



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:31 PM UTC

PDB ID : 5N0T / pdb_00005n0t
Title : Crystal structure of OphA-DeltaC6 mutant Y76F in complex with SAM
Authors : Song, H.; Naismith, J.H.
Deposited on : 2017-02-03
Resolution : 1.78 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

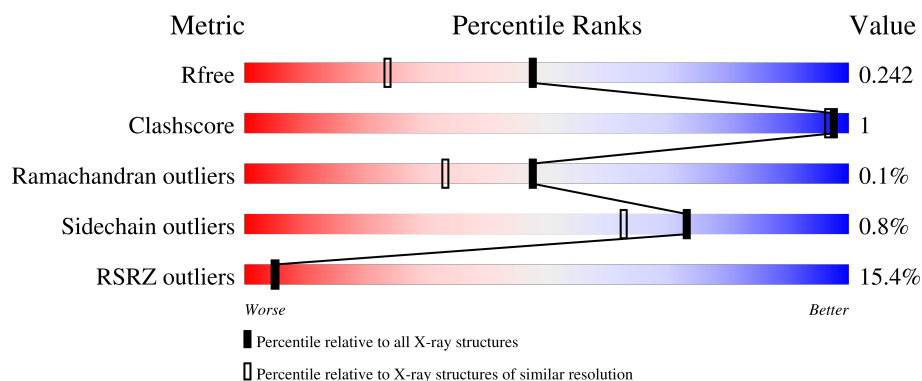
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	410	16% 95%
1	B	410	13% 92%

2 Entry composition [i](#)

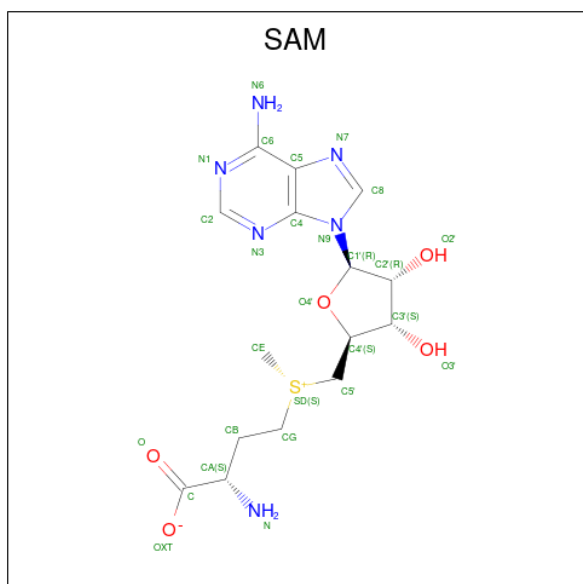
There are 3 unique types of molecules in this entry. The entry contains 6868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	6	0
			3099	1975	530	577	17			
1	B	394	Total	C	N	O	S	0	9	0
			3107	1977	531	581	18			

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

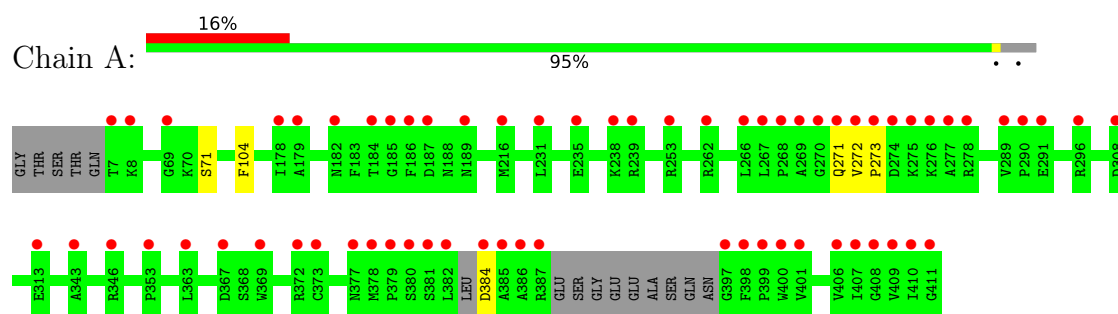
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	317	Total 317	O 317	0	0
3	B	291	Total 291	O 291	0	0

