Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2026 – 12:59 pm GMT

PDB ID	:	9SZ4 / pdb_00009sz4
Title	:	Crystal structure of the human METTL3-METTL14 in complex with COD_ME_04
Authors	:	Bedi, R.K.; Caflisch, A.
Deposited on	:	2025-10-14
Resolution	:	1.59 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:

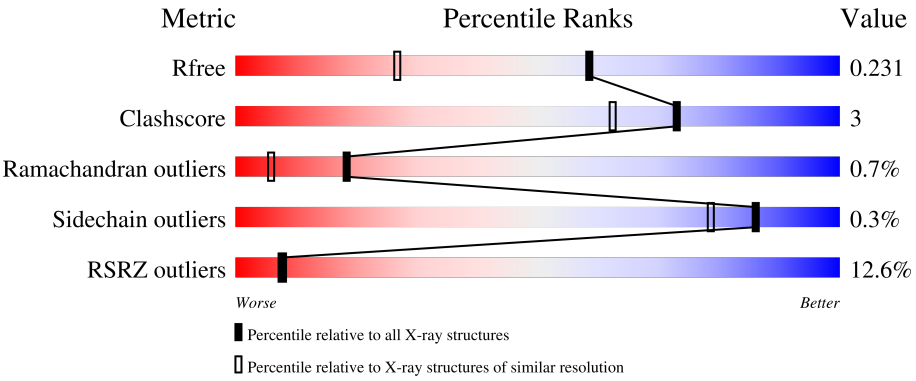
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 <=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	228	9% 84% 6% 10%
2	B	307	12% 73% 7% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3816 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 N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1606	1032	280	284	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	MET	-	initiating methionine	UNP Q86U44

- Molecule 2 is a protein called N(6)-adenosine-methyltransferase non-catalytic subunit METTL14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	2	0
			1899	1219	324	343	13			

There are 18 discrepancies between the modelled and reference sequences:

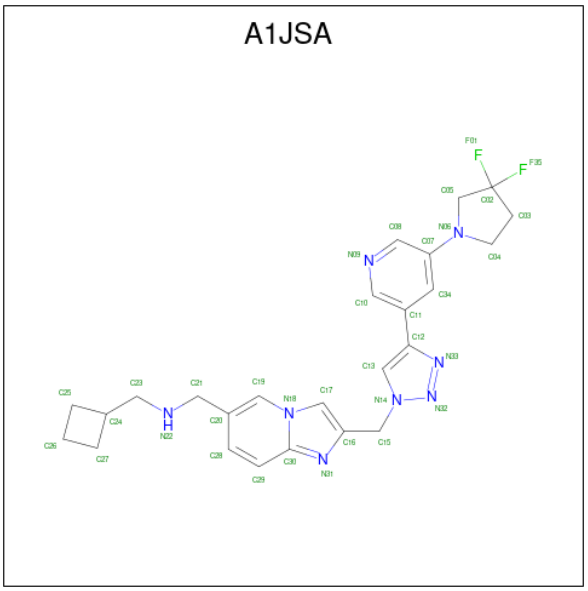
Chain	Residue	Modelled	Actual	Comment	Reference
B	89	MET	-	initiating methionine	UNP Q9HCE5
B	90	HIS	-	expression tag	UNP Q9HCE5
B	91	HIS	-	expression tag	UNP Q9HCE5
B	92	HIS	-	expression tag	UNP Q9HCE5
B	93	HIS	-	expression tag	UNP Q9HCE5
B	94	HIS	-	expression tag	UNP Q9HCE5
B	95	HIS	-	expression tag	UNP Q9HCE5
B	96	SER	-	expression tag	UNP Q9HCE5
B	97	SER	-	expression tag	UNP Q9HCE5
B	98	GLY	-	expression tag	UNP Q9HCE5
B	99	ARG	-	expression tag	UNP Q9HCE5
B	100	GLU	-	expression tag	UNP Q9HCE5
B	101	ASN	-	expression tag	UNP Q9HCE5
B	102	LEU	-	expression tag	UNP Q9HCE5

Continued on next page...

