



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:23 AM UTC

PDB ID : 9S43 / pdb_00009s43
Title : Complex of Equine Serum Albumin with Oxacillin
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Deposited on : 2025-07-25
Resolution : 2.03 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

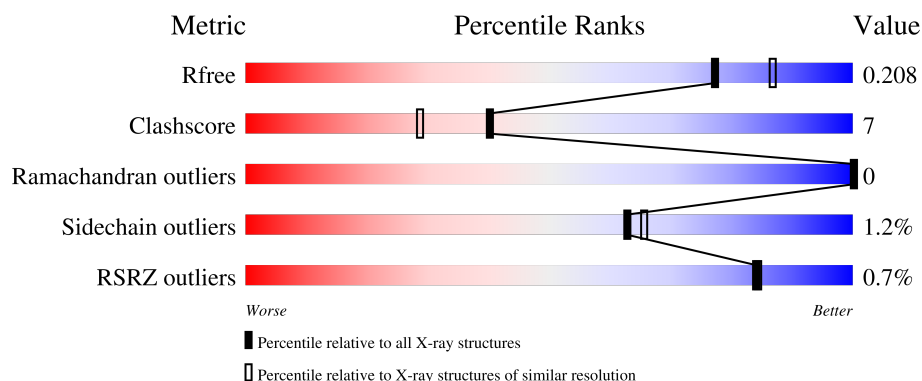
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

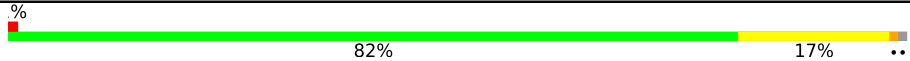
The reported resolution of this entry is 2.03 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	583	

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
5	MLI	A	610	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	A	611	-	-	X	-
5	MLI	A	613	-	X	-	-

2 Entry composition [i](#)

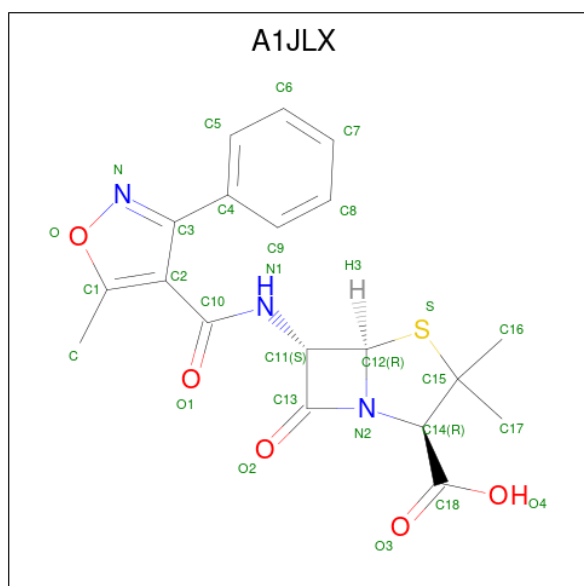
There are 9 unique types of molecules in this entry. The entry contains 4964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

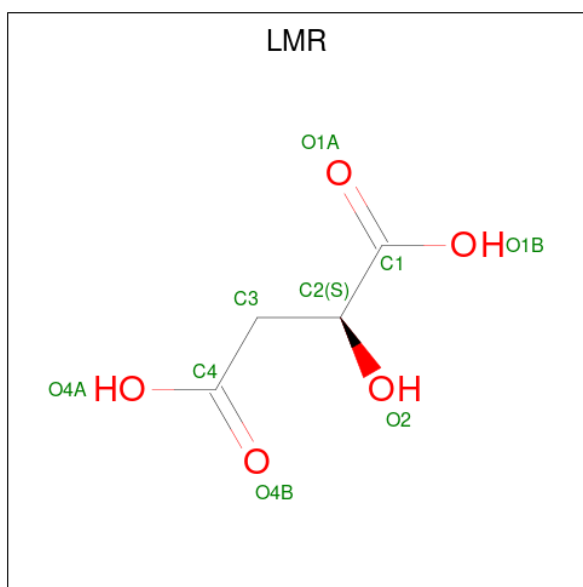
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	6	0
			4587	2900	768	884	35			

- Molecule 2 is (2 {R},5 {R},6 {S})-3,3-dimethyl-6-[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbonylamino]-7-oxidanylidene-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid (CCD ID: A1JLX) (formula: C₁₉H₁₉N₃O₅S) (labeled as "Ligand of Interest" by depositor).