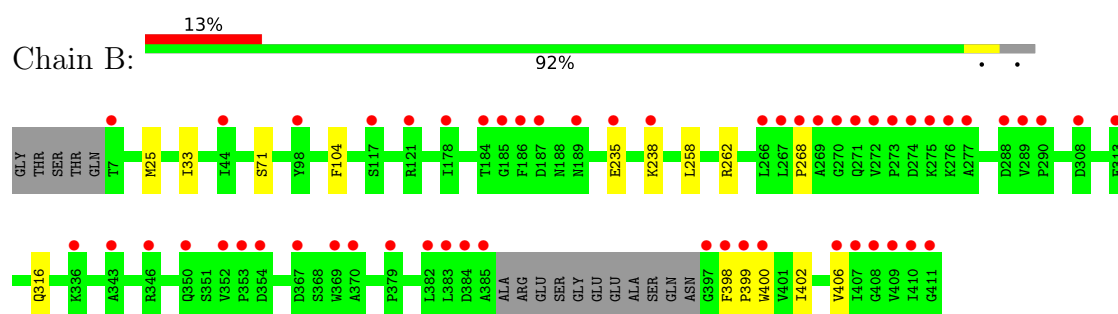
3 Residue-property plots [i](#)

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: Peptide N-methyltransferase



- Molecule 1: Peptide N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.08Å 93.54Å 86.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.00 – 1.78 83.00 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.3 (83.00-1.78) 98.3 (83.00-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.211 , 0.232 0.219 , 0.242	Depositor DCC
R_{free} test set	6242 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6868	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0150e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CSO, SAM

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	0.74	0/3172	0.88	1/4309 (0.0%)
1	B	0.74	0/3183	0.86	1/4324 (0.0%)
All	All	0.74	0/6355	0.87	2/8633 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLN	N-CA-C	5.74	119.38	112.38
1	B	406	VAL	N-CA-C	5.03	116.35	110.62

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	3099	0	3080	3	0
1	B	3107	0	3088	7	0
2	A	27	0	22	2	0
2	B	27	0	22	1	0
3	A	317	0	0	0	0
3	B	291	0	0	0	3
All	All	6868	0	6212	10	3

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 1.

All (10) 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:B:25[B]:MET:CE	1:B:33:ILE:HD12	2.21	0.71
1:A:272:VAL:N	1:A:273:PRO:HD3	2.26	0.51
1:B:104:PHE:O	2:B:501:SAM:HE2	2.14	0.47
1:A:104:PHE:O	2:A:501:SAM:HE2	2.16	0.46
1:A:272:VAL:O	1:A:272:VAL:HG12	2.17	0.45
1:B:235:GLU:HA	1:B:238:LYS:HE2	1.99	0.45
2:A:501:SAM:HE1	1:B:402:ILE:HA	2.01	0.43
1:B:398:PHE:HB3	1:B:400:TRP:CZ2	2.54	0.43
1:B:25[B]:MET:HE1	1:B:33:ILE:HD12	2.01	0.42
1:B:258:LEU:HD21	1:B:262[B]:ARG:NH2	2.35	0.41

All (3) 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)
3:B:844:HOH:O	3:B:844:HOH:O[2_565]	0.70	1.50
3:B:886:HOH:O	3:B:886:HOH:O[2_565]	1.06	1.14
3:B:879:HOH:O	3:B:879:HOH:O[2_565]	1.37	0.83

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	394/410 (96%)	374 (95%)	20 (5%)	0	100	100
1	B	398/410 (97%)	381 (96%)	16 (4%)	1 (0%)	36	22
All	All	792/820 (97%)	755 (95%)	36 (4%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	PRO