Continued from previous page...

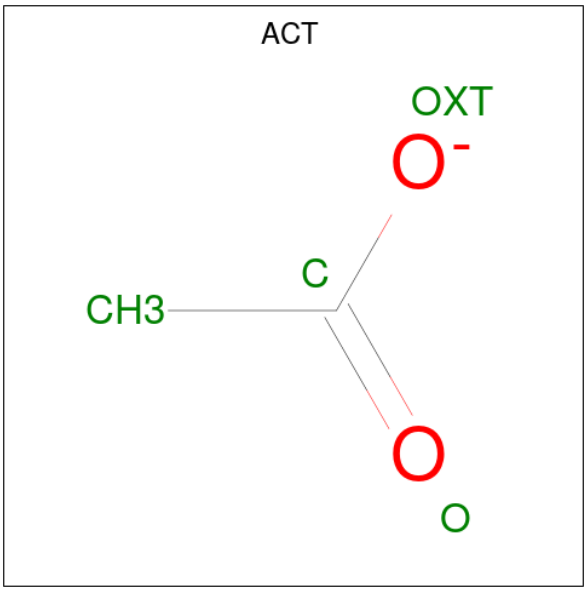
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	TYR	-	expression tag	UNP Q9HCE5
B	104	PHE	-	expression tag	UNP Q9HCE5
B	105	GLN	-	expression tag	UNP Q9HCE5
B	106	GLY	-	expression tag	UNP Q9HCE5

- Molecule 3 is 1-[2-[[4-[5-[3,3-bis(fluoranyl)pyrrolidin-1-yl]pyridin-3-yl]-1,2,3-triazol-1-yl]methyl]imidazo[1,2-a]pyridin-6-yl]- {N}-(cyclobutylmethyl)methanamine (CCD ID: A1JSA) (formula: $C_{25}H_{28}F_2N_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			35	25	2	8		

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



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

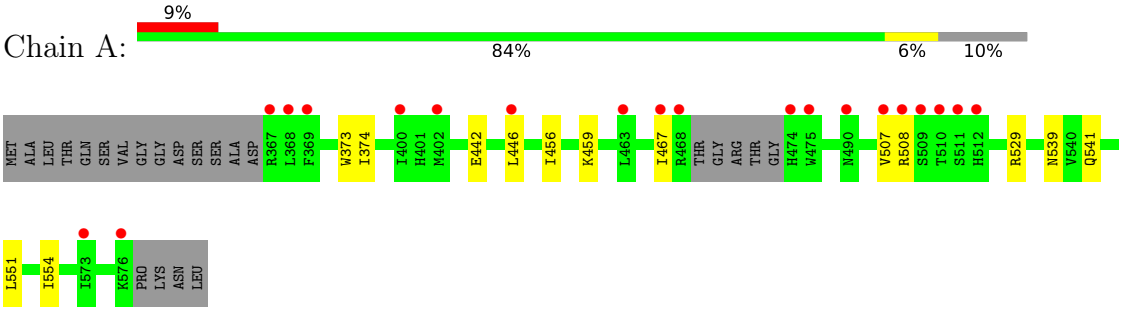
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	147	Total O 147 147	0	0

