



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 09:15 PM EDT

PDB ID : 1P0Y
Title : Crystal structure of the SET domain of LSM1 bound to MeLysine and AdoHcy
Authors : Trievel, R.C.; Flynn, E.M.; Houtz, R.L.; Hurley, J.H.
Deposited on : 2003-04-11
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

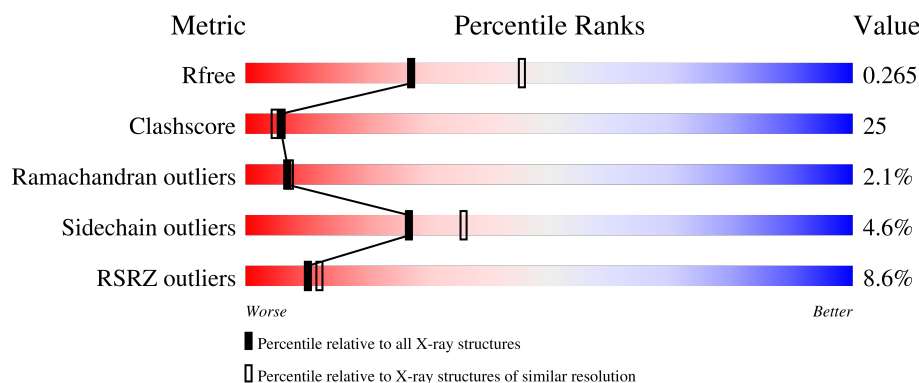
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	444	<div> <div>12%</div> <div>54%</div> <div>38%</div> <div>5%</div> <div>.</div> </div>
1	B	444	<div> <div>9%</div> <div>58%</div> <div>38%</div> <div>.</div> <div>..</div> </div>
1	C	444	<div> <div>5%</div> <div>60%</div> <div>34%</div> <div>.</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11308 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.

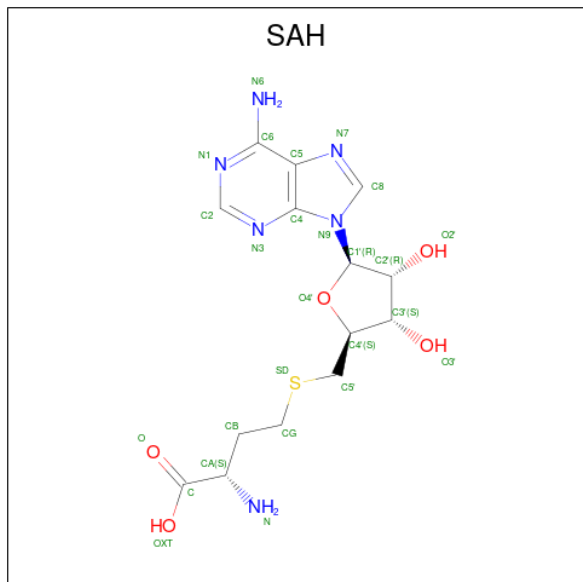
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3464	2217	573	667	7			
1	B	441	Total	C	N	O	S	0	0	0
			3549	2275	586	681	7			
1	C	439	Total	C	N	O	S	0	0	0
			3532	2265	583	677	7			

There are 21 discrepancies between the modelled and reference sequences:

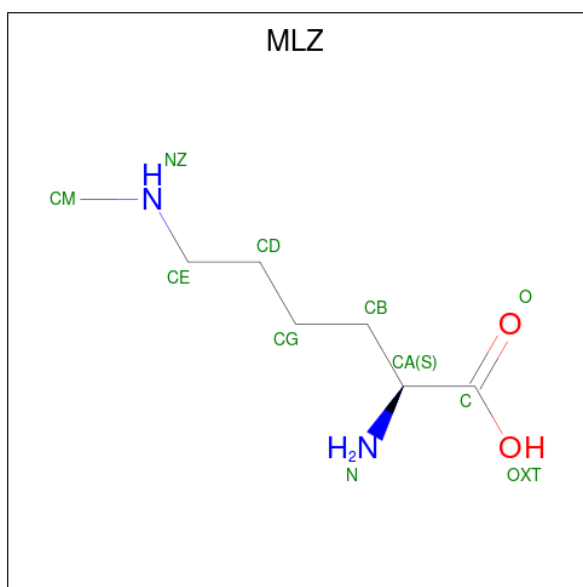
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	initiating methionine	UNP Q43088
A	483	GLU	-	engineered mutation	UNP Q43088
A	484	ASN	-	engineered mutation	UNP Q43088
A	485	LEU	-	engineered mutation	UNP Q43088
A	486	TYR	-	engineered mutation	UNP Q43088
A	487	PHE	-	engineered mutation	UNP Q43088
A	488	GLN	-	engineered mutation	UNP Q43088
B	45	MET	-	initiating methionine	UNP Q43088
B	483	GLU	-	engineered mutation	UNP Q43088
B	484	ASN	-	engineered mutation	UNP Q43088
B	485	LEU	-	engineered mutation	UNP Q43088
B	486	TYR	-	engineered mutation	UNP Q43088
B	487	PHE	-	engineered mutation	UNP Q43088
B	488	GLN	-	engineered mutation	UNP Q43088
C	45	MET	-	initiating methionine	UNP Q43088
C	483	GLU	-	engineered mutation	UNP Q43088
C	484	ASN	-	engineered mutation	UNP Q43088
C	485	LEU	-	engineered mutation	UNP Q43088
C	486	TYR	-	engineered mutation	UNP Q43088
C	487	PHE	-	engineered mutation	UNP Q43088
C	488	GLN	-	engineered mutation	UNP Q43088

- 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		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is N-METHYL-LYSINE (three-letter code: MLZ) (formula: $C_7H_{16}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			11	7	2	2		
3	C	1	Total	C	N	O	0	0
			11	7	2	2		
3	C	1	Total	C	N	O	0	0
			11	7	2	2		

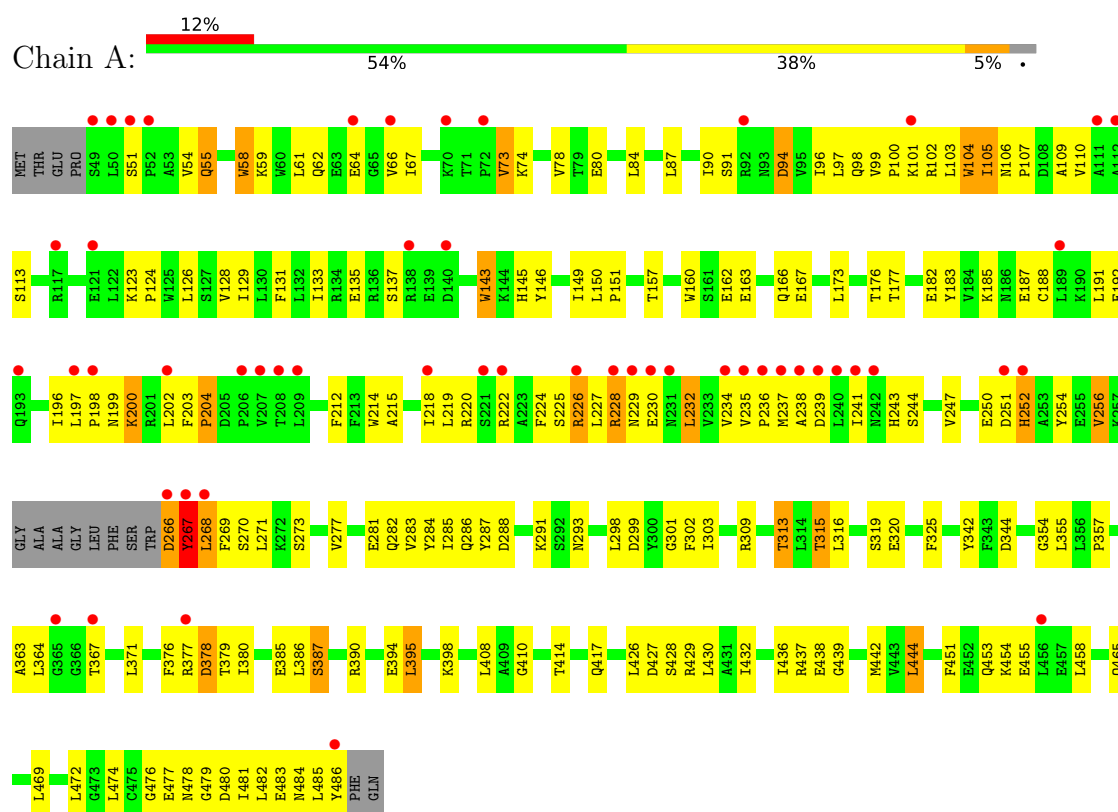
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	210	Total	O	0	0
			210	210		
4	C	221	Total	O	0	0
			221	221		