5.3.2 Protein sidechains ⓘ

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	331/337 (98%)	329 (99%)	2 (1%)	78	70
1	B	334/337 (99%)	331 (99%)	3 (1%)	70	59
All	All	665/674 (99%)	660 (99%)	5 (1%)	73	63

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	384	ASP
1	B	71	SER
1	B	316	GLN
1	B	399	PRO

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	165	HIS
1	A	219	GLN
1	B	64	GLN
1	B	165	HIS
1	B	182	ASN
1	B	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	B	175	1	3,6,7	0.59	0	1,6,8	0.33	0
1	CSO	A	175	1	3,6,7	0.56	0	1,6,8	0.14	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	CSO	B	175	1	-	0/1/5/7	-
1	CSO	A	175	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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](#)

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	SAM	A	501	-	27,29,29	1.61	3 (11%)	34,42,42	2.05	11 (32%)
2	SAM	B	501	-	27,29,29	1.43	5 (18%)	34,42,42	2.10	9 (26%)

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	SAM	A	501	-	-	3/17/33/33	0/3/3/3
2	SAM	B	501	-	-	4/17/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAM	C5-C4	4.95	1.47	1.39
2	B	501	SAM	C5-C4	3.92	1.46	1.39
2	A	501	SAM	C8-N7	2.89	1.37	1.31
2	A	501	SAM	C5-C6	2.60	1.48	1.41
2	B	501	SAM	C8-N7	2.34	1.36	1.31
2	B	501	SAM	C4-N9	-2.27	1.33	1.37
2	B	501	SAM	C5-C6	2.26	1.47	1.41
2	B	501	SAM	CE-SD	-2.09	1.65	1.78

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SAM	C5-C4-N3	-5.47	119.19	126.72
2	A	501	SAM	CG-SD-C5'	4.82	115.22	103.43
2	A	501	SAM	C5-C4-N3	-4.74	120.19	126.72
2	B	501	SAM	N3-C4-N9	4.42	134.68	127.17
2	B	501	SAM	CG-SD-C5'	4.18	113.66	103.43
2	A	501	SAM	N3-C2-N1	-3.69	123.00	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAM	N3-C4-N9	3.65	133.37	127.17
2	B	501	SAM	C2-N3-C4	3.60	120.62	111.83
2	B	501	SAM	N3-C2-N1	-3.60	123.14	128.58
2	B	501	SAM	C4-N9-C8	3.25	109.15	105.74
2	A	501	SAM	C2-N3-C4	3.21	119.67	111.83
2	A	501	SAM	C4-C5-N7	-3.07	107.07	110.58
2	B	501	SAM	C4-C5-N7	-2.87	107.31	110.58
2	A	501	SAM	C2-N1-C6	2.53	122.89	118.73
2	A	501	SAM	O4'-C1'-N9	2.47	112.84	108.09
2	A	501	SAM	C4-N9-C8	2.47	108.33	105.74
2	B	501	SAM	N9-C8-N7	-2.29	110.69	113.94
2	A	501	SAM	CB-CA-N	2.10	115.59	110.12
2	B	501	SAM	C5-N7-C8	2.07	106.71	103.45
2	A	501	SAM	C2'-C1'-N9	-2.06	108.19	113.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	SAM	C4'-C5'-SD-CE
2	B	501	SAM	CB-CG-SD-CE
2	A	501	SAM	OXT-C-CA-CB
2	B	501	SAM	CB-CG-SD-C5'
2	A	501	SAM	O-C-CA-CB
2	B	501	SAM	OXT-C-CA-CB
2	B	501	SAM	O-C-CA-CB