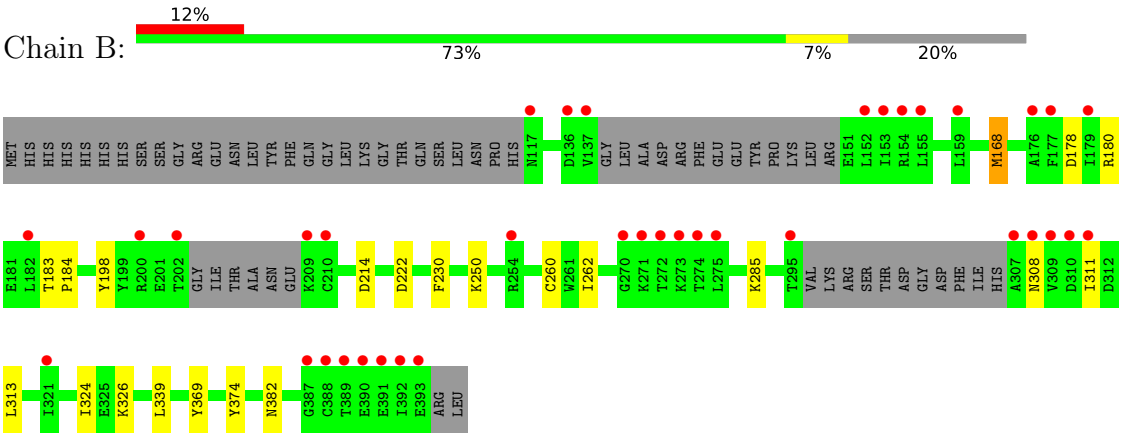
3 Residue-property plots (i)

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: N6-adenosine-methyltransferase catalytic subunit



• Molecule 2: N(6)-adenosine-methyltransferase non-catalytic subunit METTL14



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	63.96Å 63.96Å 225.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.72 – 1.59 49.72 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.72-1.59) 99.6 (49.72-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.198 , 0.231 0.198 , 0.231	Depositor DCC
R_{free} test set	2011 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: ACT, A1JSA

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	0.28	0/1649	0.51	0/2248
2	B	0.30	0/1953	0.49	0/2659
All	All	0.29	0/3602	0.50	0/4907

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	1606	0	1525	7	0
2	B	1899	0	1757	16	0
3	A	35	0	0	0	0
4	B	4	0	3	0	0
5	A	125	0	0	1	0
5	B	147	0	0	6	0
All	All	3816	0	3285	22	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 3.

All (22) 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)
2:B:250:LYS:NZ	5:B:502:HOH:O	2.13	0.80
2:B:222:ASP:OD2	5:B:501:HOH:O	2.10	0.69
2:B:178:ASP:OD1	2:B:180:ARG:NH2	2.36	0.58
2:B:168:MET:HE3	2:B:369:TYR:HA	1.85	0.57
2:B:198:TYR:HB3	2:B:324:ILE:HG22	1.86	0.56
2:B:260[B]:CYS:SG	2:B:285:LYS:HD2	2.49	0.53
2:B:326:LYS:NZ	5:B:509:HOH:O	2.41	0.52
1:A:373:TRP:HB2	1:A:551:LEU:HD13	1.92	0.52
2:B:183:THR:OG1	5:B:503:HOH:O	2.19	0.51
1:A:539:ASN:O	1:A:541:GLN:HG2	2.11	0.50
1:A:529:ARG:HG3	5:A:750:HOH:O	2.18	0.44
2:B:382:ASN:ND2	5:B:504:HOH:O	2.29	0.43
1:A:442:GLU:O	1:A:446:LEU:HG	2.19	0.43
1:A:456:ILE:HD13	2:B:260[B]:CYS:SG	2.59	0.43
1:A:459:LYS:HB3	1:A:507:VAL:CG2	2.50	0.42
2:B:311:ILE:HG23	2:B:313:LEU:H	1.85	0.42
2:B:168:MET:HE1	2:B:374:TYR:HB2	2.03	0.41
2:B:230:PHE:CE1	2:B:339:LEU:HD22	2.56	0.41
2:B:262:ILE:CD1	2:B:313:LEU:HD22	2.51	0.41
2:B:184:PRO:HD2	2:B:374:TYR:CD2	2.57	0.40
2:B:214:ASP:HB2	5:B:590:HOH:O	2.21	0.40
1:A:374:ILE:HG23	1:A:554:ILE:HG12	2.03	0.40