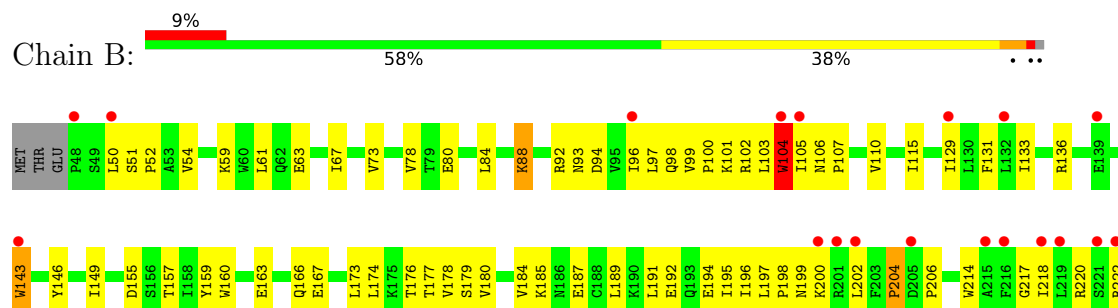
3 Residue-property plots

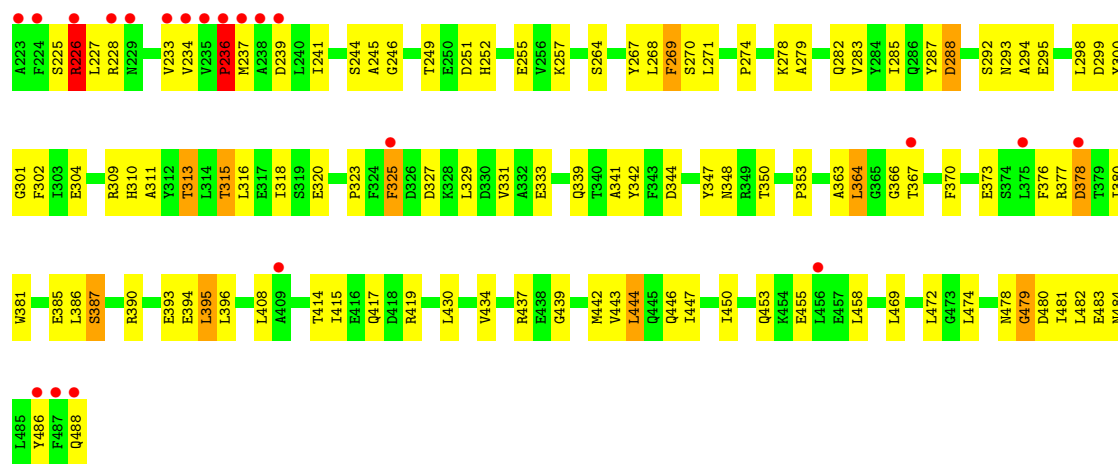
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast

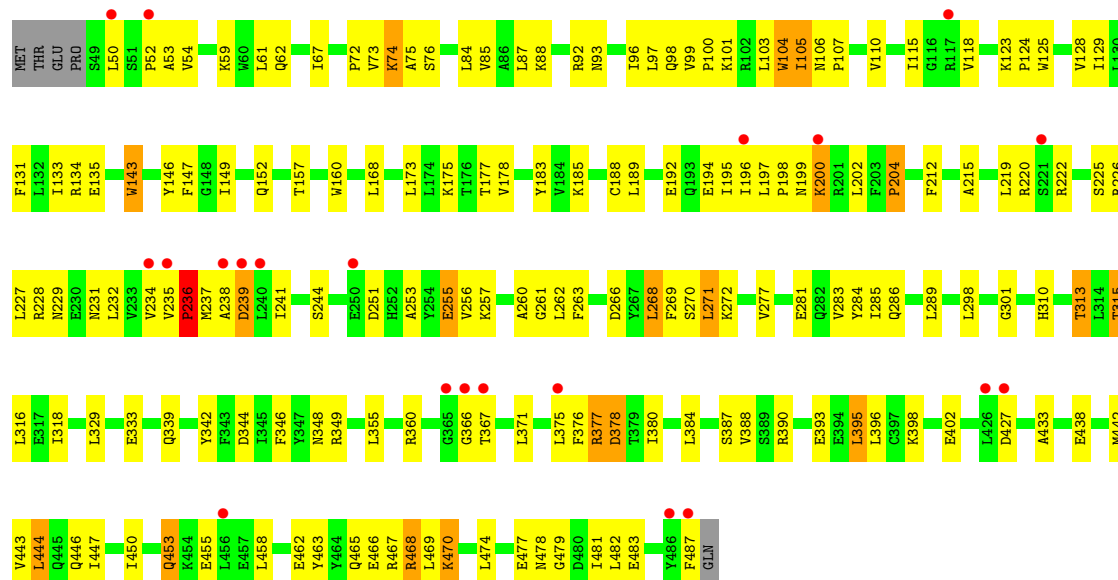


- Molecule 1: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast





- Molecule 1: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.41Å 153.19Å 266.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 2.55 29.65 – 2.55	Depositor EDS
% Data completeness (in resolution range)	85.1 (29.65-2.55) 85.2 (29.65-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.269 0.225 , 0.265	Depositor DCC
R_{free} test set	3761 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	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	0.94	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: SAH, MLZ

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	0/3534	0.60	1/4793 (0.0%)
1	B	0.39	0/3625	0.61	2/4917 (0.0%)
1	C	0.38	0/3607	0.60	0/4894
All	All	0.38	0/10766	0.60	3/14604 (0.0%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	TYR	N-CA-C	-5.37	96.51	111.00
1	B	269	PHE	N-CA-C	-5.24	96.84	111.00
1	B	104	TRP	CA-CB-CG	5.01	123.22	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	TYR	Sidechain

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	3464	0	3432	212	0
1	B	3549	0	3509	168	0
1	C	3532	0	3493	174	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
2	C	26	0	19	1	0
3	C	33	0	45	5	0
4	A	221	0	0	22	0
4	B	210	0	0	15	0
4	C	221	0	0	23	0
All	All	11308	0	10536	530	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 25.

The worst 5 of 530 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:395:LEU:HD22	1:C:469:LEU:HD12	1.42	1.01
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.42	0.98
1:A:98:GLN:HB3	1:A:268:LEU:HG	1.48	0.95
1:B:367:THR:HA	4:B:803:HOH:O	1.65	0.95
1:C:74:LYS:HG2	1:C:87:LEU:HD21	1.51	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	426/444 (96%)	389 (91%)	27 (6%)	10 (2%)	6	6
1	B	439/444 (99%)	398 (91%)	30 (7%)	11 (2%)	5	5
1	C	437/444 (98%)	402 (92%)	29 (7%)	6 (1%)	11	15
All	All	1302/1332 (98%)	1189 (91%)	86 (7%)	27 (2%)	7	7

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	ARG
1	C	377	ARG
1	A	204	PRO
1	A	252	HIS
1	A	377	ARG

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	380/390 (97%)	360 (95%)	20 (5%)	22	30
1	B	387/390 (99%)	373 (96%)	14 (4%)	35	47
1	C	385/390 (99%)	366 (95%)	19 (5%)	25	34
All	All	1152/1170 (98%)	1099 (95%)	53 (5%)	27	36