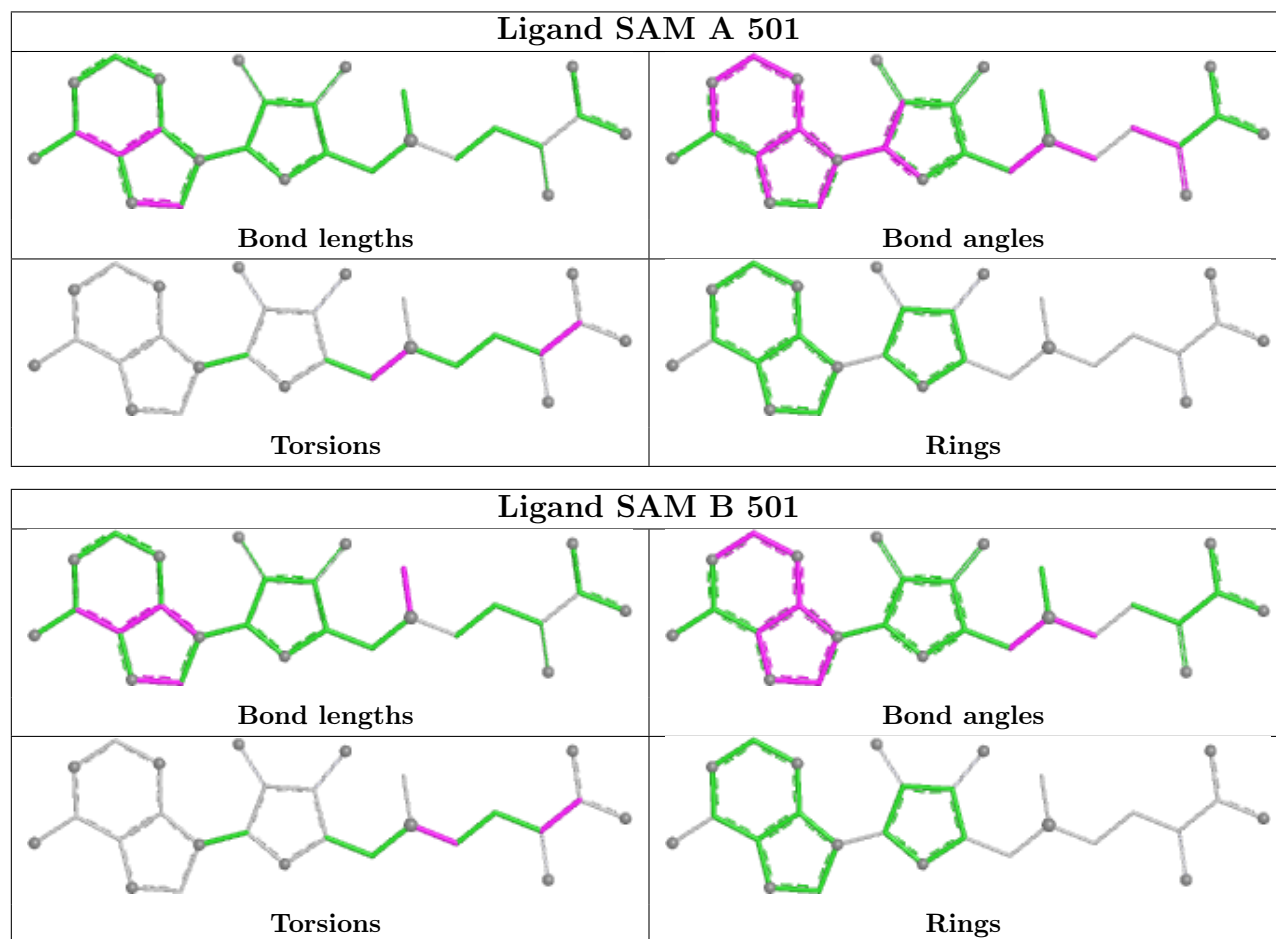
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SAM	2	0
2	B	501	SAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	394/410 (96%)	0.97	66 (16%) 4 4	11, 35, 70, 101	6 (1%)
1	B	393/410 (95%)	0.88	55 (13%) 6 7	12, 34, 66, 107	9 (2%)
All	All	787/820 (95%)	0.92	121 (15%) 5 5	11, 35, 70, 107	15 (1%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	ALA	11.2
1	A	272	VAL	10.5
1	B	272	VAL	10.0
1	A	382	LEU	8.9
1	B	400	TRP	8.8
1	A	277	ALA	8.4
1	B	409	VAL	8.4
1	A	409	VAL	8.2
1	B	410	ILE	7.5
1	A	410	ILE	7.2
1	B	273	PRO	7.2
1	A	386	ALA	7.0
1	A	400	TRP	6.6
1	A	273	PRO	6.6
1	A	384	ASP	6.6
1	A	267	LEU	6.4
1	A	268	PRO	6.4
1	A	379	PRO	6.3
1	B	186	PHE	6.1
1	B	269	ALA	6.0
1	A	269	ALA	6.0
1	B	398	PHE	6.0
1	B	270	GLY	5.8
1	A	385	ALA	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	397	GLY	5.6
1	B	268	PRO	5.4
1	A	380	SER	5.3
1	A	186	PHE	5.2
1	B	383	LEU	5.1
1	A	274	ASP	5.0
1	A	276	LYS	4.7
1	A	398	PHE	4.6
1	A	399	PRO	4.5
1	A	289	VAL	4.5
1	A	270	GLY	4.5
1	B	267	LEU	4.4
1	A	397	GLY	4.4
1	A	7	THR	4.3
1	B	274	ASP	4.3
1	B	406	VAL	4.3
1	A	266	LEU	4.2
1	A	406	VAL	4.1
1	B	385	ALA	4.0
1	B	289	VAL	4.0
1	A	407	ILE	4.0
1	B	408	GLY	4.0
1	B	407	ILE	3.9
1	B	7	THR	3.9
1	B	411	GLY	3.8
1	B	271	GLN	3.8
1	A	271	GLN	3.7
1	B	276	LYS	3.7
1	A	275	LYS	3.7
