCQ-CCM	-2.31	1.19	1.23
3	A	902	M0E	CCH-CCI	2.20	1.58	1.52
3	A	902	M0E	CBX-CBY	2.14	1.56	1.52
3	A	902	M0E	OCF-CBU	2.11	1.47	1.41
3	A	902	M0E	OCN-CCI	2.09	1.47	1.43
3	A	902	M0E	PBI-OBB	-2.09	1.45	1.55
3	A	902	M0E	O4-CBU	-2.04	1.36	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	M0E	CAS-CAO-CAQ	-19.63	95.29	111.11
3	A	902	M0E	OBH-CAV-NAT	11.92	129.11	110.58
3	A	902	M0E	OBC-CAV-NAT	-10.80	107.69	125.51
3	A	902	M0E	CAS-CAO-CAP	-9.69	99.63	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	M0E	OBA-CAO-CAP	5.92	123.71	108.18
3	A	902	M0E	CAO-CAP-CAR	4.53	121.21	112.06
3	A	902	M0E	CBU-O4-C4	-3.82	108.51	117.96
2	A	901	AIX	C4-C3-N1	3.78	119.38	114.78
3	A	902	M0E	C1-O1-CAR	-3.74	108.70	117.96
2	A	901	AIX	O3-C3-C4	-3.65	116.19	120.99
3	A	902	M0E	OBA-CAO-CAQ	3.56	114.81	107.66
3	A	902	M0E	CCH-OCE-CBX	-3.51	109.28	117.96
3	A	902	M0E	CCB-CCA-NCC	3.00	121.18	116.10
3	A	902	M0E	CBV-NCC-CCA	-2.76	116.46	123.18
3	A	902	M0E	CBZ-CBY-CBX	-2.65	109.38	113.41
2	A	901	AIX	C11-C5-C7	2.59	121.53	118.29
3	A	902	M0E	CCL-CCM-NCS	2.52	120.85	116.73
3	A	902	M0E	CBU-OCF-CBY	-2.51	109.35	113.67
3	A	902	M0E	OCG-CCA-NCC	-2.41	117.52	121.95
3	A	902	M0E	OAN-CAG-CAH	-2.28	117.82	122.06
3	A	902	M0E	O4-CBU-CBV	2.27	112.16	108.24
2	A	901	AIX	C13-C14-N1	2.19	114.75	109.98
3	A	902	M0E	O1-CAR-CAP	-2.18	101.24	106.84
3	A	902	M0E	O1-C1-O5	-2.07	104.90	110.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	M0E	CAX-OBG-PBI-OBB
3	A	902	M0E	OBC-CAV-OBH-CAP
3	A	902	M0E	NAT-CAV-OBH-CAP
3	A	902	M0E	OBS-CBJ-O6-C6
3	A	902	M0E	CBK-CBJ-O6-C6
3	A	902	M0E	OCP-CCL-CCM-NCS
3	A	902	M0E	OBS-CBN-CBO-OBT
3	A	902	M0E	CBM-CBN-CBO-OBT
3	A	902	M0E	CAX-OBG-PBI-OBF
3	A	902	M0E	O5-C5-C6-O6
3	A	902	M0E	CAX-OBG-PBI-OAZ
3	A	902	M0E	OCP-CCL-CCM-OCQ
3	A	902	M0E	CCK-CCL-CCM-OCQ
3	A	902	M0E	OCP-CCH-OCE-CBX
3	A	902	M0E	CDK-OBF-PBI-OAZ

