Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2026 – 02:08 PM JST

PDB ID	:	25VX / pdb_000025vx
Title	:	Crystal Structure of MYST histone acetyltransferase KAT6A in complex with inhibitor Compound 11
Authors	:	NarasimhaRao, K.; Vijayshankar, N.; SumalathaRani, T.; Kalishankar, B.; Chandregowda, V.; Chandrasekar, A.; Susanta, S.; Raymond, A.N.; David, C.M.
Deposited on	:	2026-04-20
Resolution	:	2.29 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 (1)) were used in the production of this report:

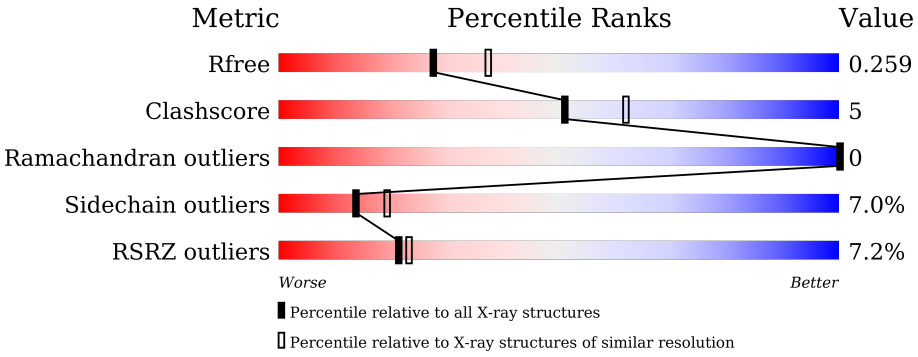
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	277	7% 78% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2337 atoms, of which 22 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.

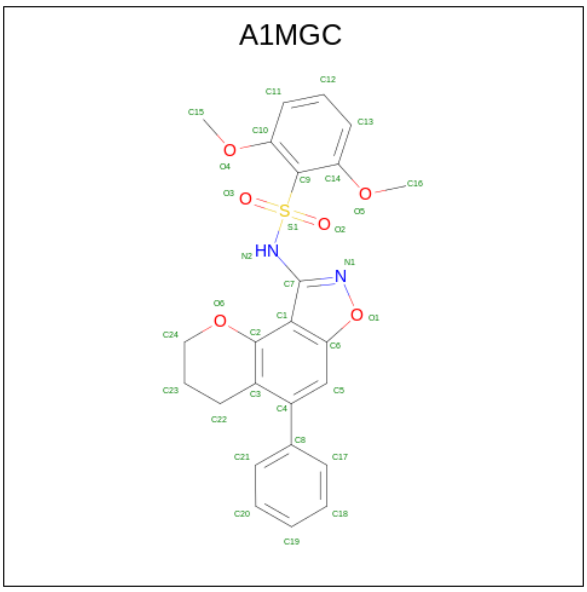
- Molecule 1 is a protein called Histone acetyltransferase KAT8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2195	1432	354	397	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	SER	-	expression tag	UNP Q9H7Z6
A	579	HIS	TYR	engineered mutation	UNP Q9H7Z6
A	645	SER	ALA	engineered mutation	UNP Q9H7Z6
A	648	MET	LEU	engineered mutation	UNP Q9H7Z6
A	649	ILE	THR	engineered mutation	UNP Q9H7Z6
A	660	ARG	LYS	engineered mutation	UNP Q9H7Z6
A	702	ASN	ILE	engineered mutation	UNP Q9H7Z6

- Molecule 2 is 2,6-dimethoxy- {N}-(5-phenyl-3,4-dihydro-2 {H}-pyrano[2,3-e][1,2]benzoxazol -9-yl)benzenesulfonamide (CCD ID: A1MGC) (formula: $C_{24}H_{22}N_2O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			55	24	22	2	6	1		

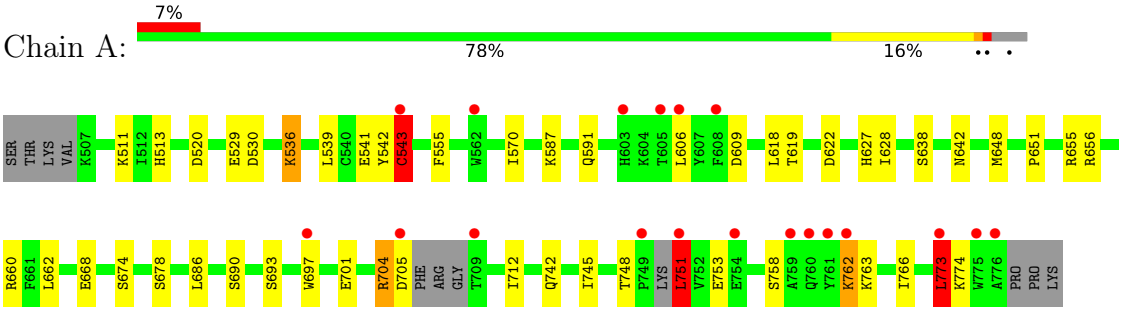
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		

