



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 8XSU / pdb_00008xsu
Title : Crystal Structure of Lymnaea stagnalis Acetylcholine-Binding Protein Q55R
Mutant Complexed with Dinotefuran
Authors : Ihara, M.; Okajima, T.; Matsuda, K.
Deposited on : 2024-01-10
Resolution : 2.63 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

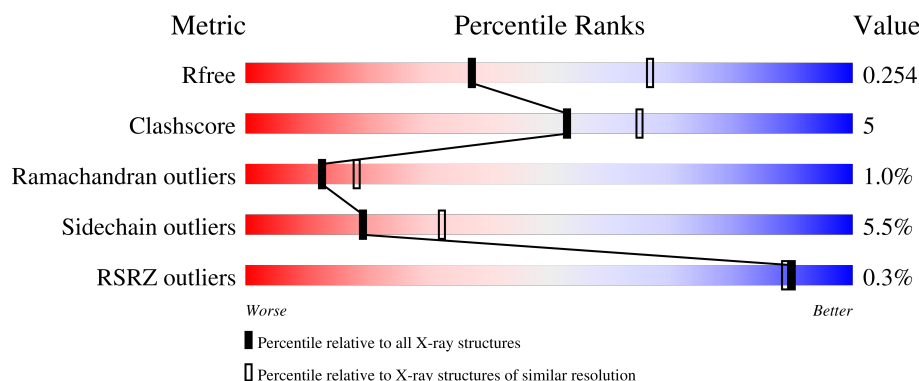
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	210	 88% 10% .
1	B	210	 88% 9% ..
1	C	210	 80% 17% ..
1	E	210	 87% 10% ..
2	D	206	 81% 15% .

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
4	NAG	E	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8481 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	1	0
			1676	1044	290	337	5			
1	B	208	Total	C	N	O	S	0	1	0
			1660	1035	288	332	5			
1	C	208	Total	C	N	O	S	0	0	0
			1661	1035	288	333	5			
1	E	208	Total	C	N	O	S	0	0	0
			1657	1033	288	331	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ARG	GLN	engineered mutation	UNP P58154
B	55	ARG	GLN	engineered mutation	UNP P58154
C	55	ARG	GLN	engineered mutation	UNP P58154
E	55	ARG	GLN	engineered mutation	UNP P58154

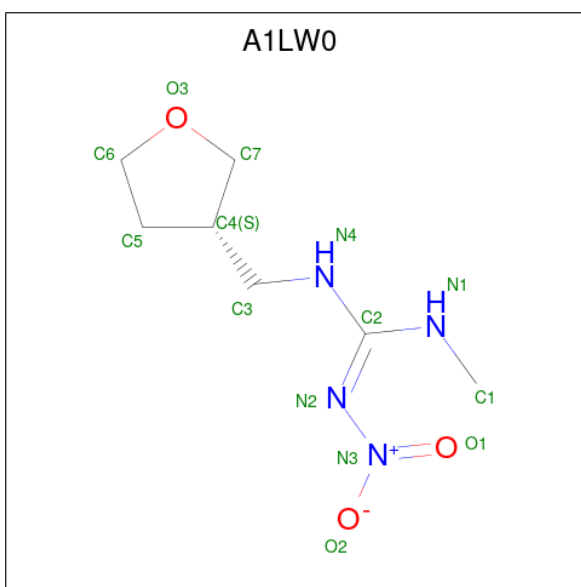
- Molecule 2 is a protein called Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	206	Total	C	N	O	S	0	0	0
			1639	1023	284	327	5			

There is a discrepancy between the modelled and reference sequences:

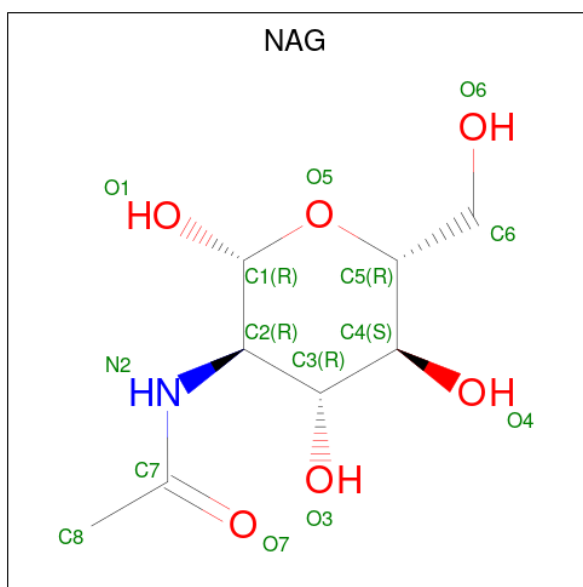
Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ARG	GLN	engineered mutation	UNP P58154

- Molecule 3 is 2-methyl-1-nitro-3-[(tetrahydro-3-furanyl) methyl] guanidine (CCD ID: A1LW0) (formula: C₇H₁₄N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	4	3		
3	B	1	Total	C	N	O	0	0
			14	7	4	3		
3	C	1	Total	C	N	O	0	0
			14	7	4	3		
3	D	1	Total	C	N	O	0	0
			14	7	4	3		
3	E	1	Total	C	N	O	0	0
			14	7	4	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	8	Total	O	0	0
			8	8		
5	C	7	Total	O	0	0
			7	7		
5	D	8	Total	O	0	0
			8	8		
5	E	12	Total	O	0	0
			12	12		

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.

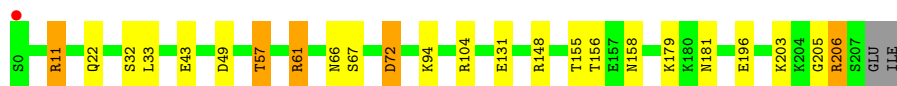
- Molecule 1: Acetylcholine-binding protein

Chain A:  88% 10% .



- Molecule 1: Acetylcholine-binding protein

Chain B:  88% 9% ..



- Molecule 1: Acetylcholine-binding protein

Chain C:  80% 17% ..



- Molecule 1: Acetylcholine-binding protein

Chain E:  87% 10% ..



- Molecule 2: Acetylcholine-binding protein

Chain D:  81% 15% .