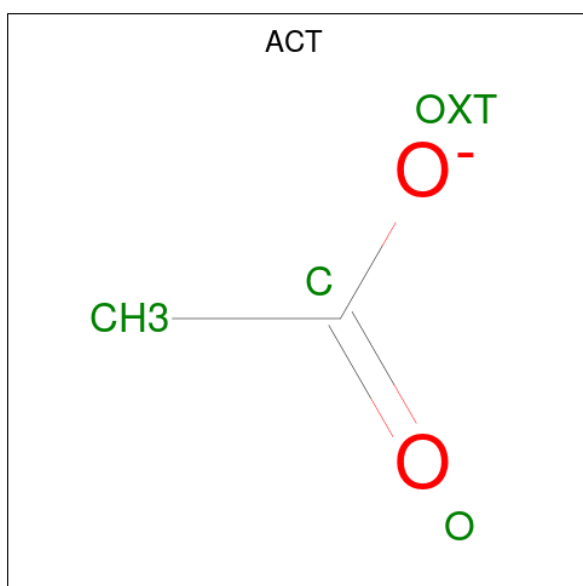
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



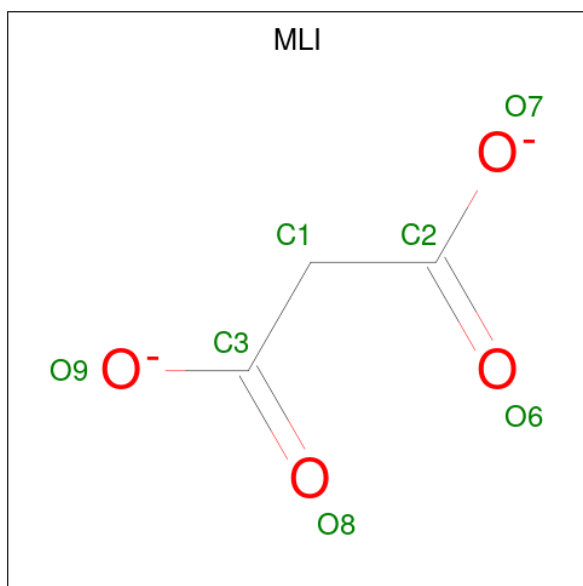
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



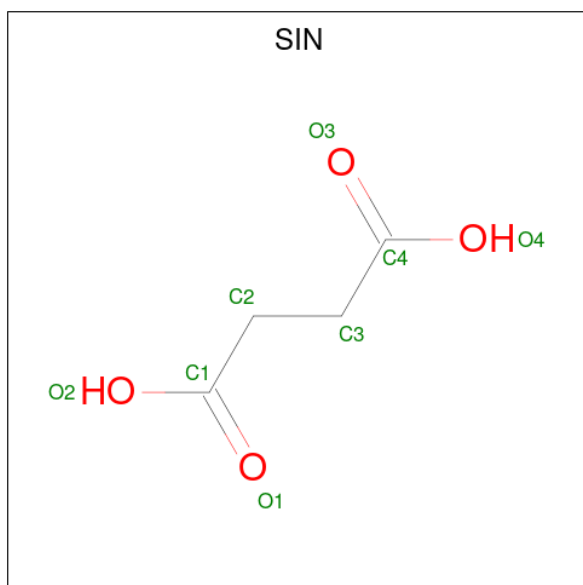
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 7 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 4 4	0	0
7	A	1	Total C O 8 4 4	0	0
7	A	1	Total C O 8 4 4	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

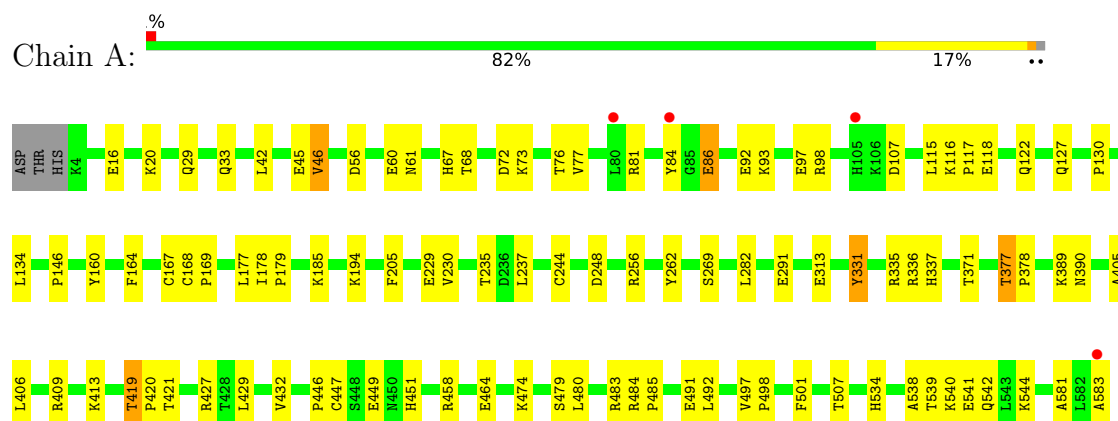
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	219	Total O 219 219	0	0