1	B	275	LYS	3.6
1	B	346	ARG	3.5
1	A	308	ASP	3.5
1	B	399	PRO	3.5
1	B	121[A]	ARG	3.4
1	B	343	ALA	3.3
1	A	411	GLY	3.3
1	B	384	ASP	3.2
1	A	369	TRP	3.2
1	A	408	GLY	3.2
1	A	387	ARG	3.1
1	A	291	GLU	3.1
1	A	178	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	178	ILE	3.1
1	B	185	GLY	3.0
1	B	382	LEU	3.0
1	A	235	GLU	2.9
1	B	369	TRP	2.9
1	B	98	TYR	2.9
1	A	377	ASN	2.8
1	A	262[A]	ARG	2.8
1	B	288	ASP	2.7
1	B	379	PRO	2.6
1	A	367	ASP	2.5
1	B	266	LEU	2.5
1	A	8	LYS	2.5
1	A	381	SER	2.5
1	B	187	ASP	2.5
1	A	185	GLY	2.5
1	A	378	MET	2.5
1	B	189	ASN	2.4
1	A	373	CYS	2.4
1	B	44	ILE	2.4
1	B	117	SER	2.4
1	B	184	THR	2.4
1	A	184	THR	2.4
1	B	313	GLU	2.3
1	A	187	ASP	2.3
1	B	290	PRO	2.3
1	A	372	ARG	2.3
1	B	352	VAL	2.3
1	B	308	ASP	2.3
1	A	353	PRO	2.3
1	A	313	GLU	2.3
1	A	179	ALA	2.2
1	A	238	LYS	2.2
1	A	182	ASN	2.2
1	B	238	LYS	2.2
1	B	350	GLN	2.2
1	A	189	ASN	2.2
1	A	216	MET	2.2
1	A	290	PRO	2.2
1	B	354	ASP	2.1
1	A	343	ALA	2.1
1	A	239	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	367	ASP	2.1
1	B	235	GLU	2.1
1	A	401	VAL	2.1
1	B	370	ALA	2.1
1	A	278	ARG	2.1
1	A	296	ARG	2.1
1	B	353	PRO	2.1
1	B	336	LYS	2.1
1	A	69	GLY	2.0
1	A	231	LEU	2.0
1	A	363	LEU	2.0
1	A	253	ARG	2.0
1	A	346	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	175	7/8	0.89	0.14	32,34,38,40	0
1	CSO	B	175	7/8	0.95	0.11	31,32,36,38	0