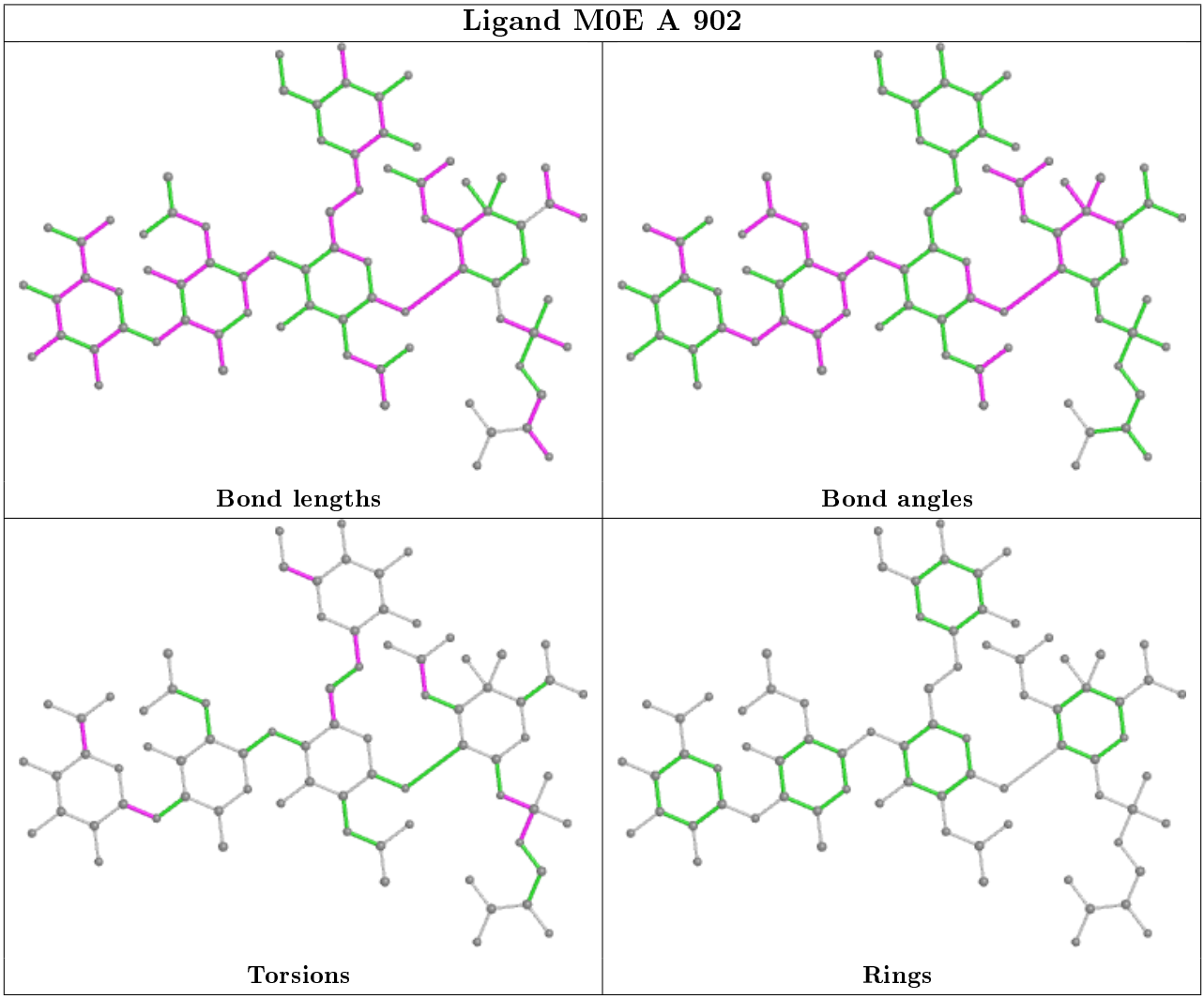
There are no ring outliers.

1 monomer is involved in 14 short contacts:

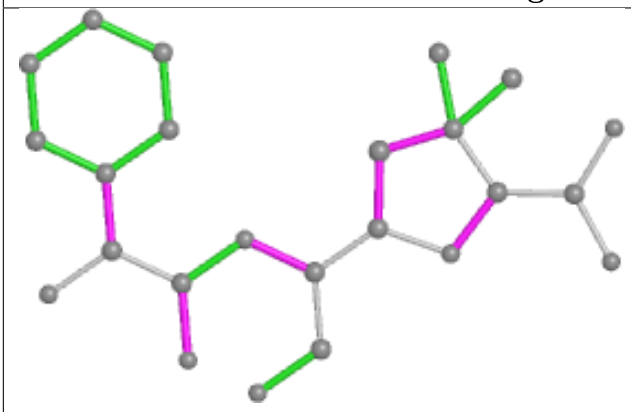
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	M0E	14	0