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	201/228 (88%)	194 (96%)	5 (2%)	2 (1%)	12 3
2	B	241/307 (78%)	233 (97%)	7 (3%)	1 (0%)	30 14
All	All	442/535 (83%)	427 (97%)	12 (3%)	3 (1%)	18 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	308	ASN
1	A	467	ILE
1	A	508	ARG

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	165/200 (82%)	165 (100%)	0	100	100
2	B	189/274 (69%)	188 (100%)	1 (0%)	81	70
All	All	354/474 (75%)	353 (100%)	1 (0%)	86	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	168	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	HIS
2	B	122	HIS

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	$\#\|Z\| > 2$
4	ACT	B	401	-	3,3,3	1.23	0	3,3,3	1.08	0
3	A1JSA	A	601	-	36,40,40	2.11	13 (36%)	39,58,58	2.53	15 (38%)

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	A1JSA	A	601	-	-	2/16/35/35	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1JSA	C30-N18	5.56	1.44	1.39
3	A	601	A1JSA	C13-N14	4.41	1.42	1.34
3	A	601	A1JSA	F35-C02	-3.90	1.31	1.38
3	A	601	A1JSA	F01-C02	-3.70	1.31	1.38
3	A	601	A1JSA	C03-C04	2.65	1.57	1.52
3	A	601	A1JSA	C29-C30	2.65	1.46	1.41
3	A	601	A1JSA	C12-N33	2.50	1.42	1.36
3	A	601	A1JSA	C15-N14	-2.44	1.43	1.46
3	A	601	A1JSA	C17-C16	2.37	1.40	1.36
3	A	601	A1JSA	C04-N06	2.22	1.50	1.47
3	A	601	A1JSA	C10-C11	2.20	1.42	1.39
3	A	601	A1JSA	C13-C12	2.16	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1JSA	C08-N09	2.04	1.38	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	A1JSA	C34-C07-C08	-6.07	114.67	119.48
3	A	601	A1JSA	C04-N06-C05	-5.88	103.94	112.36
3	A	601	A1JSA	N18-C30-N31	-5.05	107.76	110.61
3	A	601	A1JSA	C03-C04-N06	4.81	107.74	103.61
3	A	601	A1JSA	C11-C34-C07	4.47	124.68	119.59
3	A	601	A1JSA	C17-N18-C19	3.84	133.74	129.98
3	A	601	A1JSA	C13-C12-N33	-3.78	104.25	107.88
3	A	601	A1JSA	C08-N09-C10	3.08	121.69	117.48
3	A	601	A1JSA	C34-C11-C12	3.06	125.84	120.33
3	A	601	A1JSA	C12-N33-N32	2.89	112.40	109.22
3	A	601	A1JSA	C05-N06-C07	2.68	130.17	122.61
3	A	601	A1JSA	C34-C11-C10	-2.46	115.42	117.95
3	A	601	A1JSA	C29-C30-N31	2.44	134.59	130.37
3	A	601	A1JSA	C13-N14-N32	-2.06	108.62	110.73
3	A	601	A1JSA	C11-C12-C13	2.03	132.80	129.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	A1JSA	C16-C15-N14-C13
3	A	601	A1JSA	C20-C21-N22-C23

