



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 AM UTC

PDB ID : 5TEY / pdb_00005tey
Title : Human METTL3-METTLL14 complex
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Deposited on : 2016-09-23
Resolution : 1.80 Å(reported)

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

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<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

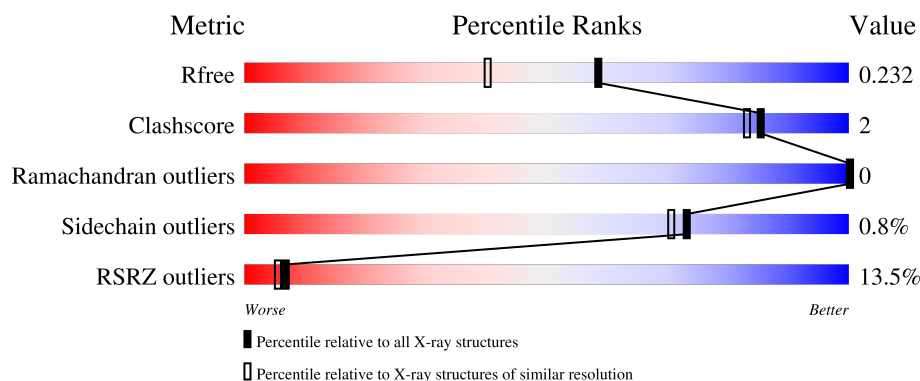
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	598	3% 34% 66%
2	B	399	11% 57% 40%

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
6	UNX	B	402	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3839 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 70 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	3	0
			1657	1063	290	295	9			

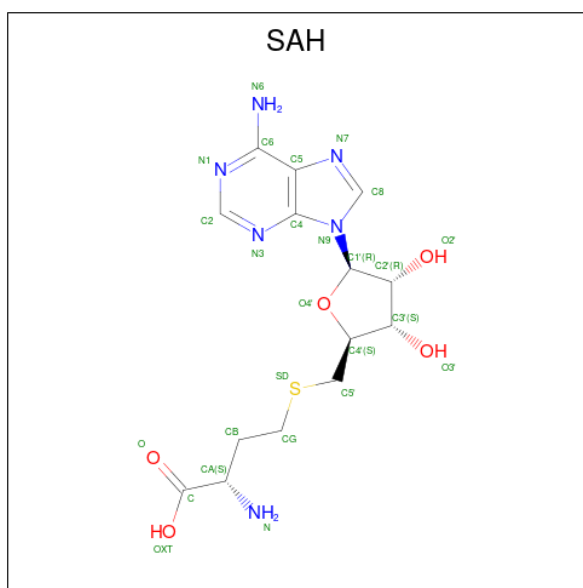
There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q86U44
A	-16	HIS	-	expression tag	UNP Q86U44
A	-15	HIS	-	expression tag	UNP Q86U44
A	-14	HIS	-	expression tag	UNP Q86U44
A	-13	HIS	-	expression tag	UNP Q86U44
A	-12	HIS	-	expression tag	UNP Q86U44
A	-11	HIS	-	expression tag	UNP Q86U44
A	-10	SER	-	expression tag	UNP Q86U44
A	-9	SER	-	expression tag	UNP Q86U44
A	-8	GLY	-	expression tag	UNP Q86U44
A	-7	ARG	-	expression tag	UNP Q86U44
A	-6	GLU	-	expression tag	UNP Q86U44
A	-5	ASN	-	expression tag	UNP Q86U44
A	-4	LEU	-	expression tag	UNP Q86U44
A	-3	TYR	-	expression tag	UNP Q86U44
A	-2	PHE	-	expression tag	UNP Q86U44
A	-1	GLN	-	expression tag	UNP Q86U44
A	0	GLY	-	expression tag	UNP Q86U44
A	568	LYS	ARG	conflict	UNP Q86U44

- Molecule 2 is a protein called N6-adenosine-methyltransferase subunit METTL14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	6	0
			1942	1243	331	354	14			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