3 Residue-property plots

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: Albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.72Å 93.72Å 141.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.86 – 2.03 46.86 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.86-2.03) 99.9 (46.86-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.161 , 0.206 0.163 , 0.208	Depositor DCC
R_{free} test set	1129 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4964	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: LMR, A1JLX, MLI, SIN, ACT, CA, FMT

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	0.95	2/4708 (0.0%)	1.23	21/6353 (0.3%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479[A]	SER	C-N	6.96	1.42	1.33
1	A	479[B]	SER	C-N	6.96	1.42	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	THR	CA-CB-OG1	-7.09	98.96	109.60
1	A	449	GLU	CB-CG-CD	6.18	123.11	112.60
1	A	419	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	507	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	235	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	230	VAL	N-CA-CB	5.94	117.10	110.51
1	A	421	THR	CA-CB-OG1	-5.91	100.74	109.60
1	A	68	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	390	ASN	CB-CA-C	5.73	119.87	110.88
1	A	331	TYR	CB-CA-C	5.69	119.72	110.96
1	A	483	ARG	N-CA-CB	-5.54	101.98	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	541	GLU	N-CA-CB	5.49	118.29	110.16
1	A	464	GLU	CB-CA-C	-5.49	102.26	110.88
1	A	291	GLU	CB-CA-C	-5.45	102.25	111.02
1	A	86	GLU	CB-CG-CD	5.19	121.43	112.60
1	A	377	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	160	TYR	CB-CA-C	5.11	118.89	110.88
1	A	269	SER	CA-C-N	-5.08	117.95	123.08
1	A	269	SER	C-N-CA	-5.08	117.95	123.08
1	A	107	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	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	4587	0	4494	59	0
2	A	28	0	0	0	0
3	A	18	0	8	3	0
4	A	12	0	9	0	0
5	A	63	0	18	7	0
6	A	12	0	6	1	0
7	A	24	0	12	4	0
8	A	1	0	0	0	0
9	A	219	0	0	6	0
All	All	4964	0	4547	61	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 7.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD12	5:A:610:MLI:H12	1.78	0.64
1:A:237:LEU:HD13	5:A:613:MLI:H11	1.82	0.61
1:A:377:THR:HB	1:A:378:PRO:HD3	1.84	0.60
1:A:458:ARG:HH22	6:A:616:FMT:H	1.67	0.59
1:A:538:ALA:HB2	1:A:583:ALA:H	1.67	0.59
1:A:540:LYS:HB2	3:A:602:LMR:O4A	2.03	0.58
1:A:544:LYS:HB2	3:A:602:LMR:H2	1.86	0.57
1:A:474:LYS:HE3	9:A:858:HOH:O	2.04	0.56
1:A:46:VAL:HG23	1:A:73:LYS:HG3	1.89	0.54
1:A:130:PRO:O	1:A:134:LEU:HG	2.09	0.53
1:A:405:ALA:HA	3:A:602:LMR:H3A	1.90	0.52
1:A:539:THR:OG1	1:A:542:GLN:HG3	2.08	0.52
1:A:117:PRO:HB2	1:A:178:ILE:CD1	2.40	0.52
1:A:93:LYS:HE2	1:A:97:GLU:HB3	1.93	0.51
1:A:168:CYS:N	1:A:169:PRO:HD2	2.27	0.50
1:A:484:ARG:HB3	1:A:485:PRO:HD3	1.92	0.50
1:A:377:THR:HB	1:A:378:PRO:CD	2.41	0.50
1:A:256:ARG:HD3	5:A:609:MLI:O9	2.12	0.49
1:A:331:TYR:O	1:A:335:ARG:HG3	2.13	0.49
1:A:451:HIS:HE1	7:A:622:SIN:H32	1.78	0.48
1:A:178:ILE:N	1:A:179:PRO:CD	2.77	0.48
1:A:313[B]:GLU:HA	9:A:892:HOH:O	2.14	0.47
1:A:86:GLU:H	1:A:86:GLU:CD	2.19	0.47
1:A:16:GLU:O	1:A:20:LYS:HG3	2.15	0.47
1:A:122:GLN:HB3	1:A:164:PHE:CE2	2.50	0.47
1:A:427:ARG:HD3	7:A:620:SIN:H31	1.96	0.47
1:A:583:ALA:HB2	9:A:886:HOH:O	2.13	0.46
1:A:491:GLU:O	1:A:492:LEU:C	2.59	0.46
1:A:389:LYS:HE3	1:A:389:LYS:HB2	1.43	0.45
1:A:451:HIS:CE1	7:A:622:SIN:H32	2.51	0.45
1:A:205:PHE:CE2	1:A:480:LEU:HG	2.52	0.45
1:A:446:PRO:O	1:A:447:CYS:C	2.60	0.44
1:A:33:GLN:HB2	1:A:84:TYR:CZ	2.53	0.43
5:A:608:MLI:O6	5:A:608:MLI:O8	2.34	0.43
1:A:194:LYS:NZ	5:A:611:MLI:C1	2.82	0.43
1:A:67:HIS:NE2	1:A:248:ASP:OD1	2.52	0.43
1:A:229:GLU:HG3	9:A:747:HOH:O	2.18	0.43
1:A:377:THR:N	1:A:378:PRO:HD2	2.34	0.43
1:A:262:TYR:CD2	1:A:262:TYR:C	2.97	0.43
1:A:406:LEU:HD13	1:A:429:LEU:HB3	2.00	0.43
1:A:429:LEU:O	1:A:432:VAL:HB	2.19	0.43
1:A:42:LEU:HD11	1:A:77:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:NZ	5:A:611:MLI:H12	2.34	0.42
1:A:167:CYS:HB2	1:A:177:LEU:HD13	2.00	0.42
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.55	0.42
1:A:56:ASP:OD1	1:A:56:ASP:C	2.63	0.42
1:A:60:GLU:O	1:A:61:ASN:HB2	2.20	0.41
7:A:622:SIN:H32	9:A:729:HOH:O	2.19	0.41
1:A:29:GLN:HG2	1:A:146:PRO:HA	2.02	0.41
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.91	0.41
1:A:115:LEU:HD12	5:A:610:MLI:C1	2.49	0.41
1:A:419:THR:HB	1:A:420:PRO:HD3	2.02	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.21	0.41
1:A:45:GLU:HB3	1:A:73:LYS:HE2	2.03	0.40
1:A:33:GLN:HB2	1:A:84:TYR:CE2	2.56	0.40
1:A:336:ARG:HG3	1:A:337:HIS:CD2	2.57	0.40
1:A:542:GLN:NE2	1:A:581:ALA:O	2.50	0.40
1:A:98:ARG:NH1	9:A:703:HOH:O	2.39	0.40
1:A:409:ARG:CG	1:A:413:LYS:HE2	2.52	0.40
1:A:116:LYS:HD3	1:A:116:LYS:HA	1.95	0.40
1:A:497:VAL:O	1:A:498:PRO:C	2.64	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	584/583 (100%)	572 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/508 (100%)	502 (99%)	6 (1%)	63	65