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: Histone acetyltransferase KAT8



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.19Å 57.62Å 122.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.02 – 2.29 61.02 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.02-2.29) 99.5 (61.02-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.199 , 0.266 0.207 , 0.259	Depositor DCC
R_{free} test set	776 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2337	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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: A1MGC, ALY

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	1.11	5/2245 (0.2%)	1.21	11/3039 (0.4%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	CYS	CA-CB	13.32	1.75	1.53
1	A	543	CYS	CA-C	7.99	1.63	1.52
1	A	543	CYS	N-CA	7.11	1.55	1.46
1	A	543	CYS	CB-SG	5.87	2.00	1.81
1	A	555	PHE	C-O	-5.10	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	751	LEU	N-CA-CB	11.50	130.05	110.50
1	A	543	CYS	N-CA-C	-9.29	101.05	111.82
1	A	542	TYR	CA-C-N	9.28	134.41	120.31
1	A	542	TYR	C-N-CA	9.28	134.41	120.31
1	A	766	ILE	N-CA-C	-7.00	100.55	109.30
1	A	638	SER	CA-C-N	6.41	126.62	119.32
1	A	638	SER	C-N-CA	6.41	126.62	119.32
1	A	758	SER	N-CA-C	6.08	118.14	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	651	PRO	CA-C-N	-5.30	114.63	119.82
1	A	651	PRO	C-N-CA	-5.30	114.63	119.82
1	A	773	LEU	O-C-N	5.14	129.16	123.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	656	ARG	Sidechain
1	A	748	THR	Peptide

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	2195	0	2158	22	0
2	A	33	22	0	2	0
3	A	87	0	0	0	0
All	All	2315	22	2158	23	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 (23) 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:543:CYS:CB	1:A:543:CYS:CA	1.75	1.59
1:A:541:GLU:OE1	1:A:627:HIS:HD2	1.76	0.68
1:A:704:ARG:HD3	1:A:753:GLU:OE2	1.96	0.64
1:A:606:LEU:HD21	1:A:609:ASP:O	1.97	0.64
1:A:622:ASP:OD1	1:A:627:HIS:HE1	1.86	0.59
1:A:660:ARG:HH22	1:A:697:TRP:CD1	2.20	0.59
1:A:570:ILE:O	1:A:773:LEU:HD23	2.08	0.54
1:A:618:LEU:HB2	1:A:662:LEU:HD21	1.89	0.54
1:A:543:CYS:CB	1:A:543:CYS:HA	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HG2	1:A:763:LYS:N	2.26	0.51
1:A:513:HIS:HB2	1:A:536:LYS:HE3	1.93	0.51
1:A:587:LYS:HE2	1:A:591:GLN:NE2	2.25	0.51
1:A:642:ASN:HA	1:A:678:SER:O	2.11	0.51
1:A:704:ARG:HG2	1:A:705:ASP:OD2	2.16	0.46
1:A:751:LEU:HD13	1:A:751:LEU:HA	1.97	0.45
1:A:543:CYS:CB	1:A:543:CYS:C	2.81	0.45
1:A:511:LYS:NZ	1:A:520:ASP:OD1	2.51	0.43
1:A:655:ARG:N	2:A:900:A1MGC:N1	2.62	0.43
1:A:648:MET:HE3	1:A:648:MET:HB3	1.97	0.42
1:A:541:GLU:OE1	1:A:627:HIS:CD2	2.66	0.41
2:A:900:A1MGC:C22	2:A:900:A1MGC:C21	2.98	0.41
1:A:619:THR:HG22	1:A:628:ILE:HA	2.04	0.40
1:A:712:ILE:HG13	1:A:745:ILE:HG13	2.04	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	259/277 (94%)	251 (97%)	8 (3%)	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	243/256 (95%)	226 (93%)	17 (7%)	14 19