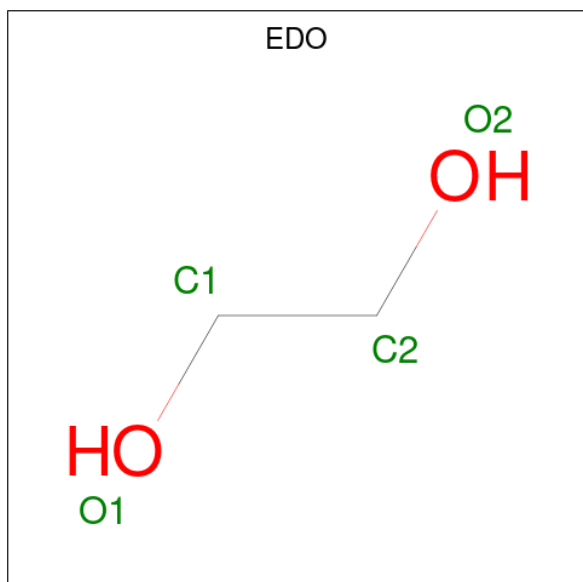


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

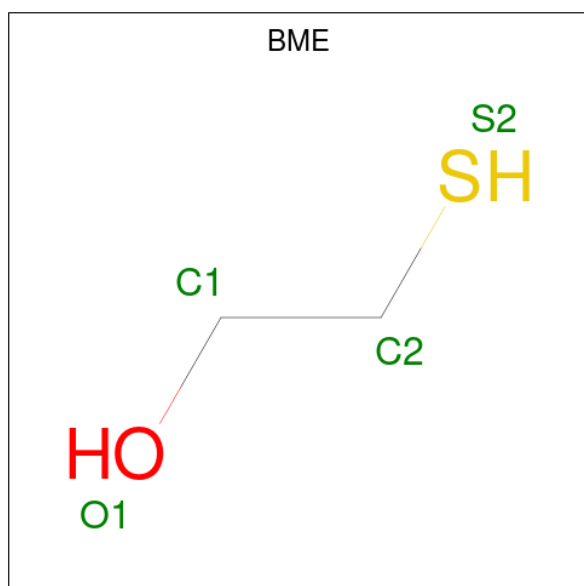


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	X	0	0
			2	2		
6	B	6	Total	X	0	0
			6	6		

- Molecule 7 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	89	Total	O	0	0
			89	89		
8	B	107	Total	O	0	1
			108	108		

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.

- Chain A:  34%  66%

Chain	Residue	Label	Color
Chain A	1	GLY	Green
	2	ASP	Red
	3	LYS	Green
	4	ASN	Green
	5	LEU	Green
	6	LEU	Green
	7	THR	Green
	8	GLN	Green
	9	GLU	Green
	10	VAL	Green
	11	GLY	Green
	12	ARG	Green
	13	THR	Green
	14	GLU	Green
	15	ASN	Green
	16	LEU	Green
	17	THR	Green
	18	TYR	Green
	19	LEU	Green
	20	ALA	Green
Chain B	1	GLY	Green
	2	ASP	Red
	3	LYS	Green
	4	ASN	Green
	5	LEU	Green
	6	LEU	Green
	7	THR	Green
	8	GLN	Green
	9	GLU	Green
	10	VAL	Green
	11	GLY	Green
	12	ARG	Green
	13	THR	Green
	14	GLU	Green
	15	ASN	Green
	16	LEU	Green
	17	THR	Green
	18	TYR	Green
	19	LEU	Green
	20	ALA	Green

- Chain B:
-
- 11%
57%
40%
- MET ASP SER ARG LEU GLN GLY ILE ARG GLY ARG GLN LYS LEU ALA GLN LEU GLY ALA MET GLN ASP SER ILE VAL LEU ASN SER LYS ASP GLY GLN ARG THR ARG CYS ARG ALA SER TYR ASP THR PRO
- ASN ALA LYS ARG LYS TVR LEU ASP GLY ASP MET LYS MET GLY TYR LYS ASP GLY MET ASN GLY THR PHE LEU LYS GLY THR GLN SER LEU ASN PRO HIS N117 D136 H137
- GLY LEU ASP ASP PHE GLY GLY TYR PRO LYS L149 R150 E151 L152 I153 R154 L155 M188 D173 A176 F177 D178 I179 Y199 K200 THR THR GLY ILE THR ALA ASN ASN GLU K209 C210 R254 R255 C256 C260 W261 L262 N267 N268 P269 G270 K271 T272 L275 D276



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.88Å 63.88Å 225.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.80) 99.9 (50.00-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.198 , 0.224 0.207 , 0.232	Depositor DCC
R_{free} test set	1180 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3839	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: BME, UNX, MG, EDO, SAH

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	0.65	0/1701	0.81	0/2311
2	B	0.68	0/1995	0.79	0/2705
All	All	0.67	0/3696	0.80	0/5016

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	1657	0	1627	4	0
2	B	1942	0	1829	15	0
3	A	26	0	19	0	0
4	A	1	0	0	0	0
5	A	4	0	6	0	0
6	A	2	0	0	0	0
6	B	6	0	0	2	0
7	B	4	0	6	2	0
8	A	89	0	0	0	0
8	B	108	0	0	0	0
All	All	3839	0	3487	16	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 2.