6.3 Carbohydrates [i](#)

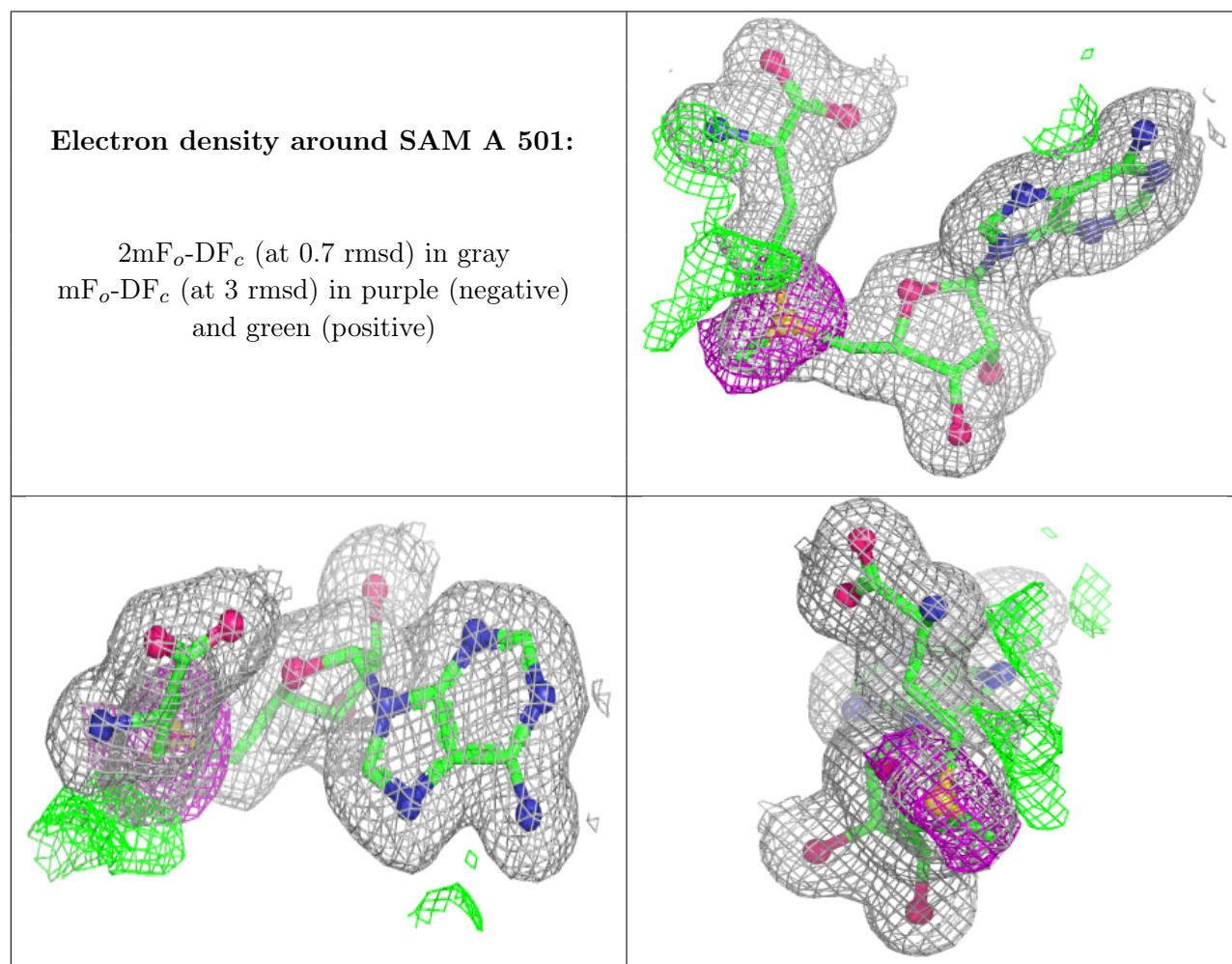
There are no oligosaccharides in this entry.