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	529	GLU
1	A	530	ASP
1	A	536	LYS
1	A	539	LEU
1	A	543	CYS
1	A	668	GLU
1	A	674	SER
1	A	686	LEU
1	A	690	SER
1	A	693	SER
1	A	701	GLU
1	A	704	ARG
1	A	742	GLN
1	A	751	LEU
1	A	762	LYS
1	A	773	LEU
1	A	774	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	GLN
1	A	603	HIS
1	A	627	HIS
1	A	723	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	ALY	A	604	1	10,11,12	0.68	0	7,12,14	1.04	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
1	ALY	A	604	1	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	604	ALY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	A1MGC	A	900	-	37,37,37	2.58	5 (13%)	46,54,54	3.17	19 (41%)

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	A1MGC	A	900	-	-	10/19/26/26	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	A1MGC	C7-N1	11.10	1.36	1.29
2	A	900	A1MGC	C9-S1	-7.60	1.67	1.79
2	A	900	A1MGC	O1-C6	-5.71	1.31	1.36
2	A	900	A1MGC	C7-N2	-2.65	1.34	1.39
2	A	900	A1MGC	O2-S1	-2.00	1.41	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	A1MGC	C9-S1-N2	8.20	118.00	106.76
2	A	900	A1MGC	O6-C2-C1	-7.45	110.93	117.49
2	A	900	A1MGC	C22-C3-C2	-7.39	112.38	120.37
2	A	900	A1MGC	N2-C7-N1	7.15	132.07	118.62
2	A	900	A1MGC	O6-C2-C3	6.55	128.92	120.98
2	A	900	A1MGC	O1-C6-C5	5.54	129.75	125.78
2	A	900	A1MGC	C15-O4-C10	4.18	123.84	117.53
2	A	900	A1MGC	O2-S1-O3	-4.01	114.61	119.55
2	A	900	A1MGC	C16-O5-C14	3.79	123.24	117.53
2	A	900	A1MGC	C5-C6-C1	-3.38	120.89	124.81
2	A	900	A1MGC	O5-C14-C13	-3.30	118.72	124.37
2	A	900	A1MGC	C24-O6-C2	3.30	122.41	113.99
2	A	900	A1MGC	O4-C10-C11	-3.23	118.83	124.37
2	A	900	A1MGC	C6-O1-N1	2.58	108.71	107.48
2	A	900	A1MGC	C11-C10-C9	2.49	122.36	119.04
2	A	900	A1MGC	C22-C3-C4	2.48	126.54	121.50
2	A	900	A1MGC	C4-C3-C2	2.33	121.08	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	A1MGC	O2-S1-N2	-2.32	100.23	106.74
2	A	900	A1MGC	C13-C14-C9	2.24	122.03	119.04

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	A1MGC	C7-N2-S1-C9
2	A	900	A1MGC	C1-C7-N2-S1
2	A	900	A1MGC	C3-C4-C8-C21
2	A	900	A1MGC	C3-C4-C8-C17
2	A	900	A1MGC	C7-N2-S1-O2
2	A	900	A1MGC	C5-C4-C8-C17
2	A	900	A1MGC	C5-C4-C8-C21
2	A	900	A1MGC	C14-C9-S1-O3
2	A	900	A1MGC	C10-C9-S1-O3
2	A	900	A1MGC	C7-N2-S1-O3

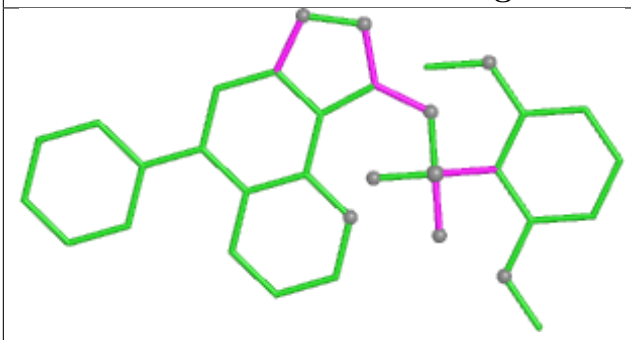
There are no ring outliers.

1 monomer is involved in 2 short contacts:

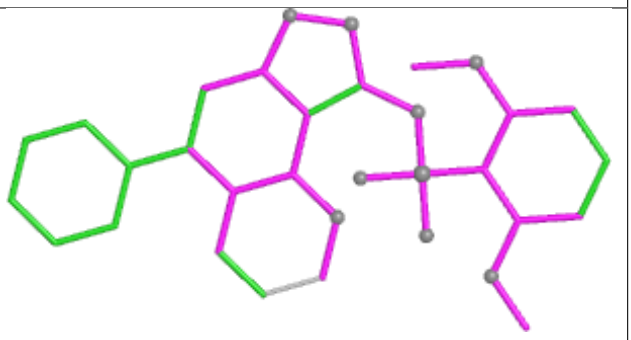
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	A1MGC	2	0

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 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.

