WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 03:07 am BST

PDB ID	:	5N0V
Title	:	Crystal structure of OphA-DeltaC6 mutant Y76F in complex with SAH
Authors	:	Song, H.; Naismith, J.H.
Deposited on	:	2017-02-03
Resolution	:	1.91 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.91 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.
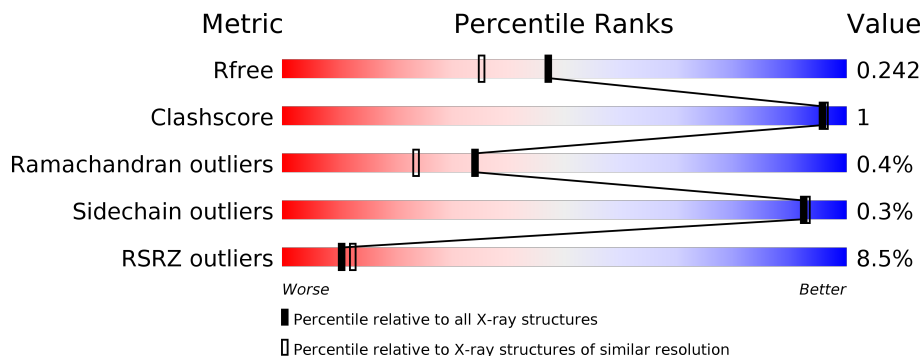
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on 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	410	6% / 91% / · 6%
1	B	410	10% / 92% / · 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6602 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	385	Total	C	N	O	S	0	6	0
			3043	1940	517	569	17			
1	B	391	Total	C	N	O	S	0	5	0
			3072	1958	523	574	17			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
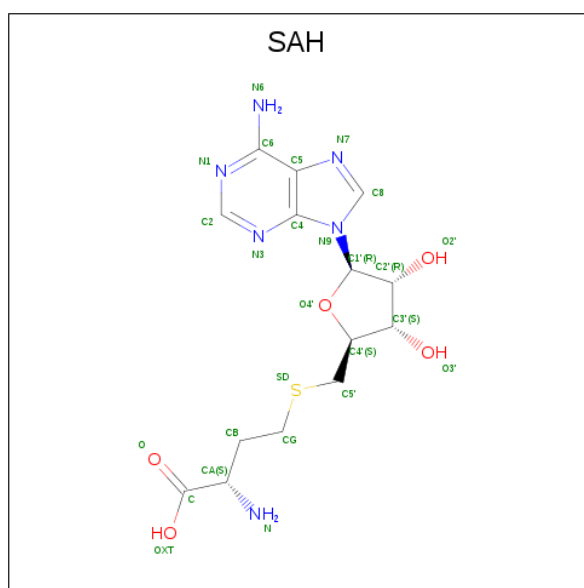
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	226	Total O 226 226	0	0
3	B	209	Total O 209 209	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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
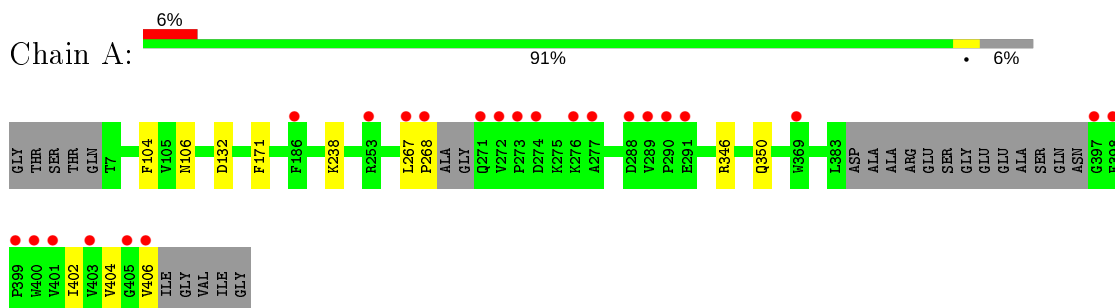
- Molecule 1: Peptide N-methyltransferase
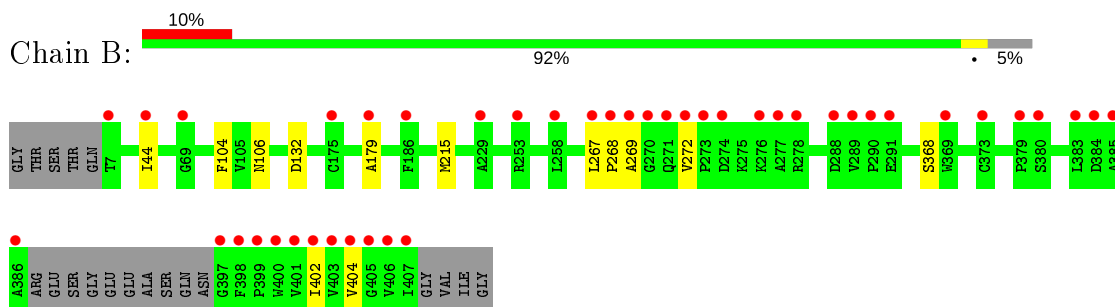
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.74Å 91.92Å 85.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.62 – 1.91 80.15 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (85.62-1.91) 99.4 (80.15-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.218 , 0.237 0.225 , 0.242	Depositor DCC
R_{free} test set	4893 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6602	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 75.92 % 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 1.1504e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/3115	0.62	0/4235
1	B	0.39	0/3145	0.63	0/4279
All	All	0.39	0/6260	0.62	0/8514