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

Mol	Chain	Res	Type
1	A	46	VAL
1	A	92	GLU
1	A	118	GLU
1	A	127	GLN
1	A	244	CYS
1	A	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

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	LMR	A	602	-	8,8,8	1.33	1 (12%)	10,10,10	1.37	1 (10%)
5	MLI	A	614	8	6,6,6	2.12	3 (50%)	7,7,7	1.12	0
6	FMT	A	619	-	2,2,2	1.09	0	1,1,1	0.25	0
3	LMR	A	603	-	8,8,8	1.49	2 (25%)	10,10,10	1.84	3 (30%)
5	MLI	A	607	-	6,6,6	1.47	1 (16%)	7,7,7	1.11	0
4	ACT	A	606	-	3,3,3	1.25	0	3,3,3	0.85	0
7	SIN	A	621	-	7,7,7	1.32	1 (14%)	8,8,8	0.96	0
5	MLI	A	613	-	6,6,6	2.20	3 (50%)	7,7,7	1.45	1 (14%)
5	MLI	A	615	-	6,6,6	1.48	2 (33%)	7,7,7	1.20	0
6	FMT	A	616	-	2,2,2	1.37	0	1,1,1	0.31	0
6	FMT	A	617	-	2,2,2	0.86	0	1,1,1	0.19	0
7	SIN	A	622	-	7,7,7	1.20	0	8,8,8	1.18	0
5	MLI	A	610	-	6,6,6	1.90	3 (50%)	7,7,7	0.84	0
2	A1JLX	A	601	-	31,31,31	2.08	10 (32%)	46,48,48	2.85	19 (41%)
5	MLI	A	612	-	6,6,6	1.59	1 (16%)	7,7,7	1.12	0
6	FMT	A	618	-	2,2,2	1.20	0	1,1,1	0.29	0
5	MLI	A	611	-	6,6,6	1.11	0	7,7,7	1.56	1 (14%)
5	MLI	A	609	-	6,6,6	1.92	3 (50%)	7,7,7	1.01	0
4	ACT	A	604	-	3,3,3	1.61	1 (33%)	3,3,3	0.76	0
7	SIN	A	620	-	7,7,7	1.14	0	8,8,8	1.05	0
5	MLI	A	608	-	6,6,6	2.13	4 (66%)	7,7,7	0.87	0
4	ACT	A	605	-	3,3,3	1.04	0	3,3,3	0.87	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	LMR	A	602	-	-	0/8/8/8	-
5	MLI	A	609	-	-	0/4/4/4	-
2	A1JLX	A	601	-	-	7/16/47/47	0/4/4/4
5	MLI	A	611	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SIN	A	621	-	-	2/5/5/5	-
5	MLI	A	614	8	-	0/4/4/4	-
5	MLI	A	613	-	-	3/4/4/4	-
5	MLI	A	615	-	-	0/4/4/4	-
7	SIN	A	622	-	-	0/5/5/5	-
7	SIN	A	620	-	-	3/5/5/5	-
5	MLI	A	608	-	-	0/4/4/4	-
5	MLI	A	612	-	-	2/4/4/4	-
3	LMR	A	603	-	-	3/8/8/8	-
5	MLI	A	610	-	-	0/4/4/4	-
5	MLI	A	607	-	-	4/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1JLX	C2-C1	5.81	1.47	1.36
2	A	601	A1JLX	C3-N	4.25	1.39	1.31
2	A	601	A1JLX	C2-C3	3.63	1.50	1.43
5	A	613	MLI	C1-C2	3.52	1.56	1.51
5	A	614	MLI	O8-C3	3.20	1.32	1.22
5	A	614	MLI	C1-C3	3.12	1.55	1.51
5	A	608	MLI	O6-C2	3.08	1.32	1.22
3	A	603	LMR	O1A-C1	2.76	1.30	1.22