All (16) 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:210:CYS:SG	6:B:402:UNX:UNK	1.69	1.12
1:A:456:ILE:HD11	2:B:262:ILE:HD11	1.47	0.96
1:A:456:ILE:HD11	2:B:262:ILE:CD1	2.19	0.73
2:B:256:CYS:SG	7:B:401:BME:S2	2.61	0.70
1:A:456:ILE:CD1	2:B:262:ILE:HD11	2.24	0.66
2:B:173[A]:ASP:OD1	2:B:173[A]:ASP:C	2.53	0.51
2:B:210:CYS:HG	6:B:402:UNX:UNK	0.53	0.50
2:B:325:GLU:CD	2:B:349:ARG:HH11	2.19	0.50
2:B:338:CYS:O	2:B:386:THR:OG1	2.30	0.50
2:B:260[A]:CYS:SG	2:B:287:HIS:CE1	3.09	0.45
1:A:419:ILE:N	1:A:420:PRO:CD	2.80	0.45
2:B:168[A]:MET:HE3	2:B:369:TYR:HA	1.99	0.45
2:B:168[A]:MET:CE	2:B:369:TYR:HD1	2.30	0.44
2:B:168[A]:MET:HE3	2:B:168[A]:MET:HB3	1.80	0.42
2:B:386:THR:HG23	2:B:388:CYS:H	1.84	0.42
2:B:256:CYS:CB	7:B:401:BME:HS2	2.26	0.41

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	202/598 (34%)	199 (98%)	3 (2%)	0	100	100
2	B	237/399 (59%)	234 (99%)	3 (1%)	0	100	100
All	All	439/997 (44%)	433 (99%)	6 (1%)	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	179/518 (35%)	178 (99%)	1 (1%)	78	77
2	B	200/357 (56%)	197 (98%)	3 (2%)	57	49
All	All	379/875 (43%)	375 (99%)	4 (1%)	73	60

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	ASN
2	B	168[A]	MET
2	B	168[B]	MET
2	B	321	ILE

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	445	ASN
1	A	550	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](#)

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

Of 12 ligands modelled in this entry, 1 is monoatomic and 8 are unknown - leaving 3 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
7	BME	B	401	-	3,3,3	0.37	0	2,2,2	0.25	0
3	SAH	A	601	-	27,28,28	1.45	4 (14%)	36,40,40	2.04	9 (25%)
5	EDO	A	603	-	3,3,3	0.68	0	2,2,2	0.20	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
7	BME	B	401	-	-	0/1/1/1	-
3	SAH	A	601	-	-	1/15/31/31	0/3/3/3
5	EDO	A	603	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	SAH	C5-C4	4.36	1.46	1.39
3	A	601	SAH	C5-N7	-2.59	1.34	1.39
3	A	601	SAH	C5-C6	2.52	1.48	1.41
3	A	601	SAH	C4-N9	-2.36	1.32	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	SAH	C5-C4-N3	-5.34	119.37	126.72
3	A	601	SAH	N3-C4-N9	4.61	135.01	127.17
3	A	601	SAH	N3-C2-N1	-4.26	122.13	128.58
3	A	601	SAH	C2-N3-C4	4.24	122.18	111.83
3	A	601	SAH	C4-N9-C8	2.85	108.73	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	SAH	C4-C5-N7	-2.67	107.53	110.58
3	A	601	SAH	C6-C5-N7	2.57	137.04	132.09
3	A	601	SAH	C5-C6-N6	-2.23	117.77	123.29
3	A	601	SAH	OXT-C-O	-2.09	119.35	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