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

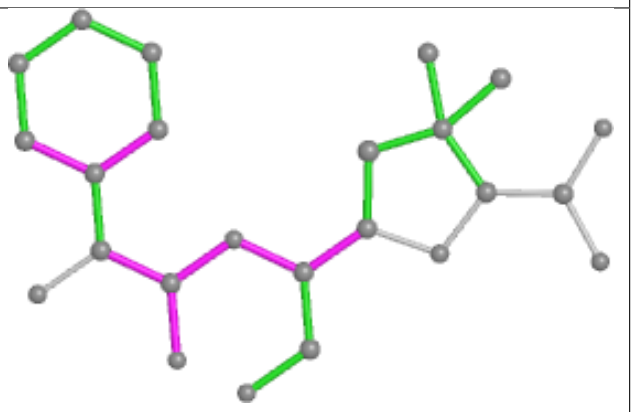
Ligand M0E A 902



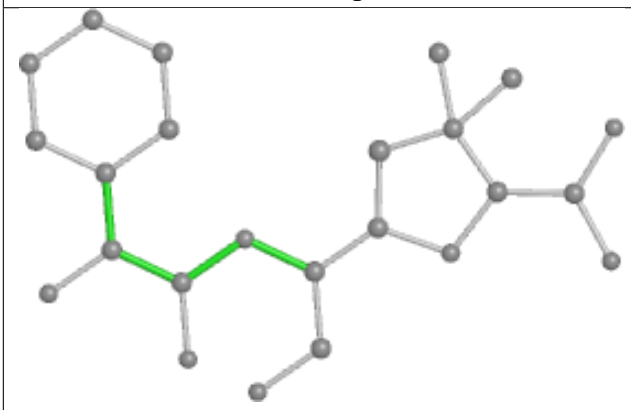
Ligand AIX A 901



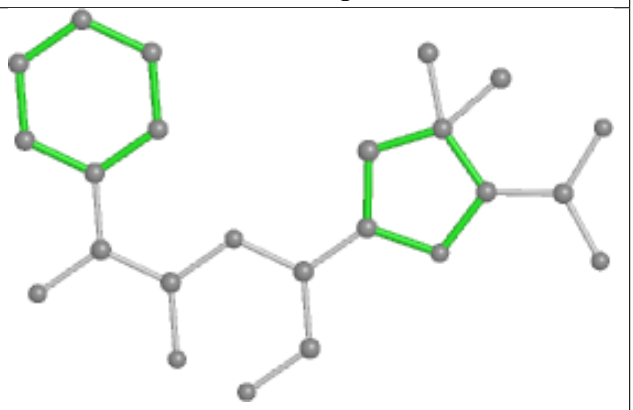
Bond lengths



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	695/747 (93%)	0.80	86 (12%) 4 3	29, 69, 144, 179	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	ASP	9.4
1	A	92	ARG	9.0
1	A	408	ILE	8.7
1	A	399	LEU	8.6
1	A	280	SER	7.5
1	A	430	VAL	7.2
1	A	89	GLN	7.0
1	A	409	SER	6.5
1	A	393	MET	6.0
1	A	796	GLN	5.9
1	A	285	TRP	5.5
1	A	212	GLN	5.0
1	A	71	LYS	5.0
1	A	403	PRO	4.9
1	A	321	ASP	4.8
1	A	91	ILE	4.7
1	A	72	LEU	4.7
1	A	96	ASP	4.6
1	A	398	PRO	4.5
1	A	93	SER	4.5
1	A	297	MET	4.4
1	A	320	GLY	4.4
1	A	319	SER	4.3
1	A	795	GLN	4.3
1	A	401	VAL	4.2
1	A	279	SER	4.2
1	A	284	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	4.1
1	A	76	PHE	4.1
1	A	90	LYS	4.1
1	A	344	LEU	4.0
1	A	68	LEU	4.0
1	A	431	LYS	4.0
1	A	295	LEU	3.9
1	A	333	TYR	3.8
1	A	322	ASN	3.8
1	A	391	TYR	3.7
1	A	363	TRP	3.6
1	A	99	VAL	3.6
1	A	85	VAL	3.5
1	A	392	ASP	3.5
1	A	286	ARG	3.4
1	A	309	LEU	3.4
1	A	98	LYS	3.4
1	A	87	LEU	3.4