C187	C188	P189	E190	K203	K204	G205	R206
------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 74.15Å 350.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.34 – 2.63 47.34 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.34-2.63) 99.9 (47.34-2.63)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.196 , 0.254 0.198 , 0.254	Depositor DCC
R_{free} test set	1629 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8481	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 3.08% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LW0, NAG

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	0.62	0/1715	1.02	3/2340 (0.1%)
1	B	0.58	0/1699	1.02	6/2317 (0.3%)
1	C	0.54	0/1697	1.05	7/2314 (0.3%)
1	E	0.59	0/1693	1.01	3/2309 (0.1%)
2	D	0.57	0/1675	1.07	9/2286 (0.4%)
All	All	0.58	0/8479	1.04	28/11566 (0.2%)

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	A	0	3
1	B	0	2
1	C	0	3
2	D	0	2
All	All	0	10

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	ASP	CB-CA-C	8.47	124.66	109.83
1	C	206	ARG	N-CA-CB	-8.37	98.83	110.38
1	A	49	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	43	GLU	CB-CG-CD	6.20	123.14	112.60
1	E	72	ASP	CA-CB-CG	5.99	118.59	112.60
1	E	57	THR	CA-CB-OG1	-5.98	100.63	109.60
2	D	49	ASP	CA-CB-CG	5.90	118.50	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	72	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	20	PRO	N-CA-CB	-5.77	98.21	102.25
2	D	161	ASP	N-CA-C	-5.75	105.76	112.89
1	A	72	ASP	CA-CB-CG	5.50	118.10	112.60
2	D	72	ASP	CA-CB-CG	5.50	118.10	112.60
2	D	155	THR	CA-CB-OG1	-5.46	101.42	109.60
1	A	57	THR	CA-CB-OG1	-5.44	101.44	109.60
1	C	94	LYS	N-CA-CB	5.43	118.04	110.11
1	B	57	THR	CA-CB-OG1	-5.41	101.49	109.60
1	C	49	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	156	THR	CA-CB-OG1	-5.38	101.53	109.60
1	C	57	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	49	ASP	CA-CB-CG	5.17	117.77	112.60
2	D	104	ARG	N-CA-CB	-5.16	102.46	110.57
2	D	172	GLU	CB-CA-C	-5.14	98.63	109.38
1	B	61	ARG	CB-CG-CD	5.13	123.10	111.30
1	C	104	ARG	N-CA-CB	-5.09	102.58	110.57
1	E	104	ARG	N-CA-CB	-5.06	102.62	110.57
1	C	160	ASP	CA-CB-CG	5.01	117.61	112.60
2	D	5	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	205	GLY	Peptide
1	B	11	ARG	Sidechain
1	B	148	ARG	Sidechain
1	C	11	ARG	Sidechain
1	C	157	GLU	Peptide
1	C	61	ARG	Sidechain
2	D	15	ARG	Sidechain
2	D	206	ARG	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	1676	0	1609	16	0
1	B	1660	0	1601	10	0
1	C	1661	0	1600	20	0
1	E	1657	0	1597	25	0
2	D	1639	0	1574	19	0
3	A	14	0	0	1	0
3	B	14	0	0	1	0
3	C	14	0	0	2	0
3	D	14	0	0	1	0
3	E	14	0	0	2	0
4	A	14	0	13	4	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	8	0
5	A	13	0	0	0	0
5	B	8	0	0	1	0
5	C	7	0	0	4	0
5	D	8	0	0	0	0
5	E	12	0	0	0	0
All	All	8481	0	8046	83	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 (83) 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:E:66:ASN:HD21	4:E:302:NAG:C1	0.96	1.61
1:A:66:ASN:HD21	4:A:302:NAG:C1	1.18	1.51
1:E:66:ASN:ND2	4:E:302:NAG:C1	1.73	1.44
1:A:66:ASN:ND2	4:A:302:NAG:C1	1.92	1.29
1:E:66:ASN:HD21	4:E:302:NAG:C2	1.65	1.08
1:E:66:ASN:CG	4:E:302:NAG:C1	2.37	0.97
1:E:66:ASN:ND2	4:E:302:NAG:C2	2.30	0.88
1:A:66:ASN:HD21	4:A:302:NAG:C2	1.86	0.88
1:B:11:ARG:HH11	1:B:11:ARG:HG3	1.44	0.81
1:C:129:ASP:O	1:C:206:ARG:NH2	2.11	0.81
1:C:55:ARG:HB2	1:C:114:MET:HE3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ASP:OD2	2:D:11:ARG:NH2	2.20	0.73
1:E:11:ARG:HH11	1:E:11:ARG:HG3	1.58	0.69
1:C:108:ASP:HB2	5:C:402:HOH:O	1.93	0.69
1:A:11:ARG:HH11	1:A:11:ARG:HG3	1.60	0.67
1:E:66:ASN:OD1	4:E:302:NAG:C1	2.43	0.66
1:E:158:ASN:O	1:E:159:SER:CB	2.43	0.65
1:C:53:TRP:HB3	1:C:114:MET:HE2	1.82	0.62
1:E:187:CYS:SG	3:E:301:A1LW0:O2	2.58	0.62
1:A:53:TRP:HB3	1:A:114:MET:HE3	1.81	0.61
1:C:108:ASP:CG	5:C:402:HOH:O	2.43	0.60
1:A:66:ASN:CG	4:A:302:NAG:C1	2.71	0.60
1:B:205:GLY:O	1:B:206:ARG:HG2	2.03	0.59
1:E:73:GLN:HE21	1:E:104:ARG:CG	2.16	0.58
2:D:22:GLN:O	2:D:25:ARG:HG2	2.04	0.58
1:E:189:PRO:HD2	1:E:190:GLU:OE1	2.05	0.57
2:D:15:ARG:HH11	2:D:15:ARG:HB2	1.69	0.56
2:D:146:HIS:CE1	2:D:148:ARG:HE	2.23	0.56
1:E:73:GLN:HE21	1:E:104:ARG:HG2	1.70	0.56
1:C:108:ASP:CB	5:C:402:HOH:O	2.51	0.55
1:E:66:ASN:ND2	4:E:302:NAG:O5	2.23	0.54
1:C:93:SER:C	2:D:98:LEU:HD12	2.34	0.53
1:C:156:THR:O	1:C:158:ASN:HA	2.09	0.52
3:A:301:A1LW0:O1	3:A:301:A1LW0:N1	2.42	0.52
2:D:11:ARG:HH11	2:D:11:ARG:HG3	1.77	0.50
1:A:17:ASP:OD2	1:B:11:ARG:NH2	2.45	0.50
1:E:53:TRP:HB3	1:E:114:MET:HE3	1.93	0.49
1:C:124:ASP:HB2	2:D:168:TYR:CE1	2.48	0.48
1:B:181:ASN:ND2	1:B:196:GLU:OE2	2.47	0.48
1:E:158:ASN:O	1:E:159:SER:HB3	2.15	0.47
1:C:94:LYS:N	2:D:98:LEU:HD12	2.30	0.47
2:D:205:GLY:O	2:D:206:ARG:C	2.57	0.47
3:C:301:A1LW0:N1	3:C:301:A1LW0:O1	2.44	0.47
1:C:53:TRP:CB	1:C:114:MET:HE2	2.45	0.46
2:D:162:SER:C	2:D:164:TYR:H	2.23	0.46
1:A:34:LYS:HD2	1:A:157:GLU:OE2	2.16	0.46
1:E:66:ASN:ND2	4:E:302:NAG:H2	2.24	0.46
1:E:158:ASN:O	1:E:159:SER:HB2	2.16	0.45
3:B:301:A1LW0:N1	3:B:301:A1LW0:O1	2.49	0.45
3:D:301:A1LW0:C1	3:D:301:A1LW0:C3	2.95	0.45
3:E:301:A1LW0:N1	3:E:301:A1LW0:O1	2.50	0.45
1:A:53:TRP:CB	1:A:114:MET:HE3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:HG2	5:B:404:HOH:O	2.16	0.44
1:A:11:ARG:HH11	1:A:11:ARG:CG	2.31	0.44
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.53	0.44
1:C:185:TYR:HD1	2:D:164:TYR:CE1	2.35	0.44
1:A:125:VAL:HG12	1:A:125:VAL:O	2.18	0.43
1:C:181:ASN:ND2	1:C:196:GLU:OE2	2.51	0.43
1:A:149:GLU:OE2	1:B:104:ARG:NH2	2.35	0.43
1:A:1:LEU:CB	1:A:4:ALA:HB3	2.49	0.42
1:E:11:ARG:HG3	1:E:11:ARG:NH1	2.30	0.42
2:D:203:LYS:HB2	2:D:203:LYS:HE3	1.79	0.42
2:D:30:SER:HB2	2:D:57:THR:OG1	2.19	0.42
1:E:33:LEU:HD12	1:E:33:LEU:N	2.35	0.42
1:B:11:ARG:HH11	1:B:11:ARG:CG	2.23	0.42
2:D:137:ARG:NH1	1:E:168:TYR:OH	2.53	0.42
1:E:67:SER:HB3	1:E:107:SER:OG	2.19	0.42
2:D:125:VAL:O	2:D:125:VAL:HG12	2.20	0.41
1:A:149:GLU:CD	1:B:104:ARG:HH22	2.26	0.41
1:C:149:GLU:CD	2:D:104:ARG:HH22	2.26	0.41
1:E:158:ASN:ND2	1:E:163:GLU:OE1	2.52	0.41
1:B:33:LEU:HD12	1:B:33:LEU:N	2.36	0.41
2:D:187:CYS:C	2:D:188:CYS:SG	3.04	0.41
1:E:73:GLN:NE2	1:E:104:ARG:HG2	2.35	0.41
1:B:206:ARG:HH11	1:B:206:ARG:HB2	1.85	0.41
2:D:159:SER:HB3	2:D:160:ASP:H	1.76	0.41
1:E:94:LYS:HB3	1:E:94:LYS:HE2	1.88	0.41
1:C:137:ARG:NH1	1:C:196:GLU:OE1	2.52	0.41
1:C:125:VAL:O	1:C:125:VAL:HG12	2.21	0.40
1:C:143:TRP:O	3:C:301:A1LW0:C3	2.69	0.40
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.85	0.40
1:C:18:VAL:HG21	2:D:4:ALA:HA	2.02	0.40
1:C:115:PRO:HA	5:C:403:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	209/210 (100%)	202 (97%)	6 (3%)	1 (0%)	24	36
1	B	207/210 (99%)	199 (96%)	6 (3%)	2 (1%)	12	18
1	C	206/210 (98%)	196 (95%)	7 (3%)	3 (2%)	8	11
1	E	206/210 (98%)	198 (96%)	5 (2%)	3 (2%)	8	11
2	D	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	24	36
All	All	1032/1046 (99%)	991 (96%)	31 (3%)	10 (1%)	12	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	67	SER
1	C	66	ASN
1	C	67	SER
1	E	206	ARG
2	D	157	GLU
1	E	159	SER
1	A	206	ARG
1	E	158	ASN
1	C	161	ASP

