



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:36 AM UTC

PDB ID : 6MO2 / pdb_00006mo2
Title : Structure of dengue virus protease with an allosteric Inhibitor that blocks replication
Authors : Lin, Y.-L.; Nie, S.; Hua, Y.; Wu, J.; Wu, F.; Huo, T.; Yao, Y.; Song, Y.
Deposited on : 2018-10-03
Resolution : 2.80 Å(reported)

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

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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

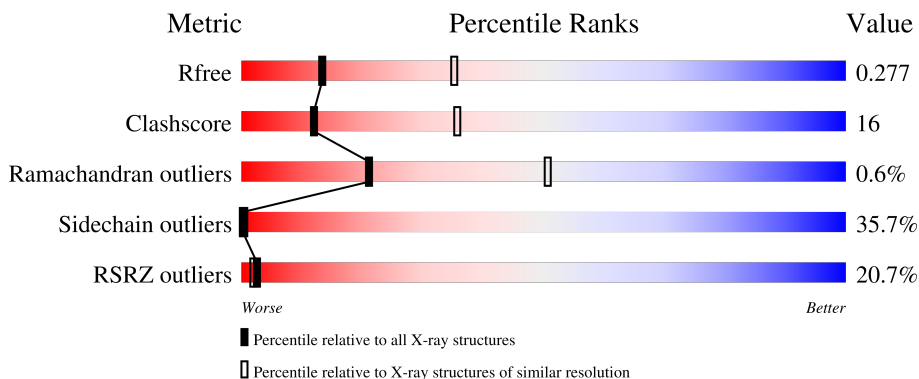
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	247	
1	B	247	

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
2	JVM	A	1201	-	X	-	-
2	JVM	B	1201	-	X	-	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2578 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 FLAVIVIRUS_NS2B/Peptidase S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1256	796	217	240	3	0	0	0
1	B	164	1256	796	217	240	3	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

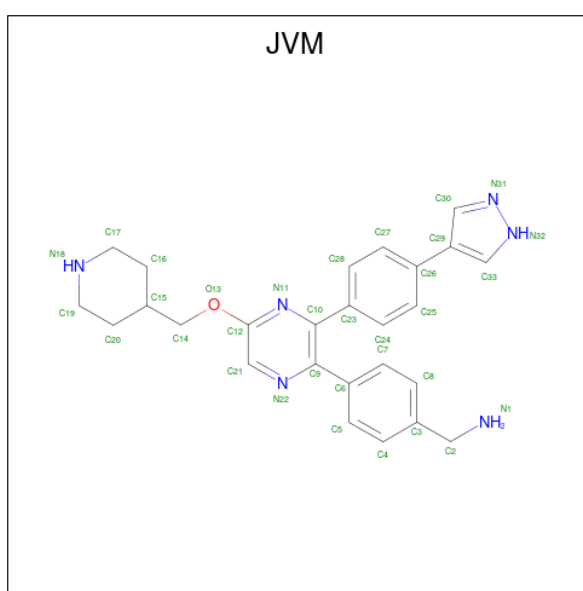
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP A0A0B4L2Y4
A	44	SER	-	expression tag	UNP A0A0B4L2Y4
A	45	HIS	-	expression tag	UNP A0A0B4L2Y4
A	46	MET	-	expression tag	UNP A0A0B4L2Y4
A	47	LEU	-	expression tag	UNP A0A0B4L2Y4
A	48	MET	-	expression tag	UNP A0A0B4L2Y4
A	992	GLY	-	linker	UNP A0A0B4L2Y4
A	993	GLY	-	linker	UNP A0A0B4L2Y4
A	994	GLY	-	linker	UNP A0A0B4L2Y4
A	995	GLY	-	linker	UNP A0A0B4L2Y4
A	996	SER	-	linker	UNP A0A0B4L2Y4
A	997	GLY	-	linker	UNP A0A0B4L2Y4
A	998	GLY	-	linker	UNP A0A0B4L2Y4
A	999	GLY	-	linker	UNP A0A0B4L2Y4
A	1000	GLY	-	linker	UNP A0A0B4L2Y4
A	1167	ASN	GLN	conflict	UNP Q91H74
B	43	GLY	-	expression tag	UNP A0A0B4L2Y4
B	44	SER	-	expression tag	UNP A0A0B4L2Y4
B	45	HIS	-	expression tag	UNP A0A0B4L2Y4
B	46	MET	-	expression tag	UNP A0A0B4L2Y4
B	47	LEU	-	expression tag	UNP A0A0B4L2Y4
B	48	MET	-	expression tag	UNP A0A0B4L2Y4
B	992	GLY	-	linker	UNP A0A0B4L2Y4
B	993	GLY	-	linker	UNP A0A0B4L2Y4
B	994	GLY	-	linker	UNP A0A0B4L2Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	995	GLY	-	linker	UNP A0A0B4L2Y4
B	996	SER	-	linker	UNP A0A0B4L2Y4
B	997	GLY	-	linker	UNP A0A0B4L2Y4
B	998	GLY	-	linker	UNP A0A0B4L2Y4
B	999	GLY	-	linker	UNP A0A0B4L2Y4
B	1000	GLY	-	linker	UNP A0A0B4L2Y4
B	1167	ASN	GLN	conflict	UNP Q91H74

- Molecule 2 is 1-(4-{5-[(piperidin-4-yl)methoxy]-3-[4-(1H-pyrazol-4-yl)phenyl]pyrazin-2-yl}phenyl)methanamine (CCD ID: JVM) (formula: C₂₆H₂₈N₆O).