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 (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	3043	0	3008	10	0
1	B	3072	0	3041	10	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
3	A	226	0	0	0	1
3	B	209	0	0	0	1
All	All	6602	0	6087	13	2

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 (13) 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:267:LEU:HD21	1:B:272:VAL:HG23	1.69	0.74
1:A:406:VAL:HG11	1:B:179:ALA:HB2	1.91	0.52
1:B:267:LEU:HD22	1:B:269:ALA:O	2.09	0.52
1:A:402:ILE:HG22	1:B:106[A]:ASN:OD1	2.10	0.52
1:A:406:VAL:CG1	1:B:179:ALA:HB2	2.41	0.50
1:B:44:ILE:HG21	1:B:215:MET:HE1	1.96	0.47
1:A:106:ASN:OD1	1:B:402:ILE:HA	2.14	0.47
1:A:104:PHE:HD2	1:B:402:ILE:HD11	1.83	0.44
1:A:132:ASP:OD2	1:B:132:ASP:OD2	2.36	0.42
1:A:346:ARG:O	1:A:350:GLN:HG2	2.18	0.42
1:A:267:LEU:N	1:A:268:PRO:CD	2.83	0.41
1:A:104:PHE:CE2	1:A:171:PHE:HB2	2.56	0.41
1:A:402:ILE:HG23	1:B:104:PHE:C	2.41	0.40

All (2) 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:A:812:HOH:O	3:A:812:HOH:O[2_595]	1.63	0.57
3:B:805:HOH:O	3:B:805:HOH:O[2_595]	2.08	0.12

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	385/410 (94%)	372 (97%)	12 (3%)	1 (0%)	41	31
1	B	392/410 (96%)	377 (96%)	13 (3%)	2 (0%)	29	18
All	All	777/820 (95%)	749 (96%)	25 (3%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	VAL
1	A	404	VAL
1	B	268	PRO

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	328/338 (97%)	327 (100%)	1 (0%)	92	93
1	B	329/338 (97%)	328 (100%)	1 (0%)	92	93
All	All	657/676 (97%)	655 (100%)	2 (0%)	92	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
1	B	368	SER

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

Mol	Chain	Res	Type
1	A	345	HIS
1	B	345	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 carbohydrates 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	SAH	B	501	-	21,28,28	0.92	1 (4%)	20,40,40	1.41	2 (10%)
2	SAH	A	501	-	21,28,28	0.98	1 (4%)	20,40,40	1.35	2 (10%)