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	194/196 (99%)	184 (95%)	10 (5%)	21	34
1	B	193/196 (98%)	182 (94%)	11 (6%)	18	31
1	C	193/196 (98%)	182 (94%)	11 (6%)	18	31
1	E	192/196 (98%)	186 (97%)	6 (3%)	35	55
2	D	189/192 (98%)	174 (92%)	15 (8%)	11	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	961/976 (98%)	908 (94%)	53 (6%)	19	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	23	ARG
1	A	34	LYS
1	A	57	THR
1	A	61	ARG
1	A	180	LYS
1	A	183	VAL
1	A	187	CYS
1	A	188	CYS
1	A	206	ARG
1	B	22	GLN
1	B	32	SER
1	B	57	THR
1	B	61	ARG
1	B	72	ASP
1	B	94	LYS
1	B	131	GLU
1	B	155	THR
1	B	158	ASN
1	B	203	LYS
1	B	206	ARG
1	C	11	ARG
1	C	23	ARG
1	C	32	SER
1	C	57	THR
1	C	63	LEU
1	C	98	LEU
1	C	148	ARG
1	C	155	THR
1	C	180	LYS
1	C	183	VAL
1	C	206	ARG
2	D	2	ASP
2	D	15	ARG
2	D	34	LYS
2	D	57	THR
2	D	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	131	GLU
2	D	137	ARG
2	D	159	SER
2	D	160	ASP
2	D	163	GLU
2	D	170	ARG
2	D	174	LEU
2	D	179	LYS
2	D	183	VAL
2	D	190	GLU
1	E	15	ARG
1	E	32	SER
1	E	34	LYS
1	E	57	THR
1	E	131	GLU
1	E	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	66	ASN
1	A	146	HIS
1	B	9	ASN
1	B	146	HIS
1	C	9	ASN
2	D	12	GLN
2	D	22	GLN
2	D	146	HIS
2	D	200	ASN
1	E	66	ASN
1	E	73	GLN
1	E	158	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	A1LW0	D	301	-	11,14,14	0.79	0	10,17,17	2.48	3 (30%)
3	A1LW0	A	301	-	11,14,14	0.67	0	10,17,17	3.77	4 (40%)
4	NAG	E	302	-	14,14,15	0.38	0	17,19,21	1.32	2 (11%)
4	NAG	A	302	-	14,14,15	0.33	0	17,19,21	0.65	0
4	NAG	C	302	1	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
3	A1LW0	E	301	-	11,14,14	0.55	0	10,17,17	4.04	3 (30%)
3	A1LW0	B	301	-	11,14,14	0.65	0	10,17,17	2.89	4 (40%)
4	NAG	B	302	1	14,14,15	0.45	0	17,19,21	1.21	2 (11%)
3	A1LW0	C	301	-	11,14,14	0.77	0	10,17,17	3.45	3 (30%)
4	NAG	D	302	2	14,14,15	0.43	0	17,19,21	0.89	1 (5%)