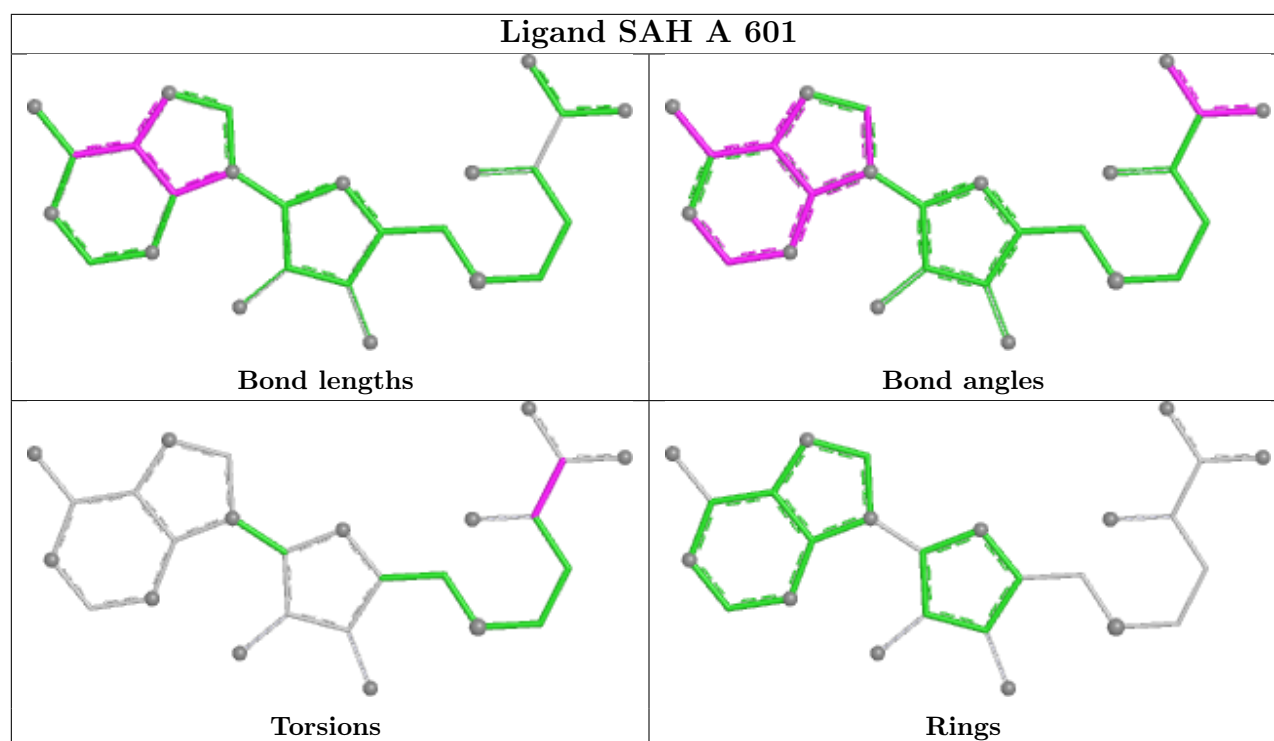
Mol	Chain	Res	Type	Atoms
3	A	601	SAH	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	401	BME	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	205/598 (34%)	0.55	17 (8%) 17 15	13, 26, 54, 62	3 (1%)
2	B	241/399 (60%)	0.74	43 (17%) 4 3	9, 24, 56, 75	6 (2%)
All	All	446/997 (44%)	0.65	60 (13%) 7 5	9, 26, 56, 75	9 (2%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	149	LEU	10.2
2	B	392	ILE	6.0
2	B	275	LEU	5.6
1	A	406	TYR	5.6
1	A	368	LEU	5.3
2	B	272	THR	4.8
1	A	469	THR	4.7
1	A	367	ARG	4.4
2	B	137	VAL	4.3
1	A	473	GLY	4.2
2	B	295	THR	4.1
2	B	322	GLY	4.1
1	A	475	TRP	4.1
2	B	117	ASN	3.9
2	B	200	ARG	3.8
2	B	390	GLU	3.8
2	B	389	THR	3.8
2	B	391	GLU	3.7
1	A	577	PRO	3.7
2	B	321	ILE	3.6
2	B	386	THR	3.5
1	A	471	ARG	3.4
2	B	388	CYS	3.3
1	A	400	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	150	ARG	3.2
2	B	276	ASP	3.2
2	B	152	LEU	3.2
2	B	155	LEU	3.2
2	B	153	ILE	3.1
1	A	369	PHE	3.1
2	B	151	GLU	3.1
1	A	468	ARG	3.0
1	A	573	ILE	2.9
1	A	574	ILE	2.9
2	B	179	ILE	2.8
2	B	209	LYS	2.7
2	B	176	ALA	2.7
1	A	463	LEU	2.7
1	A	380	TYR	2.7
2	B	380	ALA	2.6
2	B	310	ASP	2.6
2	B	384	TYR	2.6
2	B	177	PHE	2.5
2	B	210	CYS	2.5
2	B	199	TYR	2.5
2	B	311	ILE	2.4
2	B	269	PRO	2.3
2	B	270	GLY	2.3
2	B	383	SER	2.3
2	B	154	ARG	2.2
2	B	254[A]	ARG	2.2
2	B	136	ASP	2.2
2	B	379	SER	2.2
1	A	576	LYS	2.2
2	B	271	LYS	2.2
2	B	267	ASN	2.1
2	B	325	GLU	2.1
2	B	323	ASN	2.0
2	B	173[A]	ASP	2.0
1	A	472	THR	2.0