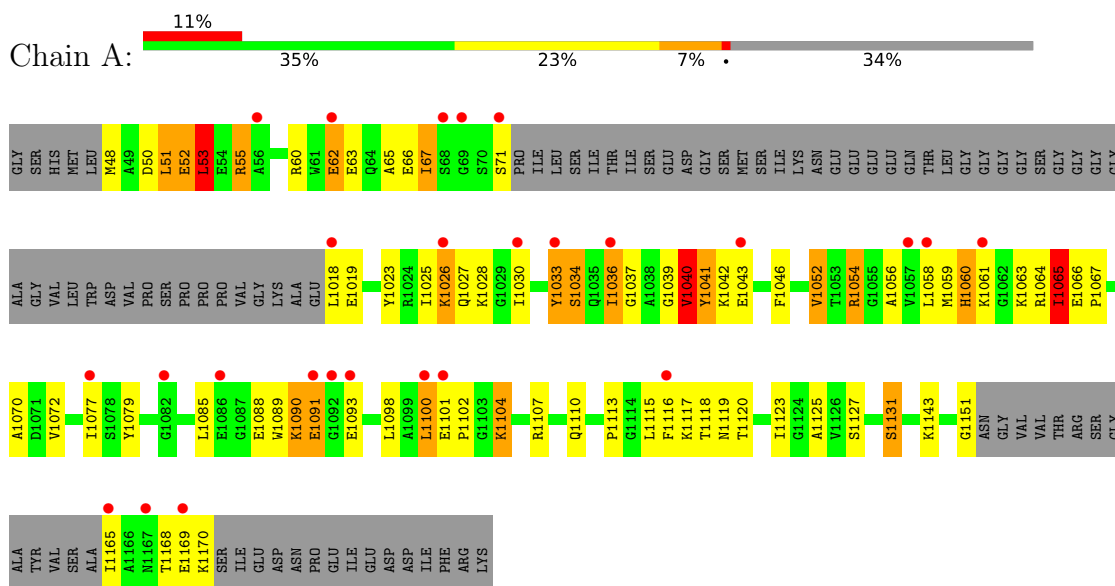


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	26	6	1	0	0
2	B	1	33	26	6	1	0	0

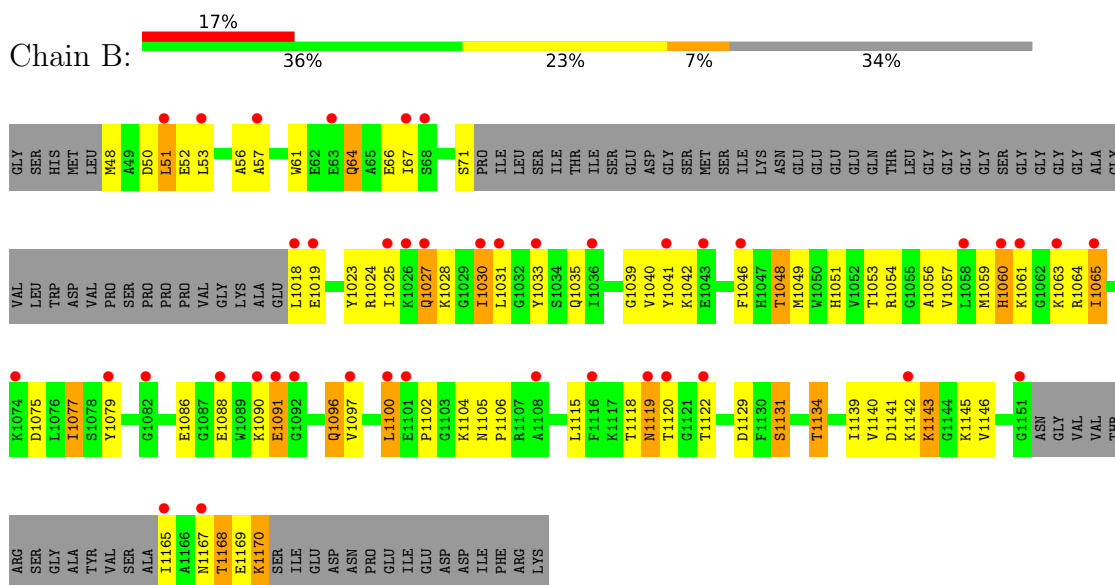
3 Residue-property plots i

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: FLAVIVIRUS_NS2B/Peptidase S7