5	A	609	MLI	C1-C3	2.72	1.55	1.51
5	A	607	MLI	O9-C3	-2.61	1.22	1.30
2	A	601	A1JLX	O1-C10	-2.55	1.18	1.23
5	A	613	MLI	C1-C3	2.54	1.55	1.51
2	A	601	A1JLX	C13-N2	-2.49	1.32	1.37
5	A	608	MLI	O9-C3	-2.48	1.22	1.30
5	A	609	MLI	O9-C3	-2.47	1.22	1.30
2	A	601	A1JLX	C15-S	-2.47	1.80	1.85
5	A	614	MLI	C1-C2	2.46	1.54	1.51
5	A	610	MLI	O9-C3	-2.45	1.22	1.30
5	A	612	MLI	O9-C3	-2.44	1.22	1.30
5	A	615	MLI	C1-C3	2.44	1.54	1.51
3	A	602	LMR	O1A-C1	2.40	1.29	1.22
2	A	601	A1JLX	C12-S	-2.34	1.77	1.81
2	A	601	A1JLX	C4-C3	2.23	1.51	1.48
5	A	608	MLI	O8-C3	2.21	1.29	1.22
2	A	601	A1JLX	O2-C13	2.20	1.26	1.22
5	A	609	MLI	O7-C2	-2.17	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	615	MLI	C1-C2	2.17	1.54	1.51
4	A	604	ACT	CH3-C	2.14	1.57	1.49
5	A	610	MLI	O7-C2	-2.13	1.23	1.30
7	A	621	SIN	O4-C4	-2.13	1.23	1.30
5	A	608	MLI	C1-C3	2.13	1.54	1.51
5	A	613	MLI	O9-C3	-2.12	1.23	1.30
3	A	603	LMR	C3-C2	2.10	1.57	1.52
5	A	610	MLI	C1-C2	2.04	1.54	1.51
2	A	601	A1JLX	O-N	-2.04	1.38	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1JLX	O-C1-C2	-7.85	103.26	109.38
2	A	601	A1JLX	C1-O-N	6.44	115.67	108.51
2	A	601	A1JLX	C2-C3-N	-5.91	105.19	111.43
2	A	601	A1JLX	C4-C3-N	5.76	128.04	118.75
2	A	601	A1JLX	C3-C2-C1	4.73	107.73	104.58
2	A	601	A1JLX	O2-C13-N2	4.36	137.76	131.75
2	A	601	A1JLX	C18-C14-N2	4.31	119.26	112.10
2	A	601	A1JLX	S-C12-N2	-4.23	99.21	104.93
2	A	601	A1JLX	C14-N2-C13	3.56	136.25	126.38
2	A	601	A1JLX	O4-C18-C14	3.54	122.63	112.47
3	A	603	LMR	O1A-C1-C2	-3.51	115.58	122.60
2	A	601	A1JLX	C11-C12-N2	-3.30	84.07	88.01
5	A	611	MLI	C3-C1-C2	-3.10	102.00	112.95
2	A	601	A1JLX	C12-N2-C13	3.10	97.72	93.92
2	A	601	A1JLX	C12-N2-C14	2.84	120.63	117.30
2	A	601	A1JLX	C11-C12-S	-2.83	114.79	119.22
3	A	602	LMR	O1A-C1-C2	-2.80	117.01	122.60
3	A	603	LMR	O1B-C1-C2	2.59	118.22	112.74
5	A	613	MLI	C3-C1-C2	2.41	121.45	112.95
2	A	601	A1JLX	C-C1-C2	2.40	138.06	134.27
2	A	601	A1JLX	O3-C18-C14	-2.31	115.75	122.89
2	A	601	A1JLX	C12-C11-N1	-2.27	113.79	118.49
2	A	601	A1JLX	C15-S-C12	2.19	99.16	93.42
2	A	601	A1JLX	O-N-C3	2.09	108.14	105.91
3	A	603	LMR	C2-C3-C4	-2.04	106.76	112.08