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	SAH	B	501	-	-	1/7/31/31	0/3/3/3
2	SAH	A	501	-	-	0/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	SAH	C5-C4	2.47	1.47	1.40
2	A	501	SAH	C5-C4	2.17	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	SAH	N3-C2-N1	-4.23	122.06	128.68
2	A	501	SAH	N3-C2-N1	-3.86	122.65	128.68
2	B	501	SAH	C2-N1-C6	2.50	123.03	118.75
2	A	501	SAH	C4-C5-N7	-2.47	106.82	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	B	501	SAH	C3'-C4'-C5'-SD

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 SAH B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH A 501
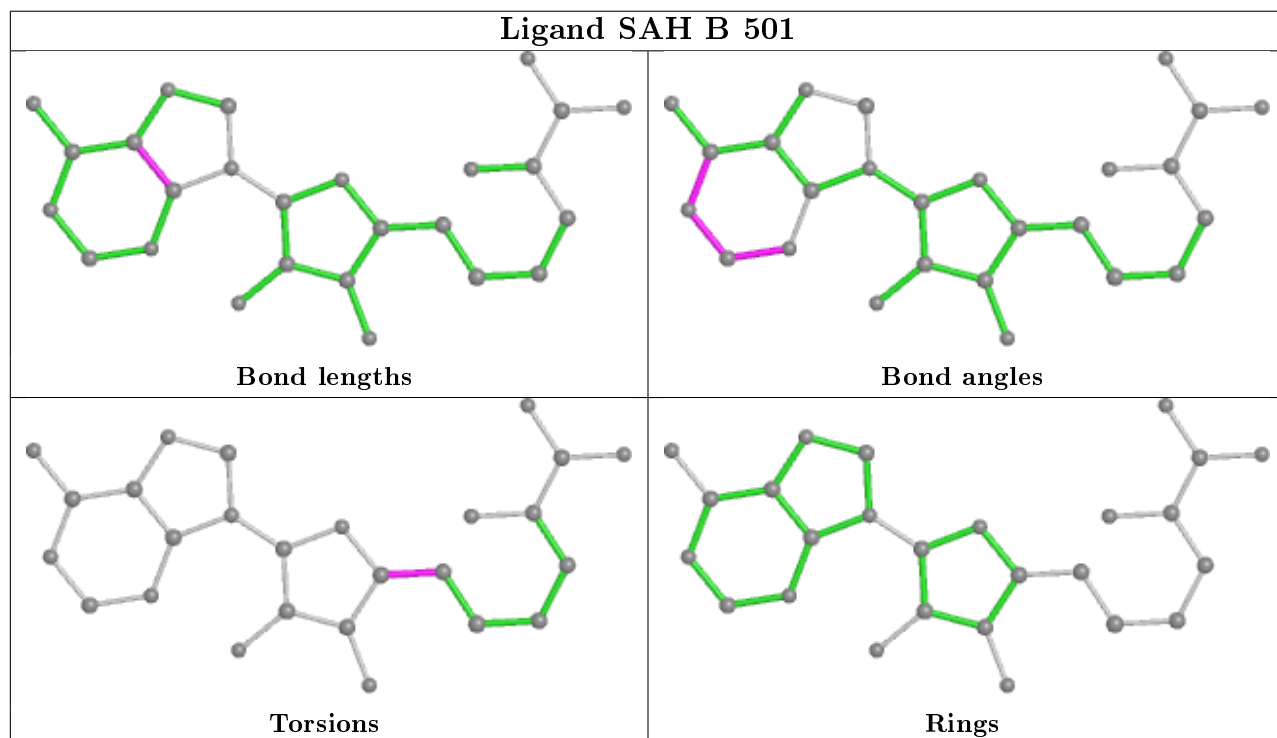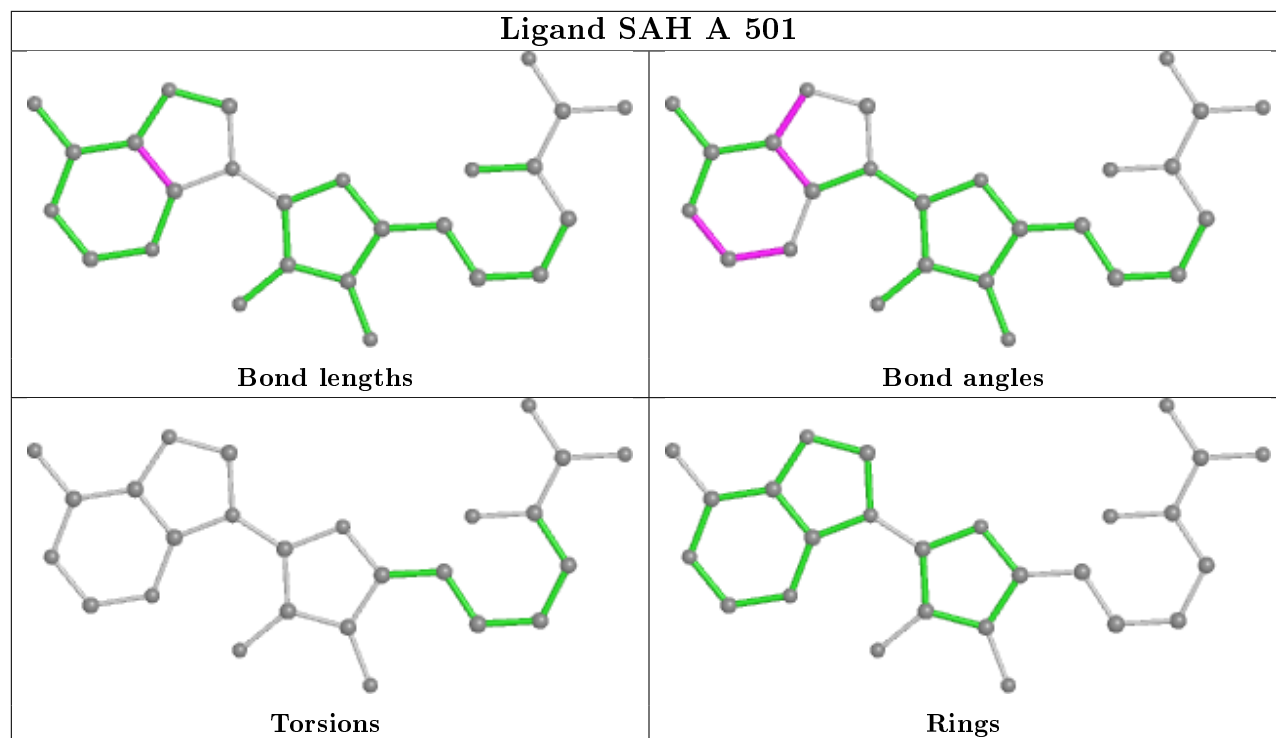
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	385/410 (93%)	0.63	23 (5%)	21	24	22, 39, 65, 100	0