- Molecule 1: FLAVIVIRUS_NS2B/Peptidase S7



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.16Å 109.16Å 76.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.31 – 2.80 47.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.31-2.80) 99.9 (47.31-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.242 , 0.310 (Not available) , 0.277	Depositor DCC
R_{free} test set	670 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.12	2/1280 (0.2%)	1.30	5/1721 (0.3%)
1	B	1.06	0/1280	1.23	0/1721
All	All	1.09	2/2560 (0.1%)	1.26	5/3442 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1040	VAL	C-O	-5.94	1.17	1.24
1	A	1102	PRO	C-O	-5.05	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LEU	CB-CA-C	7.79	123.62	109.37
1	A	1065	ILE	N-CA-CB	-5.64	104.22	110.99
1	A	1033	TYR	CB-CA-C	5.50	119.57	109.46
1	A	1131	SER	CA-C-N	5.05	124.65	119.05
1	A	1131	SER	C-N-CA	5.05	124.65	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1256	0	1252	41	6
1	B	1256	0	1252	36	5
2	A	33	0	0	5	0
2	B	33	0	0	3	0
All	All	2578	0	2504	80	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (80) 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:1090:LYS:O	1:A:1091:GLU:HB3	1.75	0.86
1:B:1090:LYS:O	1:B:1091:GLU:HB3	1.89	0.72
1:B:1165:ILE:HD12	2:B:1201:JVM:C8	2.19	0.72
1:B:1097:VAL:HG22	1:B:1139:ILE:HG12	1.77	0.65
1:A:1101:GLU:HB2	1:A:1104:LYS:HB2	1.81	0.62
1:A:1165:ILE:HD12	2:A:1201:JVM:C8	2.30	0.61
1:A:67:ILE:HA	1:A:1110:GLN:HB3	1.84	0.60
1:A:53:LEU:C	1:A:53:LEU:HD12	2.29	0.57
1:A:1151:GLY:O	2:A:1201:JVM:C2	2.53	0.56
1:B:1167:ASN:ND2	1:B:1168:THR:N	2.54	0.55
1:A:53:LEU:HD12	1:A:53:LEU:O	2.07	0.55
1:B:50:ASP:O	1:B:1027:GLN:HA	2.06	0.55
1:A:1039:GLY:HA3	1:A:1046:PHE:CZ	2.42	0.54
1:B:56:ALA:HB1	1:B:1100:LEU:HD11	1.90	0.54
1:A:53:LEU:HD11	1:A:1060:HIS:HB2	1.90	0.52
1:B:1065:ILE:HG22	1:B:1079:TYR:HB3	1.92	0.51
1:B:1100:LEU:CD2	1:B:1106:PRO:HB3	2.41	0.51
1:A:50:ASP:O	1:A:1027:GLN:HA	2.11	0.51
1:B:1090:LYS:O	1:B:1091:GLU:CB	2.56	0.51
1:A:1151:GLY:C	1:A:1165:ILE:HG21	2.36	0.50
1:A:1089:TRP:CZ2	1:A:1113:PRO:HD2	2.46	0.50
1:B:1051:HIS:ND1	1:B:1075:ASP:OD2	2.40	0.50
1:A:1036:ILE:O	1:A:1036:ILE:HG13	2.11	0.50
1:B:71:SER:HB3	1:B:1129:ASP:O	2.12	0.49
1:A:1037:GLY:HA3	1:A:1052:VAL:HG21	1.94	0.48
1:B:1143:LYS:HD2	1:B:1145:LYS:HE2	1.96	0.48
1:A:1054:ARG:HE	1:A:1054:ARG:HB2	1.54	0.48
1:A:1088:GLU:HG2	1:A:1088:GLU:O	2.14	0.47
1:A:1090:LYS:O	1:A:1091:GLU:CB	2.53	0.47
1:B:1131:SER:O	1:B:1134:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LYS:HG2	1:A:1043:GLU:HG3	1.96	0.46
1:B:1100:LEU:HD13	1:B:1100:LEU:HA	1.71	0.46
1:A:51:LEU:HD13	1:A:1056:ALA:HB3	1.97	0.46
1:A:1046:PHE:HB3	1:A:1079:TYR:HB2	1.97	0.46
1:A:1065:ILE:O	1:A:1065:ILE:HG22	2.14	0.46
1:B:61:TRP:CE2	1:B:1096:GLN:NE2	2.84	0.46
1:A:1088:GLU:HG3	1:A:1169:GLU:HB3	1.97	0.46
1:B:61:TRP:CE3	1:B:1142:LYS:HA	2.50	0.46
1:B:1049:MET:C	1:B:1077:ILE:HG22	2.41	0.46
1:A:53:LEU:C	1:A:53:LEU:CD1	2.90	0.45
1:B:1167:ASN:HD22	1:B:1168:THR:H	1.64	0.45
1:B:1170:LYS:HE3	1:B:1170:LYS:HB2	1.79	0.45
1:B:1048:THR:HG23	1:B:1077:ILE:HG23	1.98	0.45
1:B:1035:GLN:HB3	1:B:1102:PRO:HB3	1.98	0.45
1:B:1060:HIS:CD2	1:B:1065:ILE:HD11	2.51	0.45
1:A:1070:ALA:HB2	1:A:1077:ILE:HG13	1.99	0.45
2:A:1201:JVM:C7	2:A:1201:JVM:C28	2.95	0.45
1:B:1119:ASN:OD1	1:B:1119:ASN:N	2.39	0.44
1:A:1056:ALA:O	1:A:1079:TYR:OH	2.27	0.44
1:B:1039:GLY:HA3	1:B:1046:PHE:CZ	2.52	0.44
1:B:1100:LEU:HD22	1:B:1106:PRO:HB3	1.98	0.44
1:A:1027:GLN:HE22	1:A:1034:SER:HB3	1.82	0.44
1:A:1165:ILE:HD11	2:A:1201:JVM:C27	2.48	0.44
2:A:1201:JVM:C28	2:A:1201:JVM:C6	2.95	0.44
1:B:1023:TYR:CE1	1:B:1041:TYR:HB2	2.53	0.44
1:B:1141:ASP:OD2	1:B:1145:LYS:HE3	2.17	0.44
1:A:55:ARG:HG3	1:A:1023:TYR:CZ	2.54	0.43
1:B:56:ALA:O	1:B:57:ALA:HB2	2.18	0.43
1:B:1019:GLU:O	1:B:1023:TYR:OH	2.26	0.43
1:B:1143:LYS:CD	1:B:1145:LYS:HE2	2.49	0.42
1:B:1167:ASN:HD22	1:B:1168:THR:N	2.16	0.42
1:B:51:LEU:HD13	1:B:1056:ALA:HB3	2.01	0.42
1:B:1165:ILE:CD1	2:B:1201:JVM:C8	2.94	0.42
1:A:52:GLU:OE2	1:A:1026:LYS:HB2	2.19	0.42
1:B:1048:THR:OG1	1:B:1049:MET:N	2.53	0.42
2:B:1201:JVM:C28	2:B:1201:JVM:C7	2.98	0.42
1:A:1077:ILE:HD13	1:A:1079:TYR:CE1	2.55	0.42
1:A:1116:PHE:HE2	1:A:1125:ALA:HB2	1.85	0.42
1:A:62:GLU:HB3	1:A:65:ALA:HB2	2.02	0.41
1:A:1090:LYS:HE2	1:A:1093:GLU:HB3	2.01	0.41
1:A:1100:LEU:O	1:A:1101:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ILE:O	1:A:1052:VAL:HG22	2.21	0.41
1:B:64:GLN:O	1:B:64:GLN:CG	2.69	0.41
1:A:1040:VAL:O	1:A:1040:VAL:HG12	2.21	0.40
1:A:52:GLU:HA	1:A:1059:MET:O	2.22	0.40
1:A:53:LEU:HD13	1:A:1023:TYR:CD2	2.56	0.40
1:B:1077:ILE:HG12	1:B:1079:TYR:CE2	2.56	0.40
1:A:1023:TYR:CE1	1:A:1041:TYR:HB2	2.56	0.40
1:A:1067:PRO:HD3	1:A:1079:TYR:CE2	2.56	0.40
1:A:1060:HIS:O	1:A:1060:HIS:CD2	2.74	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:N	1:A:71:SER:OG[2_565]	1.17	1.03
1:A:1169:GLU:OE2	1:B:1030:ILE:CD1[6_455]	1.48	0.72
1:A:1169:GLU:CD	1:B:1030:ILE:CD1[6_455]	1.67	0.53
1:A:1169:GLU:CD	1:B:1030:ILE:CG1[6_455]	1.67	0.53
1:A:1169:GLU:OE1	1:B:1030:ILE:CG1[6_455]	1.74	0.46
1:B:48:MET:N	1:B:71:SER:OG[3_445]	1.78	0.42
1:A:1143:LYS:CG	1:A:1143:LYS:CG[5_555]	2.17	0.03