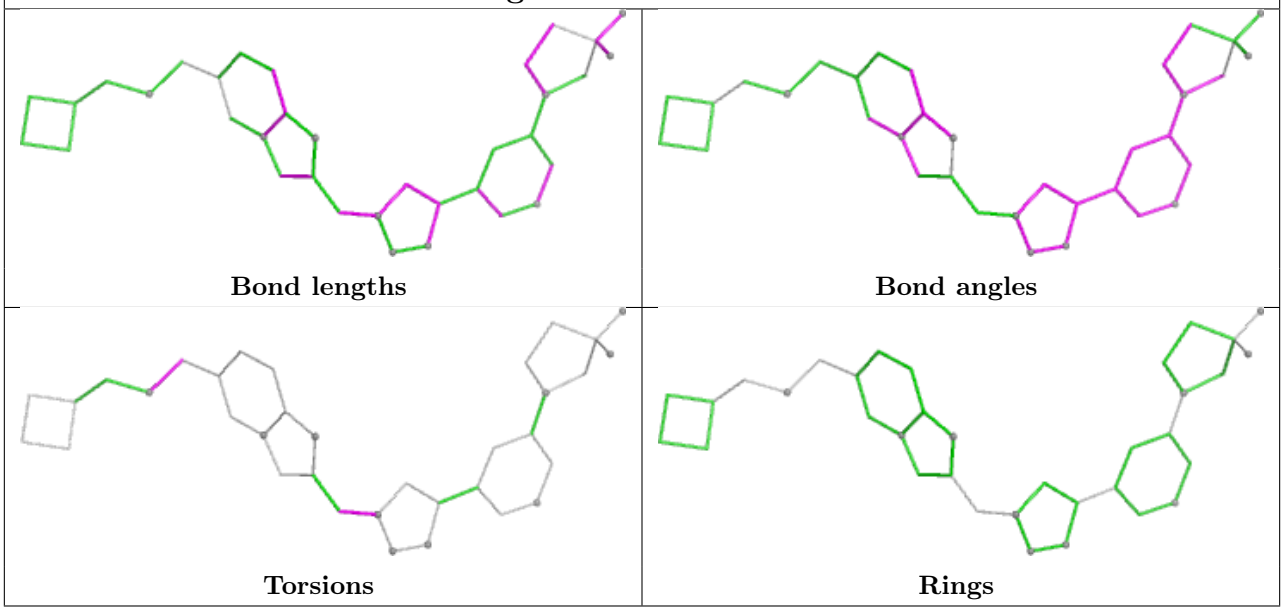
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A1JSA A 601



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, 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	205/228 (89%)	0.75	20 (9%)	13	13	25, 36, 59, 68	0
2	B	247/307 (80%)	0.98	37 (14%)	5	5	18, 36, 68, 83	2 (0%)
All	All	452/535 (84%)	0.87	57 (12%)	8	7	18, 36, 66, 83	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	307	ALA	6.1
2	B	152	LEU	6.0
2	B	153	ILE	5.4
2	B	272	THR	5.3
2	B	137	VAL	5.2
2	B	202	THR	4.7
1	A	467	ILE	4.3
2	B	177	PHE	4.2
1	A	475	TRP	4.1
2	B	274	THR	4.0
2	B	308	ASN	3.9
1	A	507	VAL	3.9
1	A	368	LEU	3.7
2	B	155	LEU	3.7
2	B	309	VAL	3.7
1	A	446	LEU	3.6
1	A	468	ARG	3.6
1	A	402	MET	3.5
2	B	388	CYS	3.5
1	A	573	ILE	3.5
1	A	510	THR	3.5
1	A	509	SER	3.4
2	B	117	ASN	3.4
2	B	295	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	387	GLY	3.4
2	B	321	ILE	3.4
2	B	392	ILE	3.3
2	B	275	LEU	3.2
1	A	508	ARG	3.2
2	B	390	GLU	3.1
1	A	474	HIS	3.1
1	A	490	ASN	3.1
2	B	154	ARG	3.0
2	B	273	LYS	2.9
2	B	270	GLY	2.8
1	A	512	HIS	2.8
2	B	311	ILE	2.8
2	B	310	ASP	2.8
2	B	179	ILE	2.7
2	B	393	GLU	2.6
1	A	463	LEU	2.6
2	B	389	THR	2.5
1	A	367	ARG	2.5
1	A	576	LYS	2.5
2	B	136	ASP	2.5
2	B	209	LYS	2.5
2	B	200	ARG	2.5
1	A	369	PHE	2.4
2	B	176	ALA	2.4
1	A	511	SER	2.4
2	B	210	CYS	2.3
2	B	271	LYS	2.3
2	B	159	LEU	2.3
2	B	182	LEU	2.3
2	B	254	ARG	2.2
1	A	400	ILE	2.1
2	B	391	GLU	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)