1	B	391/410 (95%)	0.76	43 (10%)	5	6	23, 39, 76, 102	0
All	All	776/820 (94%)	0.70	66 (8%)	10	12	22, 39, 71, 102	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	VAL	11.6
1	A	400	TRP	11.6
1	B	268	PRO	9.6
1	B	400	TRP	9.6
1	B	272	VAL	8.3
1	A	397	GLY	8.1
1	A	277	ALA	7.2
1	B	269	ALA	6.5
1	B	384	ASP	6.4
1	A	268	PRO	6.2
1	B	267	LEU	5.8
1	B	407	ILE	5.7
1	B	276	LYS	5.3
1	B	271	GLN	5.3
1	A	273	PRO	5.2
1	B	277	ALA	5.1
1	B	386	ALA	5.1
1	A	276	LYS	4.7
1	B	398	PHE	4.6
1	A	406	VAL	4.6
1	B	399	PRO	4.4
1	A	267	LEU	4.4
1	B	186	PHE	4.4
1	A	405	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	273	PRO	4.2
1	A	186	PHE	4.2
1	B	383	LEU	4.2
1	A	398	PHE	4.1
1	B	404	VAL	3.9
1	B	385	ALA	3.8
1	A	289	VAL	3.8
1	B	405	GLY	3.7