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	158/247 (64%)	148 (94%)	8 (5%)	2 (1%)	9	31
1	B	158/247 (64%)	148 (94%)	10 (6%)	0	100	100
All	All	316/494 (64%)	296 (94%)	18 (6%)	2 (1%)	21	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1091	GLU
1	A	1019	GLU

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	129/194 (66%)	84 (65%)	45 (35%)	0 0
1	B	129/194 (66%)	82 (64%)	47 (36%)	0 0
All	All	258/388 (66%)	166 (64%)	92 (36%)	0 0

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	52	GLU
1	A	53	LEU
1	A	55	ARG
1	A	60	ARG
1	A	62	GLU
1	A	63	GLU
1	A	66	GLU
1	A	67	ILE
1	A	1018	LEU
1	A	1025	ILE
1	A	1026	LYS
1	A	1028	LYS
1	A	1030	ILE
1	A	1033	TYR
1	A	1034	SER
1	A	1036	ILE
1	A	1040	VAL
1	A	1041	TYR
1	A	1052	VAL
1	A	1054	ARG
1	A	1058	LEU

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Mol	Chain	Res	Type
1	A	1060	HIS
1	A	1061	LYS
1	A	1063	LYS
1	A	1064	ARG
1	A	1065	ILE
1	A	1066	GLU
1	A	1072	VAL
1	A	1085	LEU
1	A	1090	LYS
1	A	1098	LEU
1	A	1100	LEU
1	A	1104	LYS
1	A	1107	ARG
1	A	1115	LEU
1	A	1117	LYS
1	A	1118	THR
1	A	1119	ASN
1	A	1120	THR
1	A	1123	ILE
1	A	1127	SER
1	A	1131	SER
1	A	1168	THR
1	A	1170	LYS
1	B	51	LEU
1	B	52	GLU
1	B	53	LEU
1	B	64	GLN
1	B	66	GLU
1	B	67	ILE
1	B	1018	LEU
1	B	1024	ARG
1	B	1025	ILE
1	B	1027	GLN
1	B	1028	LYS
1	B	1030	ILE
1	B	1031	LEU
1	B	1033	TYR
1	B	1040	VAL
1	B	1042	LYS
1	B	1048	THR
1	B	1053	THR
1	B	1054	ARG

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Mol	Chain	Res	Type
1	B	1057	VAL
1	B	1059	MET
1	B	1060	HIS
1	B	1061	LYS
1	B	1063	LYS
1	B	1064	ARG
1	B	1065	ILE
1	B	1077	ILE
1	B	1086	GLU
1	B	1088	GLU
1	B	1091	GLU
1	B	1096	GLN
1	B	1100	LEU
1	B	1104	LYS
1	B	1105	ASN
1	B	1115	LEU
1	B	1118	THR
1	B	1119	ASN
1	B	1120	THR
1	B	1122	THR
1	B	1131	SER
1	B	1134	THR
1	B	1140	VAL
1	B	1143	LYS
1	B	1146	VAL
1	B	1168	THR
1	B	1169	GLU
1	B	1170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	GLN
1	A	1060	HIS
1	B	64	GLN
1	B	1060	HIS
1	B	1105	ASN
1	B	1167	ASN

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](#)

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
2	JVM	B	1201	-	37,37,37	3.82	23 (62%)	49,50,50	3.04	21 (42%)
2	JVM	A	1201	-	37,37,37	3.30	21 (56%)	49,50,50	2.51	23 (46%)