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	A1LW0	D	301	-	-	1/9/18/18	0/1/1/1
3	A1LW0	A	301	-	-	3/9/18/18	0/1/1/1
4	NAG	E	302	-	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	302	-	-	4/6/23/26	0/1/1/1
4	NAG	C	302	1	-	4/6/23/26	0/1/1/1
3	A1LW0	E	301	-	-	1/9/18/18	0/1/1/1
3	A1LW0	B	301	-	-	2/9/18/18	0/1/1/1
4	NAG	B	302	1	-	4/6/23/26	0/1/1/1
3	A1LW0	C	301	-	-	5/9/18/18	0/1/1/1
4	NAG	D	302	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	A1LW0	N4-C2-N1	9.91	128.56	119.48
3	C	301	A1LW0	N4-C2-N1	9.62	128.30	119.48
3	A	301	A1LW0	N4-C2-N1	9.39	128.09	119.48
3	B	301	A1LW0	N4-C2-N1	7.30	126.17	119.48
3	E	301	A1LW0	C4-C3-N4	-6.50	101.49	112.77
3	A	301	A1LW0	C4-C3-N4	-5.74	102.81	112.77
3	D	301	A1LW0	N4-C2-N1	4.77	123.86	119.48
3	D	301	A1LW0	C4-C3-N4	-4.36	105.21	112.77
3	C	301	A1LW0	C4-C3-N4	-4.23	105.44	112.77
3	E	301	A1LW0	C3-N4-C2	4.06	131.25	123.47
3	D	301	A1LW0	C3-N4-C2	3.68	130.53	123.47
3	A	301	A1LW0	C3-N4-C2	3.39	129.97	123.47
3	B	301	A1LW0	C4-C3-N4	-3.33	107.00	112.77
3	B	301	A1LW0	C3-N4-C2	3.19	129.58	123.47
4	C	302	NAG	C1-C2-N2	3.00	115.16	110.43
4	B	302	NAG	C1-C2-N2	2.98	115.12	110.43
4	B	302	NAG	C1-O5-C5	2.89	116.06	112.19
4	E	302	NAG	C3-C4-C5	2.70	115.13	110.23
3	B	301	A1LW0	C5-C4-C7	-2.68	98.97	101.93
3	A	301	A1LW0	C5-C4-C7	-2.57	99.09	101.93
4	E	302	NAG	O5-C1-C2	-2.52	107.39	111.29
4	D	302	NAG	C1-C2-N2	2.34	114.13	110.43
3	C	301	A1LW0	N4-C2-N2	-2.02	106.54	116.60

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	A1LW0	N4-C3-C4-C5
3	B	301	A1LW0	N4-C3-C4-C7
3	C	301	A1LW0	N4-C2-N1-C1
3	C	301	A1LW0	N4-C2-N2-N3
3	D	301	A1LW0	N4-C3-C4-C7
4	A	302	NAG	O7-C7-N2-C2
4	C	302	NAG	C1-C2-N2-C7
4	C	302	NAG	C8-C7-N2-C2
4	C	302	NAG	O7-C7-N2-C2
4	D	302	NAG	C8-C7-N2-C2
4	D	302	NAG	O7-C7-N2-C2
4	A	302	NAG	C8-C7-N2-C2
4	B	302	NAG	O5-C5-C6-O6
4	B	302	NAG	C8-C7-N2-C2
4	B	302	NAG	O7-C7-N2-C2
4	C	302	NAG	O5-C5-C6-O6
4	B	302	NAG	C4-C5-C6-O6
4	D	302	NAG	C4-C5-C6-O6
3	C	301	A1LW0	N2-C2-N4-C3
3	E	301	A1LW0	N2-C2-N4-C3
4	A	302	NAG	C4-C5-C6-O6
3	C	301	A1LW0	N1-C2-N2-N3
3	A	301	A1LW0	N4-C3-C4-C5
3	A	301	A1LW0	N4-C2-N1-C1
3	C	301	A1LW0	N2-C2-N1-C1
4	A	302	NAG	O5-C5-C6-O6
4	E	302	NAG	C4-C5-C6-O6
4	D	302	NAG	O5-C5-C6-O6
3	A	301	A1LW0	N2-C2-N4-C3

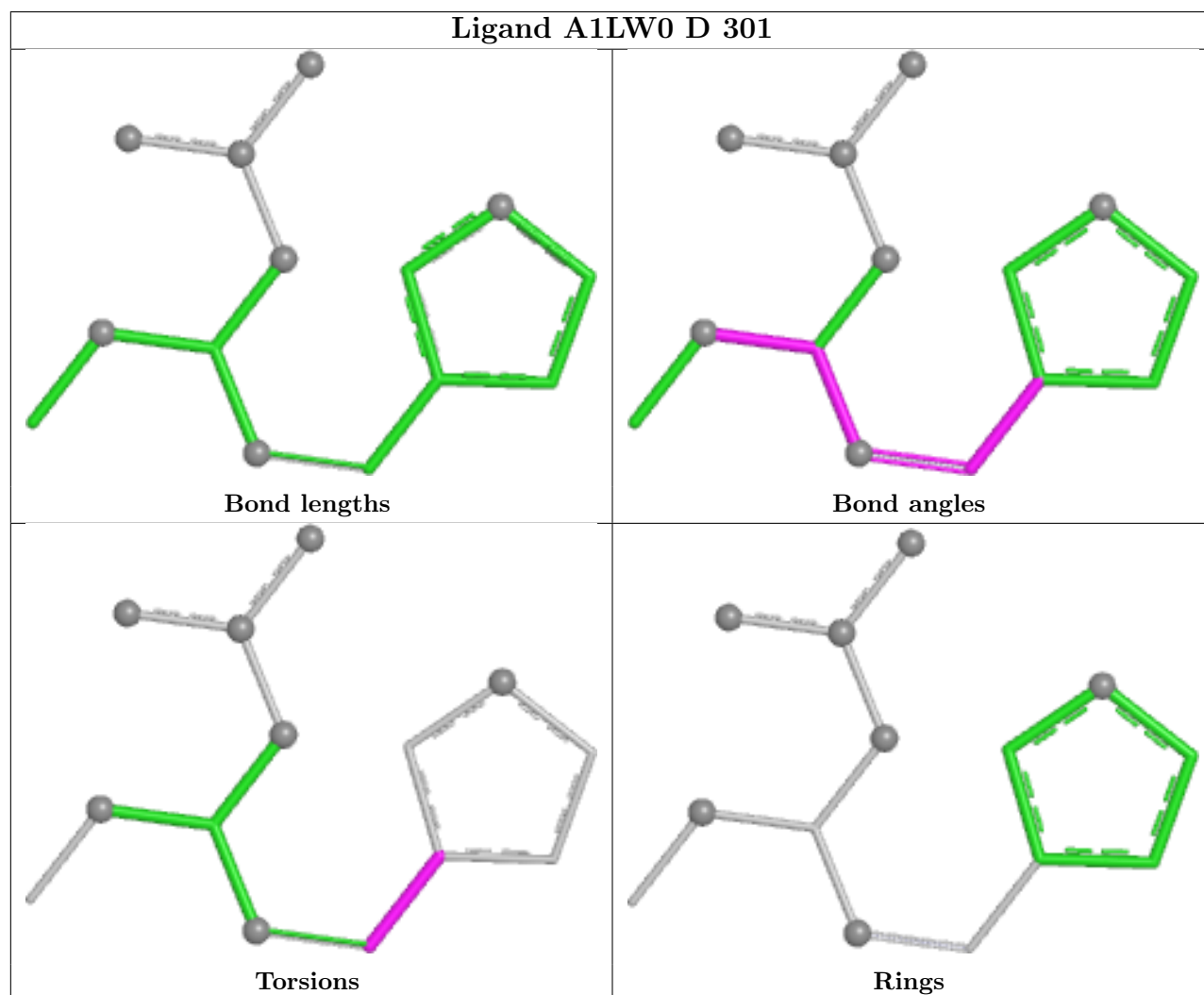
There are no ring outliers.