1	B	406	VAL	3.7
1	B	380	SER	3.7
1	B	379	PRO	3.6
1	B	288	ASP	3.6
1	A	399	PRO	3.6
1	B	397	GLY	3.5
1	B	7	THR	3.5
1	B	401	VAL	3.4
1	B	258	LEU	3.4
1	A	271	GLN	3.3
1	B	402	ILE	3.3
1	A	401	VAL	3.0
1	A	288	ASP	3.0
1	B	289	VAL	3.0
1	B	290	PRO	2.9
1	B	270	GLY	2.9
1	B	373	CYS	2.9
1	B	369	TRP	2.8
1	A	274	ASP	2.8
1	B	274	ASP	2.7
1	B	278	ARG	2.6
1	B	229	ALA	2.6
1	A	291	GLU	2.6
1	B	253	ARG	2.5
1	A	290	PRO	2.4
1	B	175	CYS	2.3
1	A	403	VAL	2.3
1	B	291	GLU	2.3
1	A	369	TRP	2.2
1	B	44	ILE	2.2
1	A	253	ARG	2.2
1	B	179	ALA	2.1
1	B	403	VAL	2.0
1	B	69	GLY	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 carbohydrates in this entry.
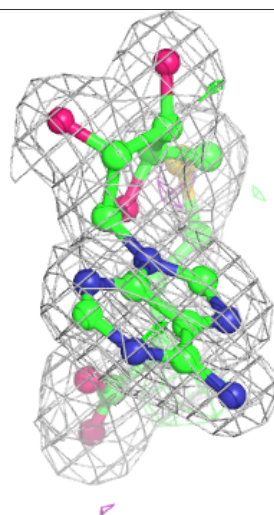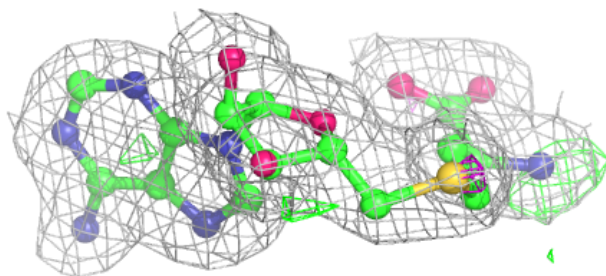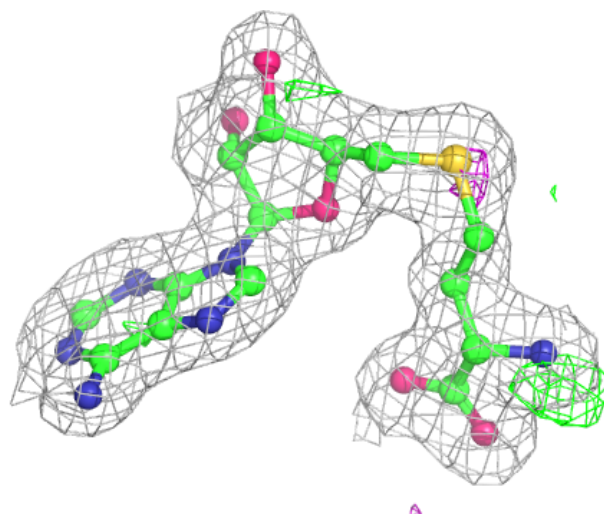
6.4 Ligands (i)