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	JVM	B	1201	-	-	7/19/27/27	0/5/5/5
2	JVM	A	1201	-	-	7/19/27/27	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	JVM	C23-C10	9.18	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	JVM	C33-C29	7.83	1.52	1.38
2	B	1201	JVM	N32-N31	7.47	1.53	1.35
2	A	1201	JVM	C23-C10	7.27	1.57	1.49
2	A	1201	JVM	C10-N11	7.27	1.46	1.34
2	B	1201	JVM	C33-N32	6.88	1.44	1.34
2	A	1201	JVM	C33-N32	6.39	1.43	1.34
2	B	1201	JVM	C30-N31	5.87	1.43	1.33
2	A	1201	JVM	C4-C5	5.73	1.48	1.38
2	B	1201	JVM	C27-C26	5.69	1.48	1.39
2	A	1201	JVM	N32-N31	5.17	1.47	1.35
2	B	1201	JVM	C27-C28	4.82	1.46	1.38
2	A	1201	JVM	C27-C26	4.71	1.46	1.39
2	B	1201	JVM	O13-C12	4.38	1.45	1.36
2	B	1201	JVM	C10-N11	4.36	1.41	1.34
2	B	1201	JVM	C8-C3	4.23	1.47	1.38
2	A	1201	JVM	C12-N11	4.14	1.40	1.33
2	B	1201	JVM	C21-N22	3.88	1.42	1.34
2	A	1201	JVM	C30-N31	3.84	1.40	1.33
2	A	1201	JVM	C24-C23	3.81	1.47	1.39
2	A	1201	JVM	C21-N22	3.79	1.42	1.34
2	B	1201	JVM	C24-C25	3.69	1.44	1.38
2	B	1201	JVM	C12-N11	3.66	1.39	1.33
2	A	1201	JVM	C27-C28	3.63	1.44	1.38
2	B	1201	JVM	C4-C5	3.51	1.44	1.38
2	B	1201	JVM	C21-C12	3.50	1.44	1.39
2	A	1201	JVM	C33-C29	3.40	1.44	1.38
2	A	1201	JVM	C4-C3	3.29	1.45	1.38
2	A	1201	JVM	O13-C12	3.26	1.42	1.36
2	B	1201	JVM	O13-C14	3.18	1.54	1.44
2	B	1201	JVM	C24-C23	3.17	1.45	1.39
2	B	1201	JVM	C9-N22	3.05	1.40	1.34
2	A	1201	JVM	C24-C25	2.96	1.43	1.38
2	B	1201	JVM	C5-C6	2.82	1.45	1.39
2	A	1201	JVM	O13-C14	2.81	1.53	1.44
2	B	1201	JVM	C25-C26	2.68	1.43	1.39
2	B	1201	JVM	C26-C29	2.53	1.53	1.48
2	A	1201	JVM	C26-C29	2.44	1.53	1.48
2	A	1201	JVM	C9-N22	2.40	1.39	1.34
2	A	1201	JVM	C5-C6	2.33	1.44	1.39
2	A	1201	JVM	C7-C6	2.11	1.43	1.39
2	B	1201	JVM	C7-C8	2.06	1.42	1.38
2	A	1201	JVM	C20-C15	2.03	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	JVM	C6-C9	-2.01	1.46	1.49

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	JVM	C14-O13-C12	-8.71	106.32	117.69
2	B	1201	JVM	C8-C7-C6	-8.37	110.38	121.12
2	B	1201	JVM	O13-C12-C21	6.36	124.85	117.94
2	A	1201	JVM	C21-C12-N11	-5.55	119.12	122.99
2	B	1201	JVM	C5-C6-C7	5.46	127.45	117.68
2	B	1201	JVM	C30-N31-N32	5.41	116.31	105.75
2	B	1201	JVM	C33-N32-N31	-5.10	100.74	111.25
2	B	1201	JVM	C6-C9-C10	-5.03	116.72	124.08
2	A	1201	JVM	C14-O13-C12	-4.83	111.38	117.69
2	B	1201	JVM	C29-C30-N31	-4.49	102.17	110.83
2	A	1201	JVM	C23-C10-N11	4.45	121.17	115.10
2	A	1201	JVM	C27-C26-C29	-4.19	115.28	121.16
2	A	1201	JVM	C33-C29-C30	3.95	112.00	104.00
2	A	1201	JVM	C5-C6-C7	3.95	124.74	117.68
2	A	1201	JVM	C17-C16-C15	-3.92	106.08	112.14
2	B	1201	JVM	C5-C4-C3	-3.91	115.86	121.00
2	B	1201	JVM	C7-C6-C9	-3.87	114.34	120.62
2	B	1201	JVM	C7-C8-C3	3.75	125.92	121.00
2	A	1201	JVM	C5-C4-C3	-3.72	116.11	121.00
2	B	1201	JVM	C33-C29-C30	3.60	111.28	104.00
2	A	1201	JVM	C8-C7-C6	-3.47	116.67	121.12
2	A	1201	JVM	C29-C30-N31	-3.45	104.17	110.83
2	A	1201	JVM	C16-C15-C14	-3.38	102.42	111.42
2	A	1201	JVM	C4-C3-C8	3.34	123.20	118.23
2	A	1201	JVM	C21-N22-C9	3.21	123.55	118.01
2	A	1201	JVM	C9-C10-N11	-3.15	115.97	120.05
2	B	1201	JVM	C6-C9-N22	3.15	120.06	115.40
2	A	1201	JVM	C30-N31-N32	3.04	111.69	105.75
2	A	1201	JVM	C24-C25-C26	-2.98	117.62	120.80
2	A	1201	JVM	C20-C15-C14	2.86	119.06	111.42
2	B	1201	JVM	C17-C16-C15	-2.84	107.75	112.14
2	A	1201	JVM	C16-C15-C20	2.76	116.03	109.29
2	B	1201	JVM	C20-C19-N18	-2.74	105.64	110.81
2	A	1201	JVM	C7-C6-C9	-2.62	116.36	120.62
2	A	1201	JVM	C4-C5-C6	-2.56	117.83	121.12
2	A	1201	JVM	C33-N32-N31	-2.55	106.00	111.25
2	A	1201	JVM	C25-C26-C27	2.39	121.60	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	JVM	C16-C17-N18	-2.28	106.51	110.81
2	B	1201	JVM	C23-C10-C9	2.27	127.40	124.08
2	B	1201	JVM	C20-C15-C14	-2.27	105.37	111.42
2	B	1201	JVM	O13-C12-N11	-2.09	112.82	118.57
2	B	1201	JVM	C27-C26-C29	-2.08	118.24	121.16
2	B	1201	JVM	C9-C10-N11	-2.05	117.39	120.05
2	B	1201	JVM	C26-C29-C30	-2.02	122.41	127.97