7 monomers are involved in 19 short contacts:

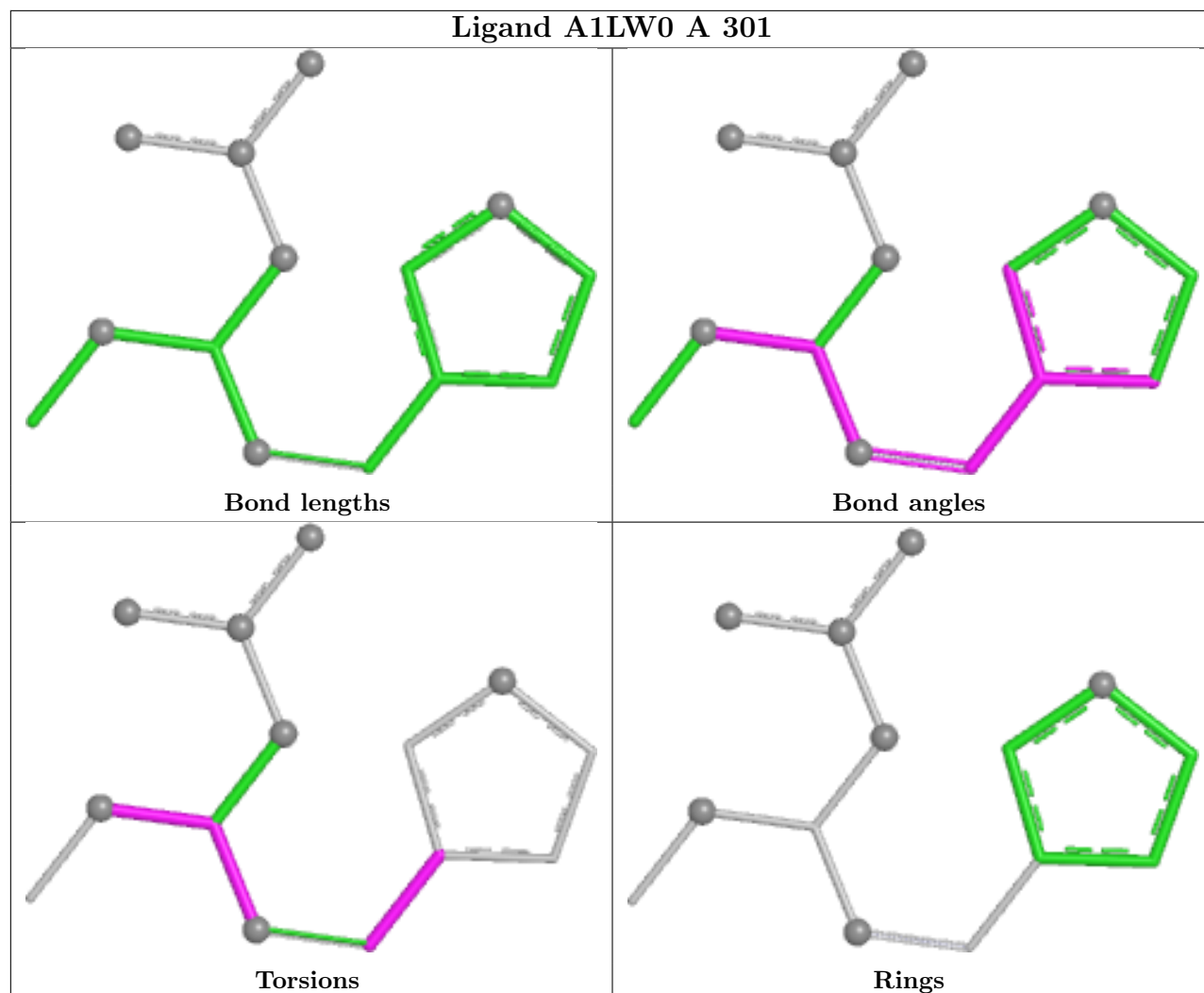
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	A1LW0	1	0
3	A	301	A1LW0	1	0
4	E	302	NAG	8	0
4	A	302	NAG	4	0
3	E	301	A1LW0	2	0
3	B	301	A1LW0	1	0
3	C	301	A1LW0	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

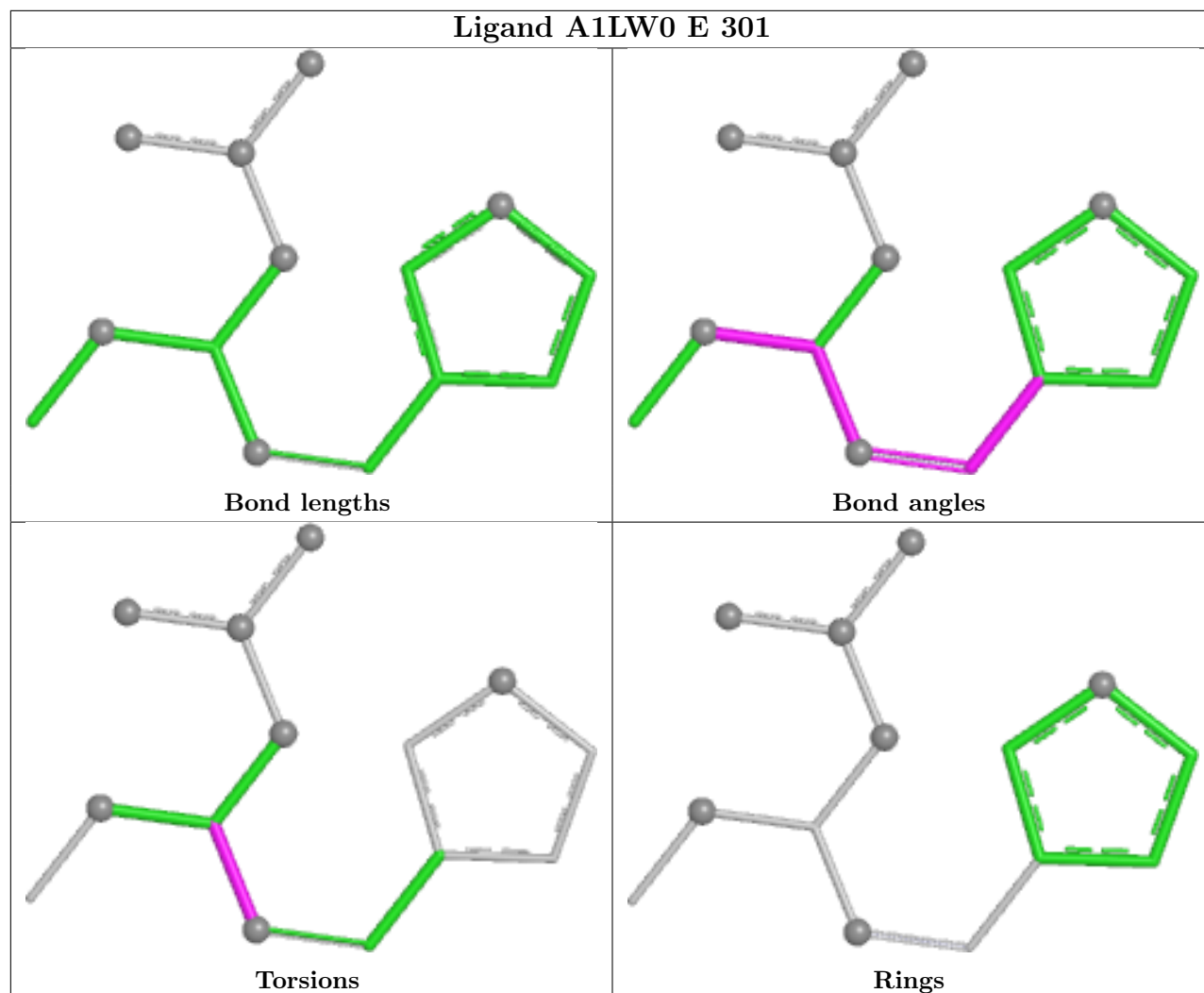
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