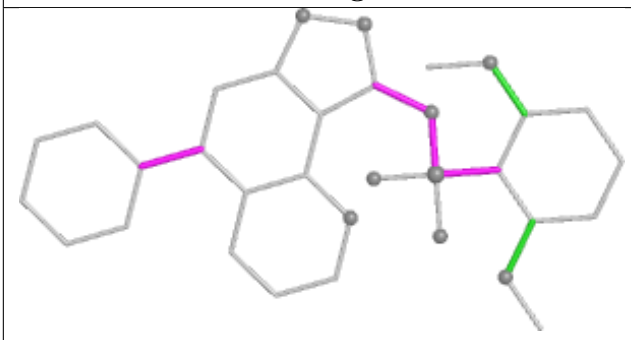
Ligand A1MGC A 900



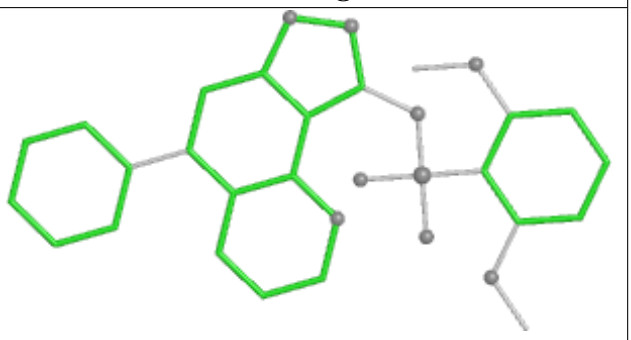
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	265/277 (95%)	0.14	19 (7%)	21	23	16, 27, 56, 128	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	776	ALA	11.8
1	A	773	LEU	5.6
1	A	751	LEU	5.6
1	A	749	PRO	5.2
1	A	709	THR	4.7
1	A	608	PHE	4.2
1	A	760	GLN	3.7
1	A	754	GLU	3.6
1	A	603	HIS	3.4
1	A	543	CYS	3.0
1	A	606	LEU	3.0
1	A	775	TRP	2.8
1	A	705	ASP	2.7
1	A	697	TRP	2.5
1	A	605	THR	2.5
1	A	759	ALA	2.3
1	A	761	TYR	2.3
1	A	562	TRP	2.2
1	A	762	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	ALY	A	604	12/13	0.90	0.11	18,29,41,47	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

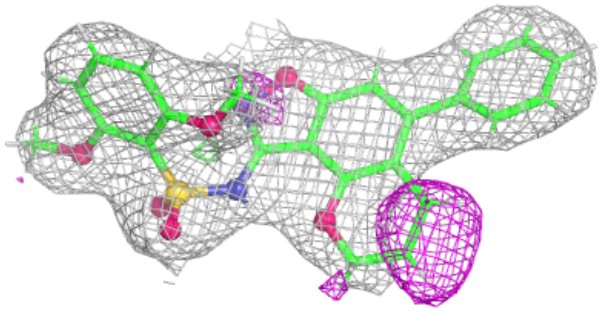
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

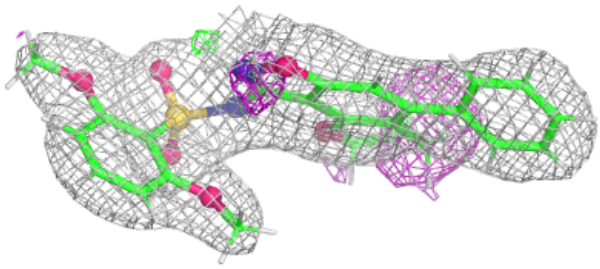
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1MGC	A	900	33/33	0.89	0.11	23,31,37,44	0

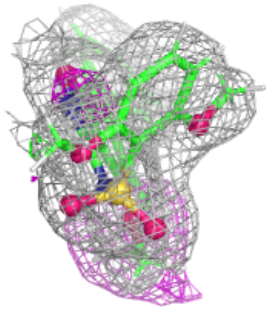
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1MGC A 900:

$2mF_o$-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

There are no such residues in this entry.