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	JVM	O13-C14-C15-C20
2	B	1201	JVM	C15-C14-O13-C12
2	B	1201	JVM	O13-C14-C15-C20
2	A	1201	JVM	C27-C26-C29-C33
2	B	1201	JVM	C27-C26-C29-C33
2	A	1201	JVM	C27-C26-C29-C30
2	A	1201	JVM	C25-C26-C29-C33
2	A	1201	JVM	O13-C14-C15-C16
2	B	1201	JVM	O13-C14-C15-C16
2	A	1201	JVM	C25-C26-C29-C30
2	B	1201	JVM	C27-C26-C29-C30
2	B	1201	JVM	C25-C26-C29-C33
2	A	1201	JVM	C15-C14-O13-C12
2	B	1201	JVM	C25-C26-C29-C30

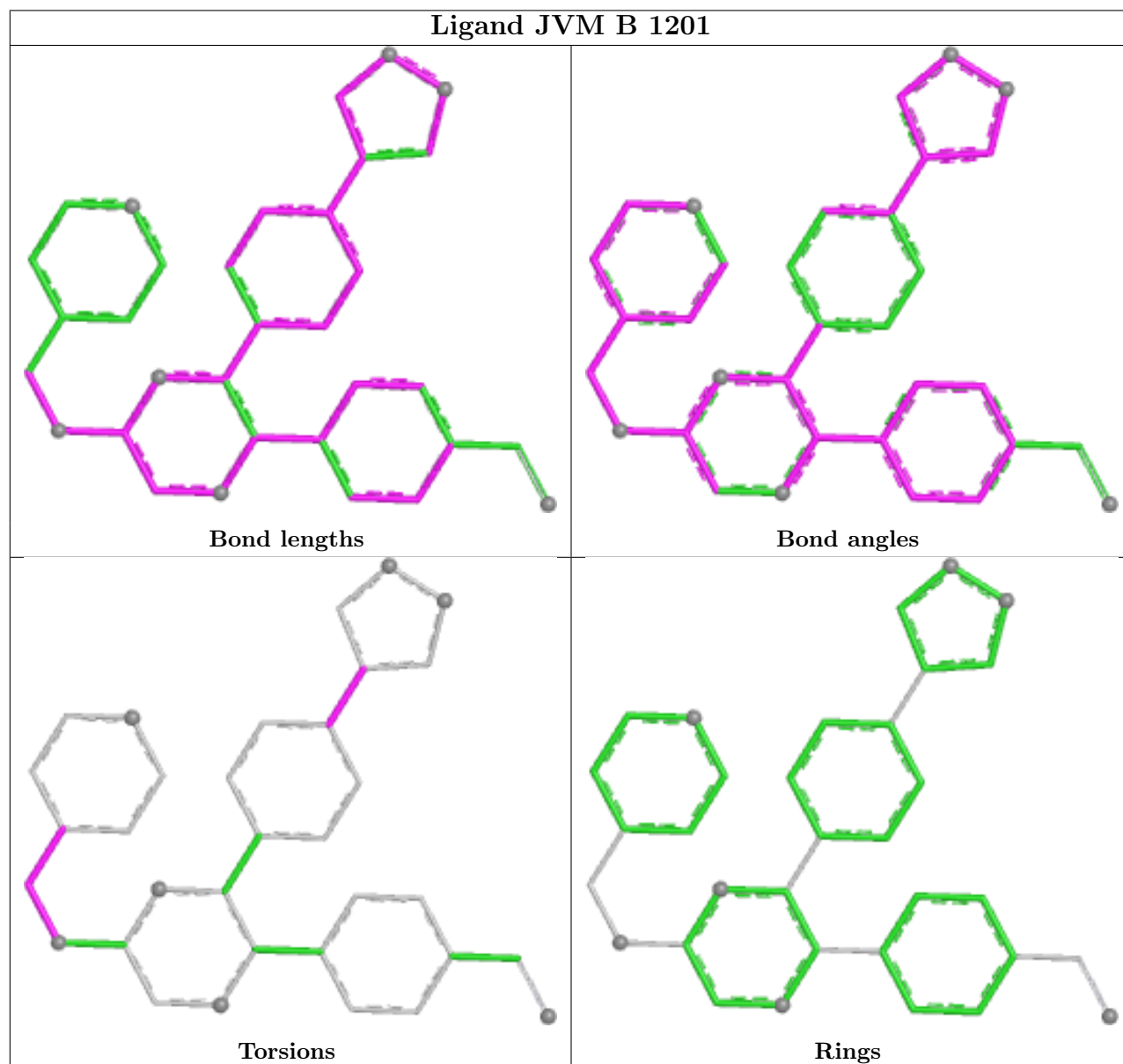
There are no ring outliers.