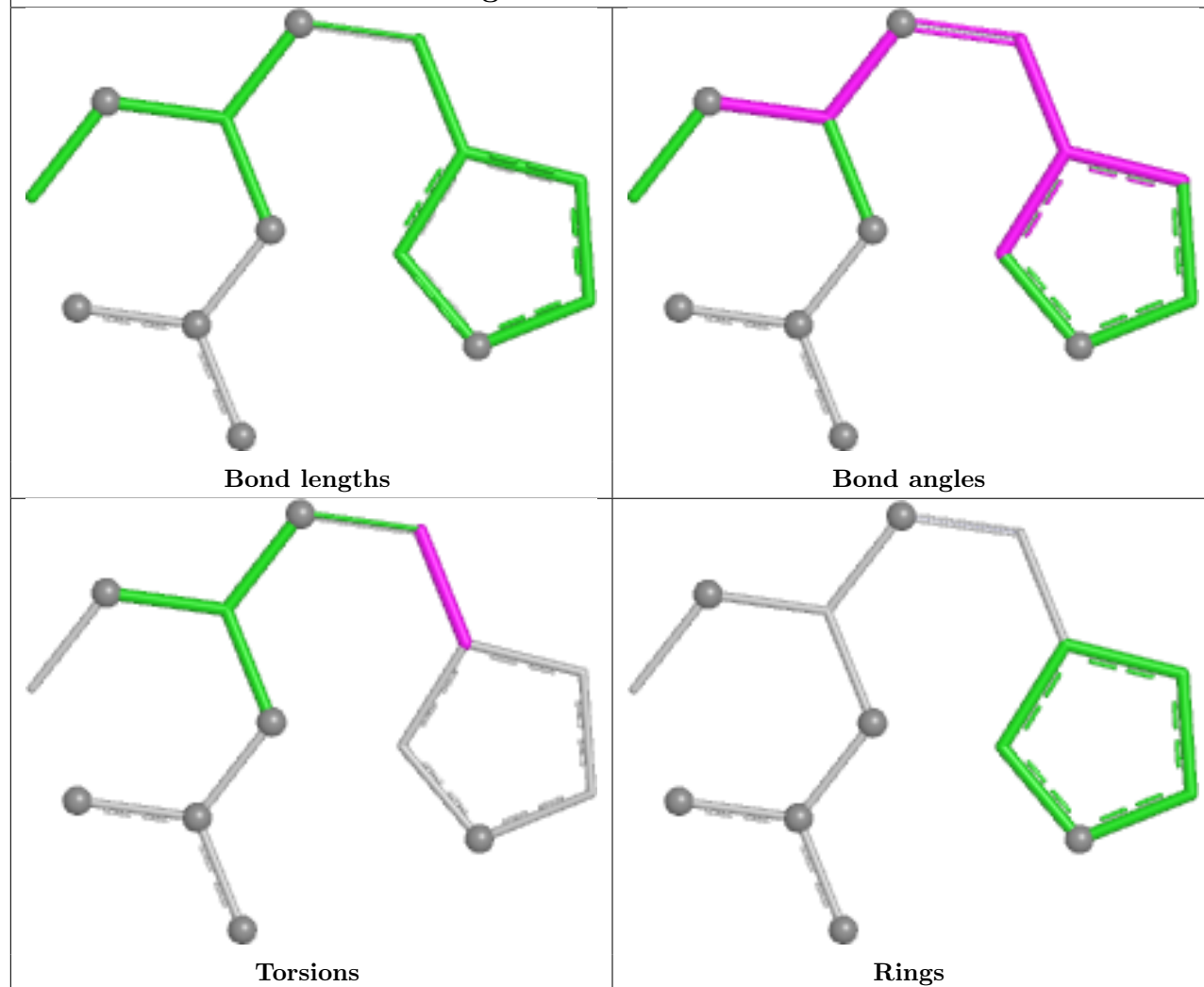
Ligand A1LW0 A 301

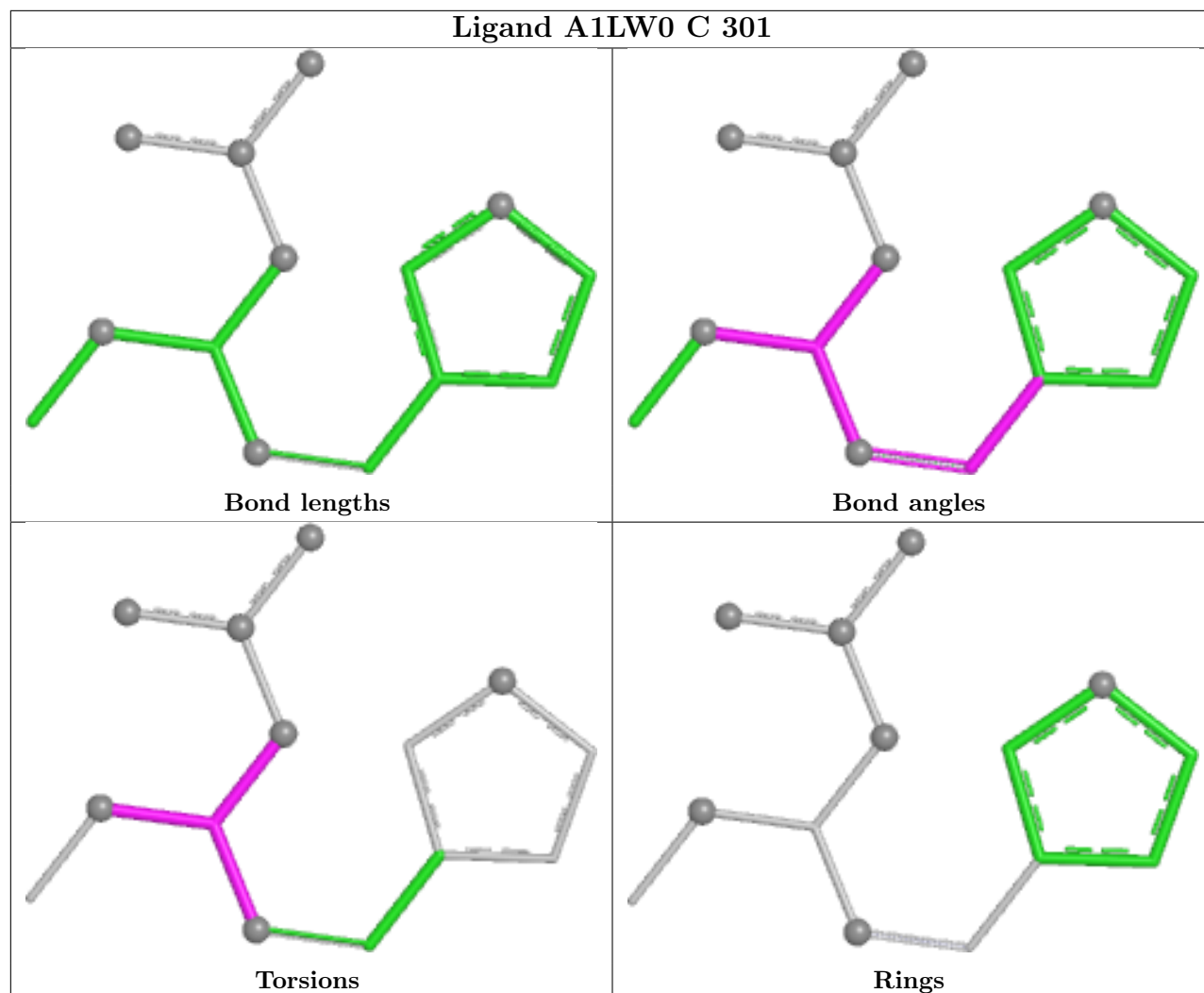


Ligand A1LW0 E 301



Ligand A1LW0 B 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	210/210 (100%)	-0.36	1 (0%) 87 85	33, 56, 124, 151	1 (0%)
1	B	208/210 (99%)	-0.25	1 (0%) 87 85	39, 62, 122, 150	1 (0%)
1	C	208/210 (99%)	-0.01	1 (0%) 87 85	48, 81, 132, 159	0
1	E	208/210 (99%)	-0.30	0 100 100	37, 62, 109, 193	0
2	D	206/206 (100%)	-0.03	0 100 100	46, 80, 137, 175	0
All	All	1040/1046 (99%)	-0.19	3 (0%) 90 89	33, 69, 128, 193	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	SER	2.5
1	A	0	SER	2.5
1	C	207	SER	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

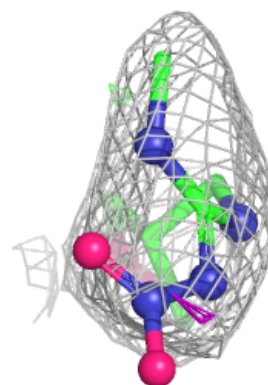
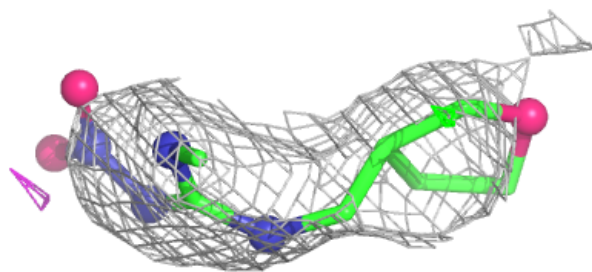