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1JLX	O1-C10-N1-C11
2	A	601	A1JLX	C2-C10-N1-C11
2	A	601	A1JLX	C12-C11-N1-C10
7	A	620	SIN	C1-C2-C3-C4
3	A	603	LMR	C1-C2-C3-C4
2	A	601	A1JLX	O1-C10-C2-C3
5	A	607	MLI	C3-C1-C2-O6
2	A	601	A1JLX	C13-C11-N1-C10
5	A	613	MLI	C3-C1-C2-O6
2	A	601	A1JLX	N1-C10-C2-C3
7	A	620	SIN	O1-C1-C2-C3
5	A	607	MLI	C2-C1-C3-O8
5	A	612	MLI	C2-C1-C3-O8
7	A	620	SIN	O2-C1-C2-C3
5	A	607	MLI	C3-C1-C2-O7
5	A	613	MLI	C3-C1-C2-O7
3	A	603	LMR	O1A-C1-C2-C3
3	A	603	LMR	O1B-C1-C2-C3
7	A	621	SIN	O2-C1-C2-C3
5	A	607	MLI	C2-C1-C3-O9
5	A	612	MLI	C2-C1-C3-O9
7	A	621	SIN	O1-C1-C2-C3
5	A	613	MLI	C2-C1-C3-O9
5	A	611	MLI	C2-C1-C3-O8
2	A	601	A1JLX	N1-C10-C2-C1