1	A	272	LEU	3.4
1	A	209	ASN	3.3
1	A	282	ARG	3.0
1	A	324	ILE	3.0
1	A	423	GLN	2.9
1	A	275	ASN	2.9
1	A	281	GLU	2.9
1	A	276	LEU	2.9
1	A	390	LEU	2.9
1	A	79	LEU	2.9
1	A	69	LEU	2.8
1	A	797	SER	2.7
1	A	213	ARG	2.7
1	A	238	TYR	2.7
1	A	336	GLY	2.7
1	A	277	PHE	2.7
1	A	278	LEU	2.6
1	A	237	PHE	2.6
1	A	292	TYR	2.5
1	A	375	LEU	2.5
1	A	342	LEU	2.4
1	A	422	LEU	2.4
1	A	388	GLN	2.4
1	A	75	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	312	ASN	2.3
1	A	211	GLU	2.3
1	A	283	SER	2.3
1	A	378	ARG	2.2
1	A	301	TYR	2.2
1	A	86	TYR	2.2
1	A	102	LEU	2.2
1	A	655	PHE	2.2
1	A	141	ARG	2.1
1	A	205	ILE	2.1
1	A	314	VAL	2.1
1	A	560	SER	2.1
1	A	94	ARG	2.1
1	A	137	SER	2.1
1	A	74	ILE	2.1
1	A	222	PRO	2.0
1	A	400	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

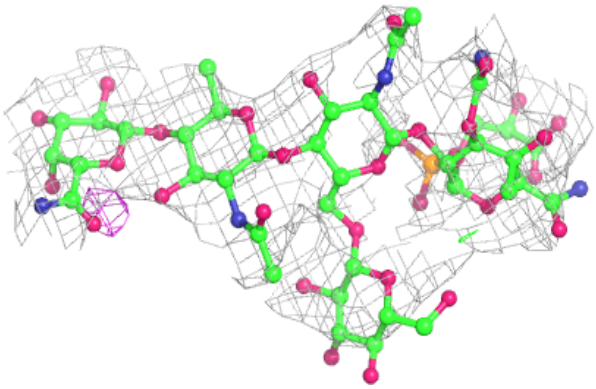
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

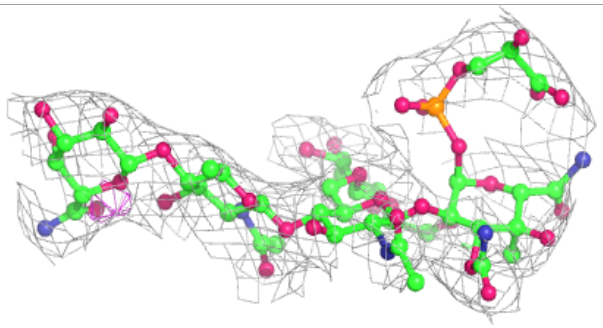
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	M0E	A	902	77/109	0.83	0.22	79,106,125,132	0
2	AIX	A	901	24/24	0.94	0.26	20,20,20,20	0

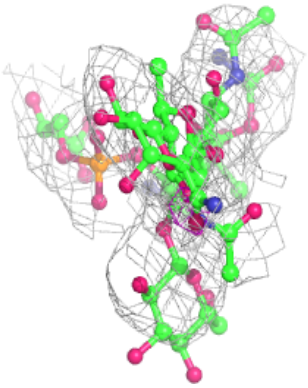
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M0E A 902:

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

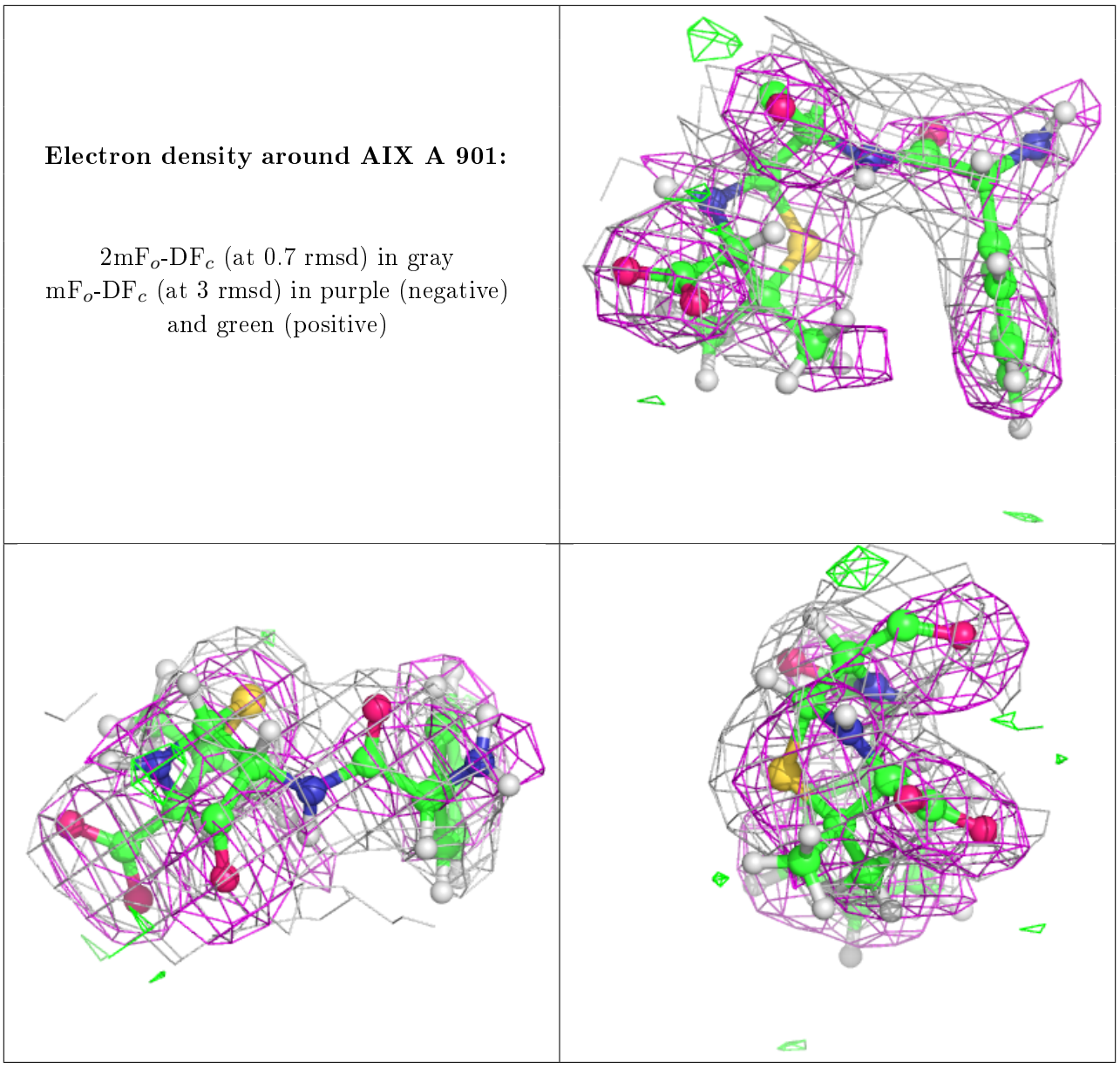






Electron density around AIX A 901:

$2mF_o$-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.