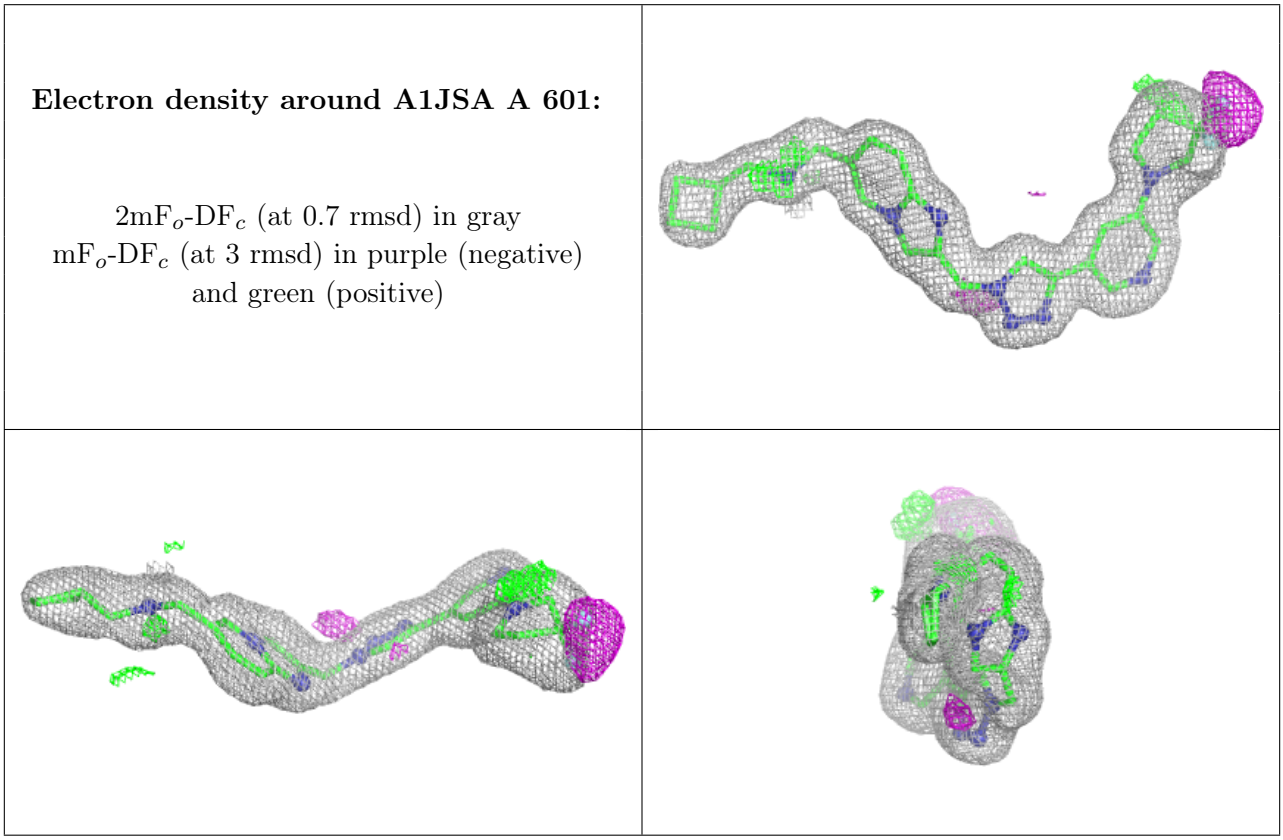
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A1JSA	A	601	35/35	0.90	0.12	30,33,46,54	0
4	ACT	B	401	4/4	0.95	0.08	31,32,33,34	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 A1JSA A 601:

$2mF_o$-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.