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

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

6.3 Carbohydrates [i](#)

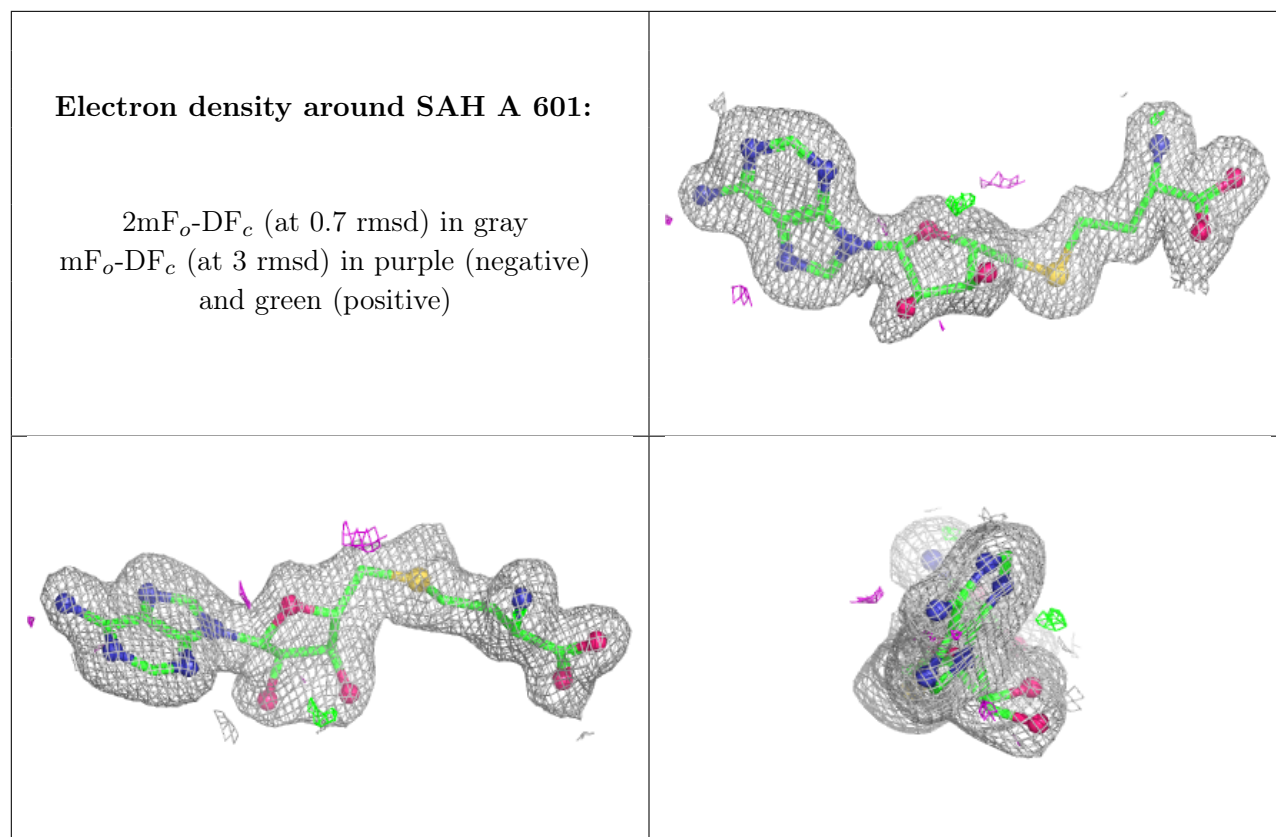
There are no oligosaccharides in this entry.

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
6	UNX	B	403	1/1	0.78	0.22	30,30,30,30	0
5	EDO	A	603	4/4	0.82	0.17	27,36,37,38	0
6	UNX	A	604	1/1	0.86	0.14	30,30,30,30	0
6	UNX	A	605	1/1	0.90	0.14	30,30,30,30	0
6	UNX	B	407	1/1	0.90	0.33	30,30,30,30	0
7	BME	B	401	4/4	0.90	0.14	46,47,48,48	0
6	UNX	B	402	1/1	0.91	0.10	30,30,30,30	0
6	UNX	B	404	1/1	0.92	0.25	30,30,30,30	0
4	MG	A	602	1/1	0.93	0.14	43,43,43,43	0
3	SAH	A	601	26/26	0.94	0.08	20,23,31,36	0
6	UNX	B	406	1/1	0.94	0.35	30,30,30,30	0
6	UNX	B	405	1/1	0.95	0.51	30,30,30,30	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 [i](#)

There are no such residues in this entry.