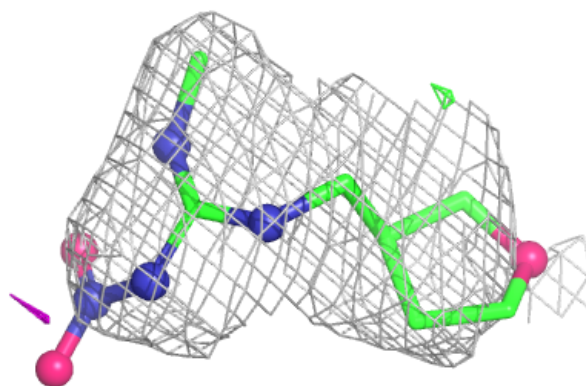
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	302	14/15	0.08	0.13	146,155,163,164	0
4	NAG	A	302	14/15	0.56	0.12	119,133,140,140	0
4	NAG	C	302	14/15	0.58	0.11	134,146,158,158	0
4	NAG	B	302	14/15	0.73	0.11	121,126,129,131	0
3	A1LW0	C	301	14/14	0.82	0.15	85,101,120,123	0
3	A1LW0	B	301	14/14	0.84	0.15	94,98,106,110	0
3	A1LW0	D	301	14/14	0.84	0.15	69,82,103,105	0
3	A1LW0	E	301	14/14	0.85	0.12	56,68,98,111	0
4	NAG	E	302	14/15	0.90	0.07	69,77,83,87	0
3	A1LW0	A	301	14/14	0.91	0.10	59,69,100,110	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.

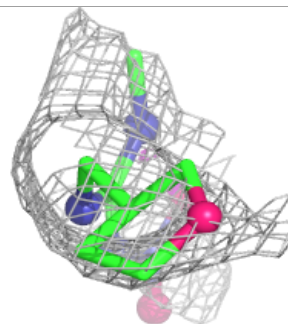
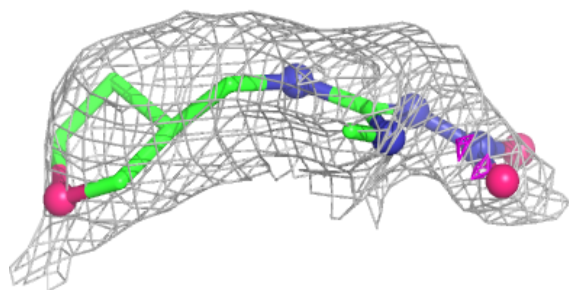
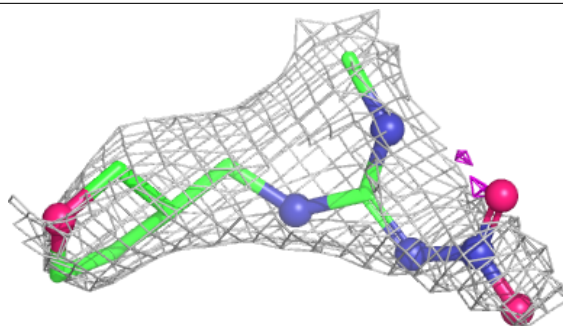
Electron density around A1LW0 C 301:

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

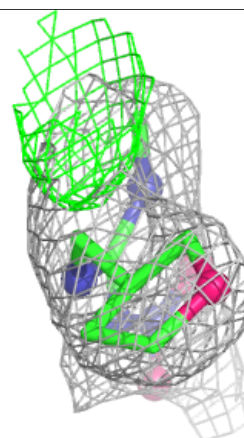
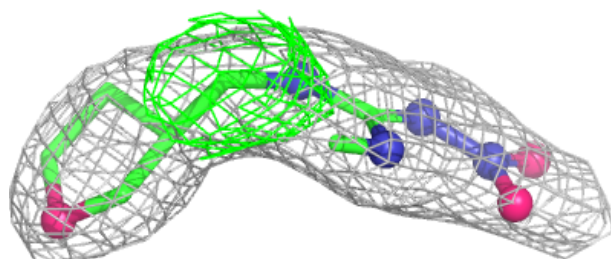
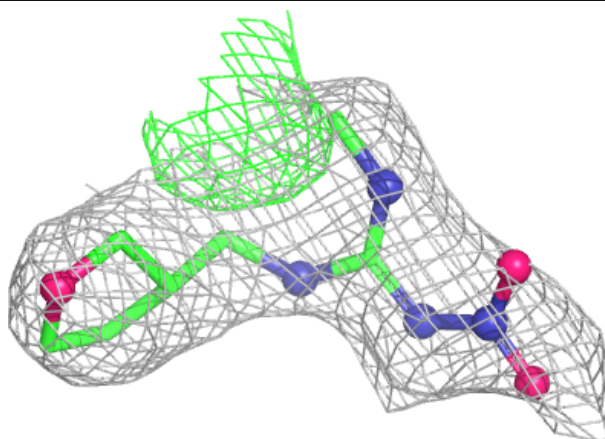


Electron density around A1LW0 B 301:

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

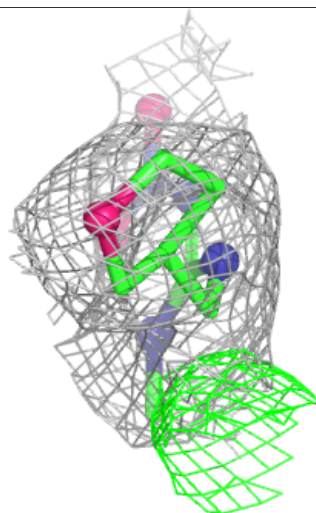
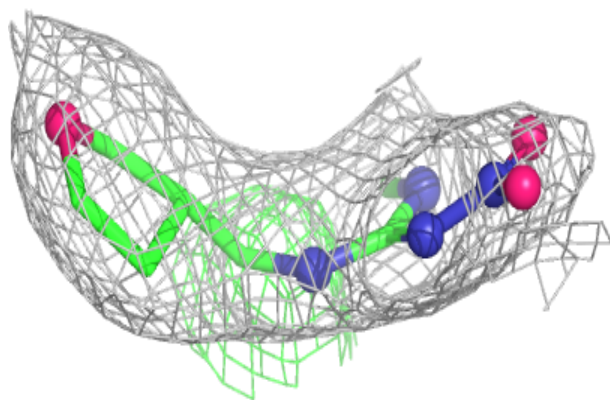
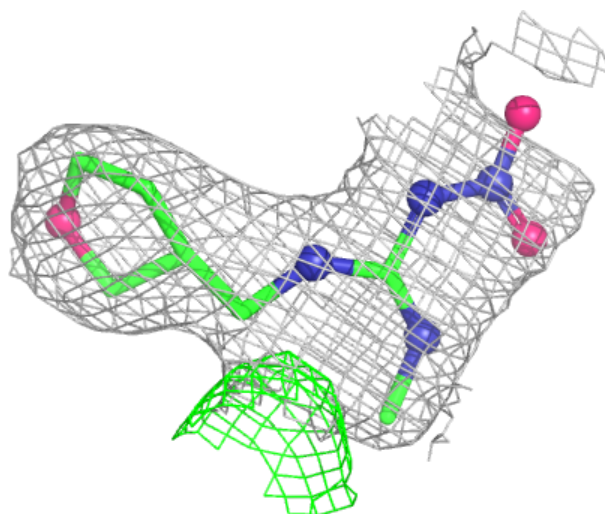
**Electron density around A1LW0 D 301:**

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



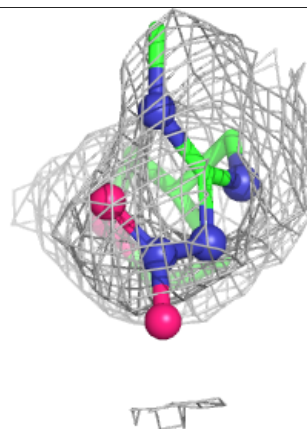
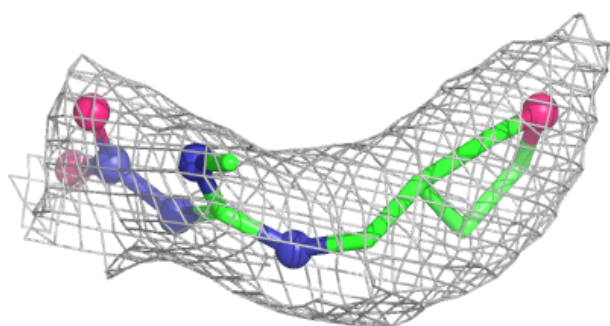
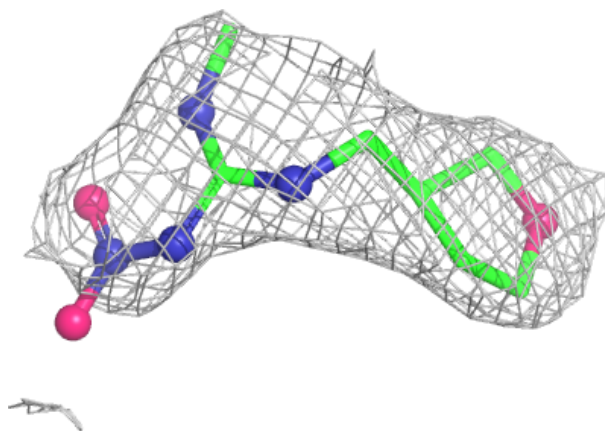
Electron density around A1LW0 E 301:

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



Electron density around A1LW0 A 301:

$2mF_o - DF_c$ (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.