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.

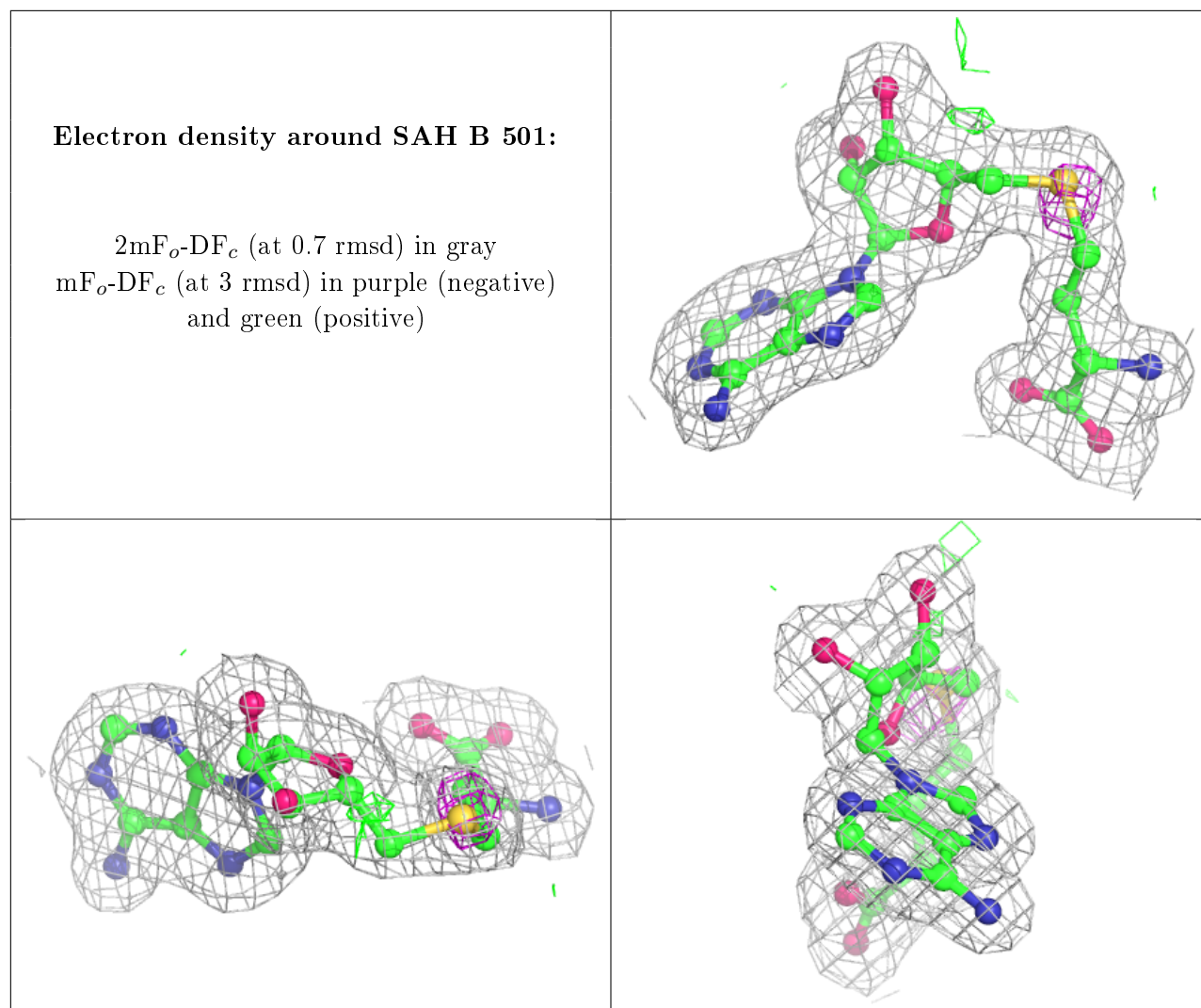| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	A	501	26/26	0.96	0.11	25,27,29,30	0
2	SAH	B	501	26/26	0.97	0.10	24,26,28,30	0

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 SAH A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SAH 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 ⓘ

There are no such residues in this entry.