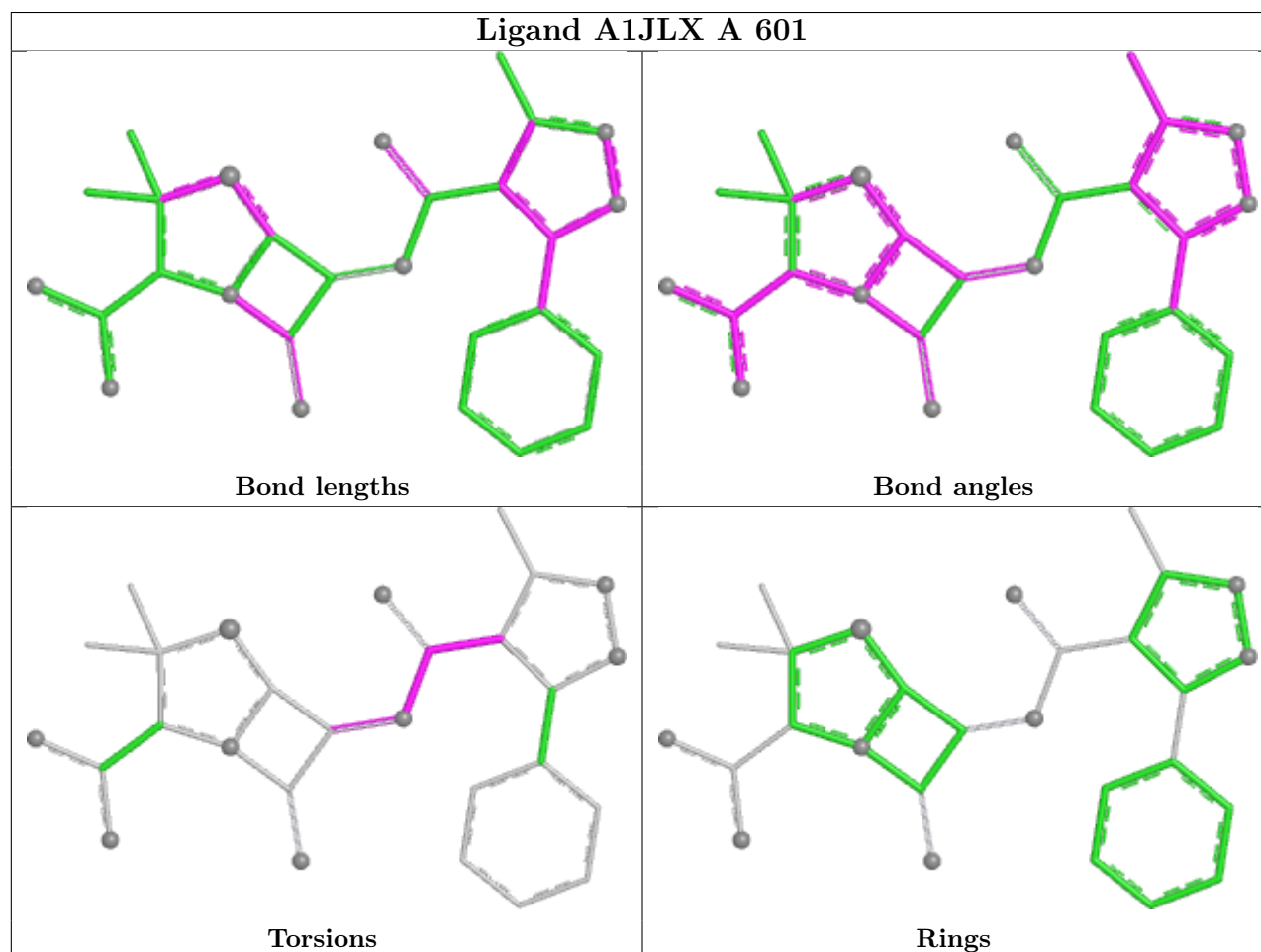
There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	LMR	3	0
5	A	613	MLI	1	0
6	A	616	FMT	1	0
7	A	622	SIN	3	0
5	A	610	MLI	2	0
5	A	611	MLI	2	0
5	A	609	MLI	1	0
7	A	620	SIN	1	0
5	A	608	MLI	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.



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	580/583 (99%)	-0.44	4 (0%) 84 84	21, 44, 73, 108	6 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	3.4
1	A	105	HIS	2.8
1	A	84	TYR	2.3
1	A	583	ALA	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.