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, 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.

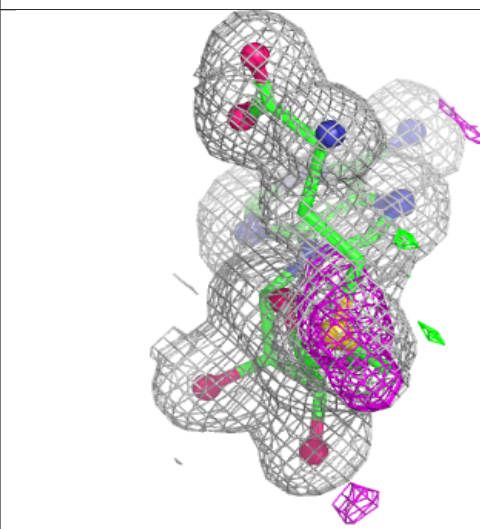
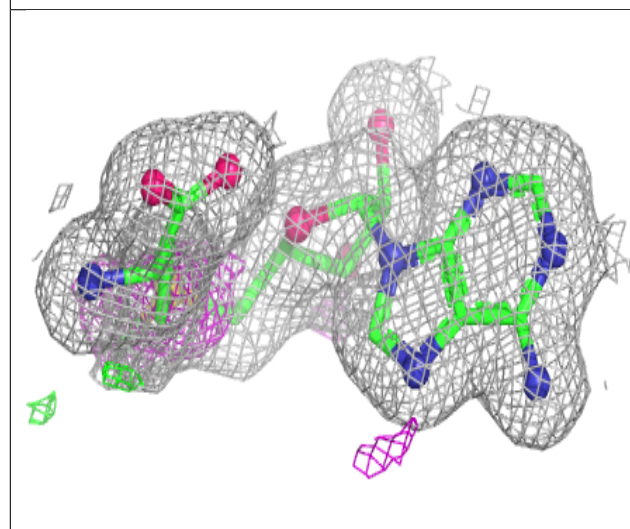
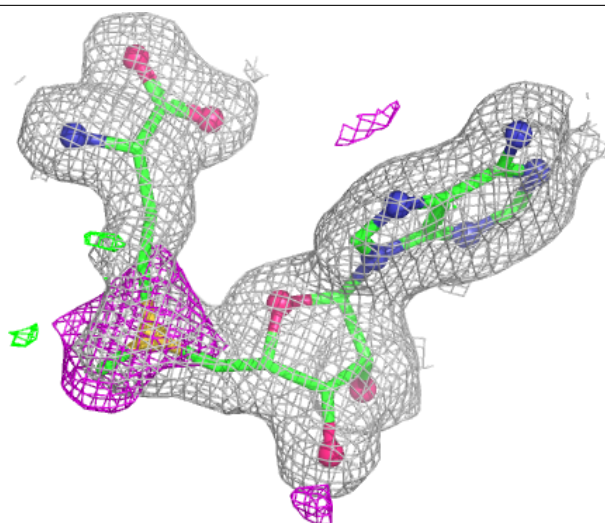
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAM	A	501	27/27	0.94	0.07	22,24,27,29	0
2	SAM	B	501	27/27	0.95	0.08	22,24,28,30	0

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.



Electron density around SAM B 501:

$2mF_o-DF_c$ (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.