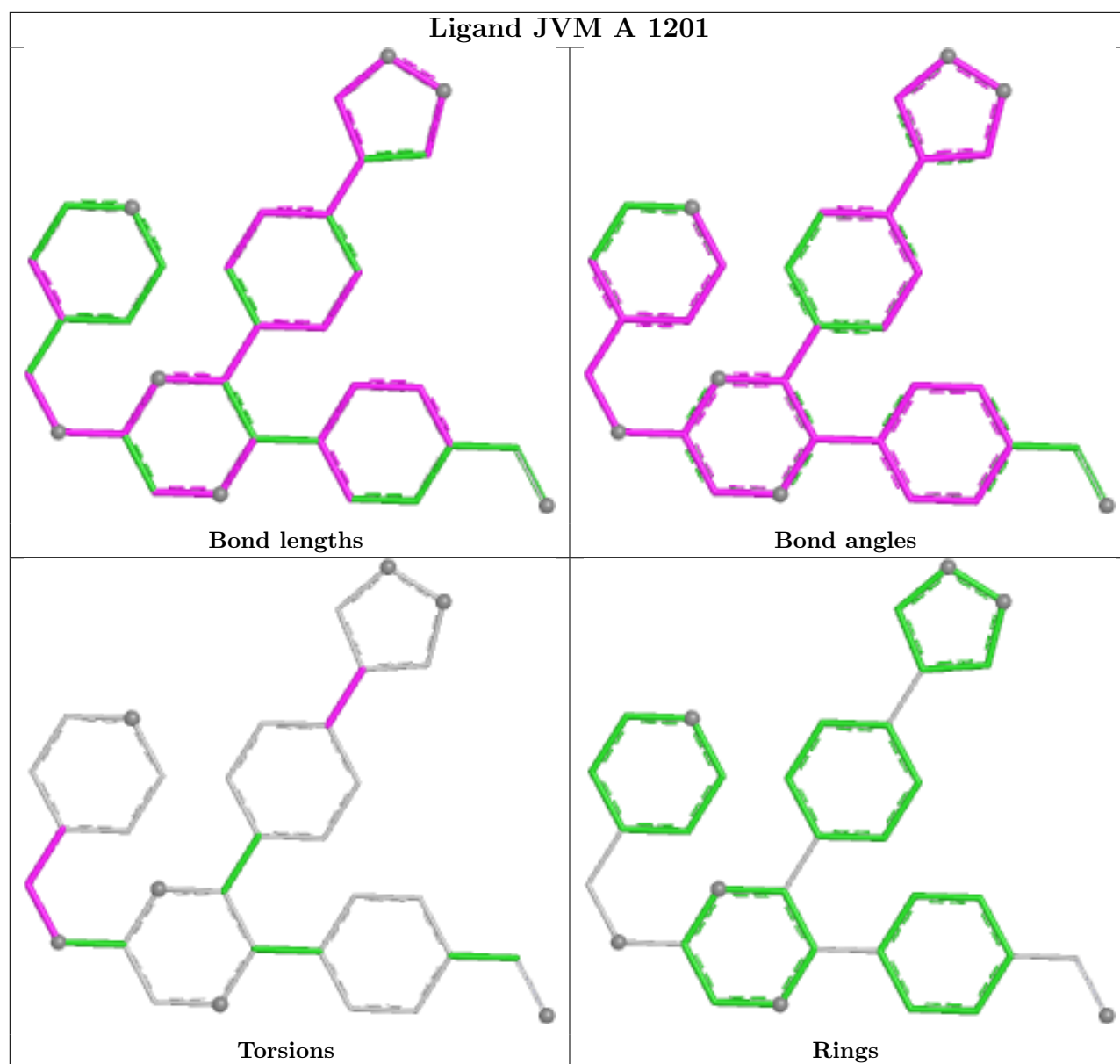
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	JVM	3	0
2	A	1201	JVM	5	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

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, 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	164/247 (66%)	0.95	26 (15%) 5 4	50, 65, 103, 118	0
1	B	164/247 (66%)	1.19	42 (25%) 1 1	50, 67, 106, 126	0
All	All	328/494 (66%)	1.07	68 (20%) 2 2	50, 66, 106, 126	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1030	ILE	6.4
1	B	1088	GLU	6.4
1	A	1169	GLU	6.1
1	B	1027	GLN	5.0
1	B	1120	THR	5.0
1	A	1165	ILE	4.7
1	B	1142	LYS	4.7
1	A	1101	GLU	4.4
1	B	1165	ILE	4.3
1	B	1122	THR	4.3
1	A	1167	ASN	4.1
1	B	1036	ILE	4.1
1	B	1101	GLU	4.1
1	A	62	GLU	3.9
1	B	1031	LEU	3.8
1	B	1167	ASN	3.7
1	A	1018	LEU	3.7
1	B	1116	PHE	3.6
1	B	1091	GLU	3.5
1	A	1091	GLU	3.3
1	B	1025	ILE	3.3
1	B	1060	HIS	3.3
1	A	1086	GLU	3.2
1	B	1043	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1018	LEU	3.1
1	B	1090	LYS	3.1
1	B	53	LEU	3.1
1	A	1077	ILE	3.0
1	A	1057	VAL	3.0
1	B	1033	TYR	2.9
1	B	1100	LEU	2.9
1	A	1093	GLU	2.9
1	A	1030	ILE	2.9
1	A	71	SER	2.9
1	A	1092	GLY	2.8
1	B	1151	GLY	2.8
1	B	51	LEU	2.7
1	B	1092	GLY	2.7
1	B	1041	TYR	2.6
1	A	1100	LEU	2.5
1	B	1079	TYR	2.5
1	A	69	GLY	2.5
1	B	1065	ILE	2.5
1	A	1058	LEU	2.4
1	B	1082	GLY	2.4
1	B	57	ALA	2.4
1	A	1043	GLU	2.4
1	B	1108	ALA	2.4
1	B	1119	ASN	2.4
1	A	68	SER	2.4
1	A	56	ALA	2.4
1	B	1063	LYS	2.3
1	B	67	ILE	2.3
1	B	1061	LYS	2.3
1	B	63	GLU	2.3
1	A	1116	PHE	2.3
1	A	1033	TYR	2.2
1	B	1026	LYS	2.2
1	B	1097	VAL	2.2
1	A	1082	GLY	2.2
1	B	1074	LYS	2.2
1	B	1046	PHE	2.2
1	B	1058	LEU	2.1
1	A	1026	LYS	2.1
1	A	1036	ILE	2.1
1	B	68	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1019	GLU	2.1
1	A	1061	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