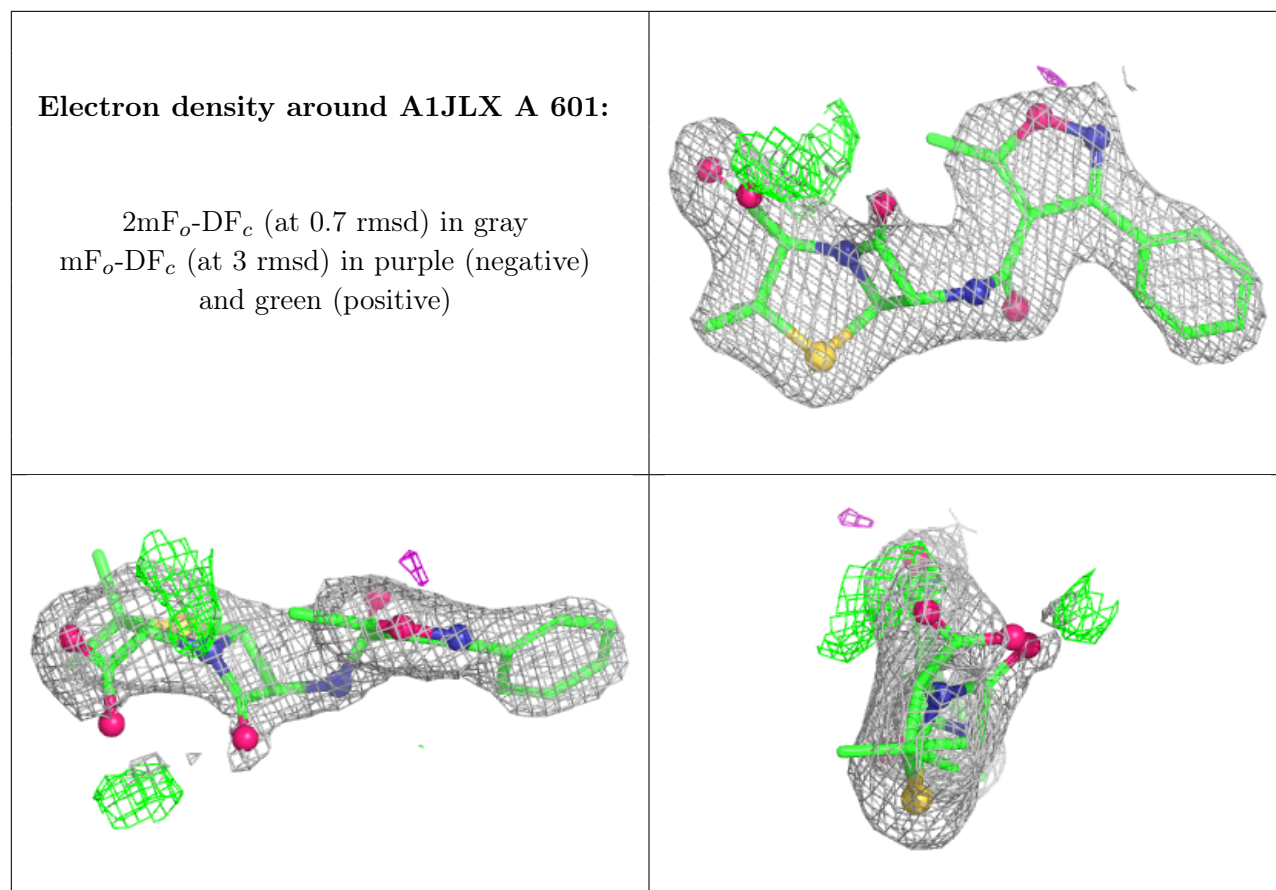
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LMR	A	602	9/9	0.79	0.19	59,76,84,87	0
7	SIN	A	620	8/8	0.81	0.16	63,76,89,113	0
3	LMR	A	603	9/9	0.83	0.10	58,63,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FMT	A	616	3/3	0.86	0.18	61,61,69,73	0
5	MLI	A	607	7/7	0.86	0.09	57,64,75,91	0
6	FMT	A	618	3/3	0.87	0.11	71,71,74,75	0
4	ACT	A	606	4/4	0.88	0.12	56,75,83,96	0
4	ACT	A	605	4/4	0.88	0.18	52,58,69,71	0
5	MLI	A	611	7/7	0.88	0.15	75,94,107,109	0
5	MLI	A	615	7/7	0.89	0.14	36,55,85,88	0
5	MLI	A	612	7/7	0.89	0.14	79,86,98,99	0
7	SIN	A	621	8/8	0.89	0.15	73,86,96,106	0
5	MLI	A	614	7/7	0.90	0.15	60,69,74,90	0
2	A1JLX	A	601	28/28	0.90	0.12	53,76,96,106	0
5	MLI	A	608	7/7	0.90	0.11	43,59,73,89	0
8	CA	A	623	1/1	0.90	0.17	96,96,96,96	0
5	MLI	A	613	7/7	0.91	0.17	48,72,87,87	0
7	SIN	A	622	8/8	0.92	0.12	59,84,98,104	0
4	ACT	A	604	4/4	0.92	0.15	57,57,58,66	0
5	MLI	A	610	7/7	0.93	0.12	53,71,91,93	0
6	FMT	A	619	3/3	0.93	0.12	74,74,87,90	0
5	MLI	A	609	7/7	0.94	0.13	56,66,75,75	0
6	FMT	A	617	3/3	0.94	0.13	72,72,79,82	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.