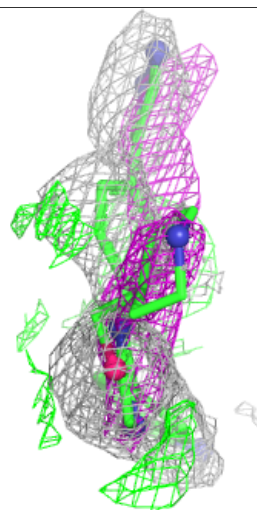
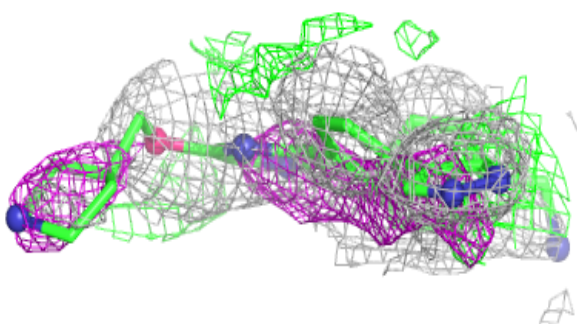
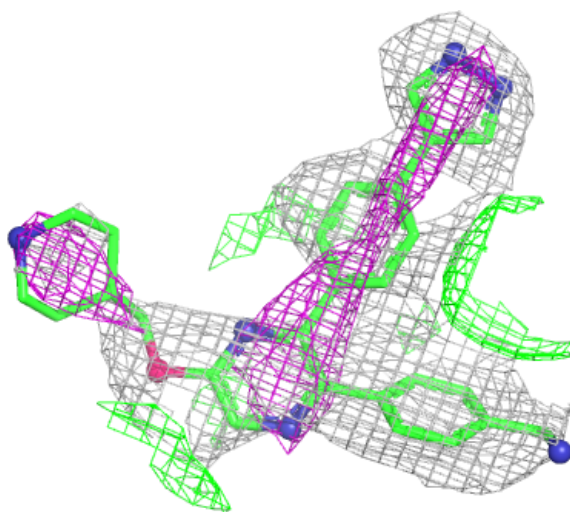
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

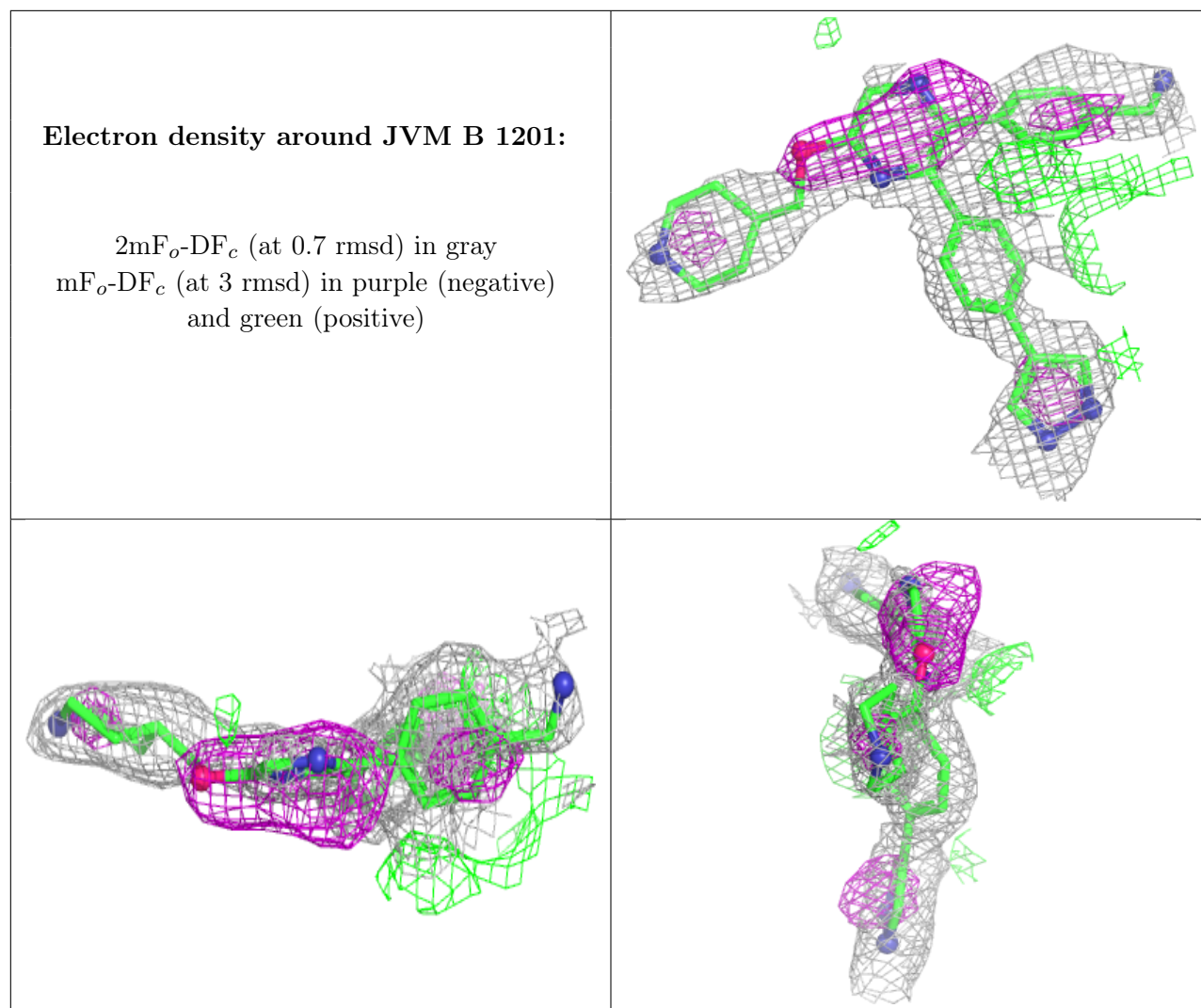
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q < 0.9
2	JVM	A	1201	33/33	0.55	0.20	37,46,52,55	0
2	JVM	B	1201	33/33	0.57	0.19	36,44,53,58	0

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 JVM A 1201:

$2mF_o-DF_c$ (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.