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	315	THR
1	C	104	TRP
1	C	453	GLN
1	B	378	ASP
1	B	453	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	460	GLN
1	C	484	ASN
1	C	98	GLN
1	C	310	HIS
1	B	488	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	MLZ	C	901	-	6,10,10	0.58	0	5,11,11	0.45	0
2	SAH	C	802	-	21,28,28	0.88	1 (4%)	20,40,40	0.89	1 (5%)
3	MLZ	C	902	-	6,10,10	0.48	0	5,11,11	0.59	0
3	MLZ	C	900	-	6,10,10	0.55	0	5,11,11	0.89	0
2	SAH	B	801	-	21,28,28	1.01	3 (14%)	20,40,40	0.92	0
2	SAH	A	800	-	21,28,28	0.89	1 (4%)	20,40,40	0.90	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
3	MLZ	C	901	-	-	3/6/10/10	-
2	SAH	C	802	-	-	1/7/31/31	0/3/3/3
3	MLZ	C	902	-	-	2/6/10/10	-
3	MLZ	C	900	-	-	3/6/10/10	-
2	SAH	B	801	-	-	2/7/31/31	0/3/3/3
2	SAH	A	800	-	-	3/7/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SAH	C2-N3	2.75	1.36	1.32
2	C	802	SAH	C2-N3	2.50	1.36	1.32
2	A	800	SAH	C2-N3	2.15	1.35	1.32
2	B	801	SAH	C4-N3	2.06	1.38	1.35
2	B	801	SAH	C8-N7	-2.06	1.31	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	SAH	C5-C6-N6	2.05	123.47	120.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	901	MLZ	CG-CD-CE-NZ
3	C	900	MLZ	CG-CD-CE-NZ
3	C	902	MLZ	CG-CD-CE-NZ
3	C	901	MLZ	CE-CD-CG-CB
3	C	900	MLZ	CE-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 7 short contacts:

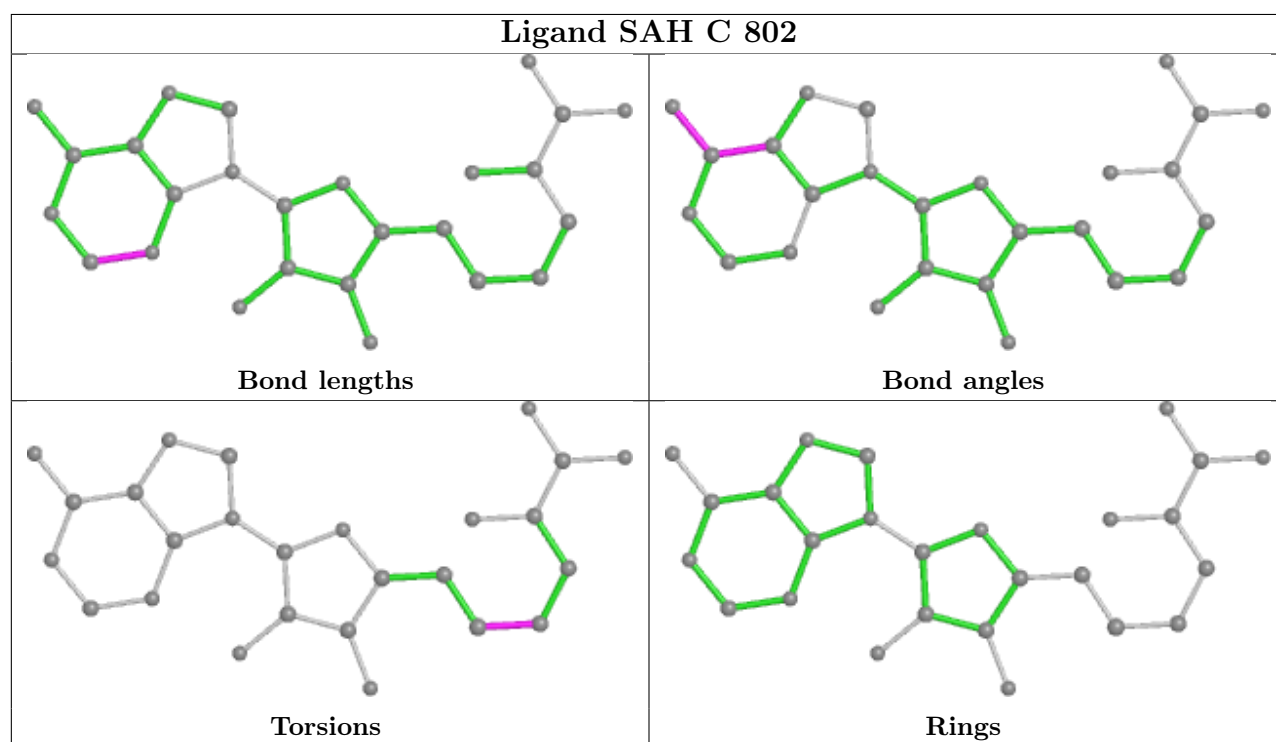
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	MLZ	2	0

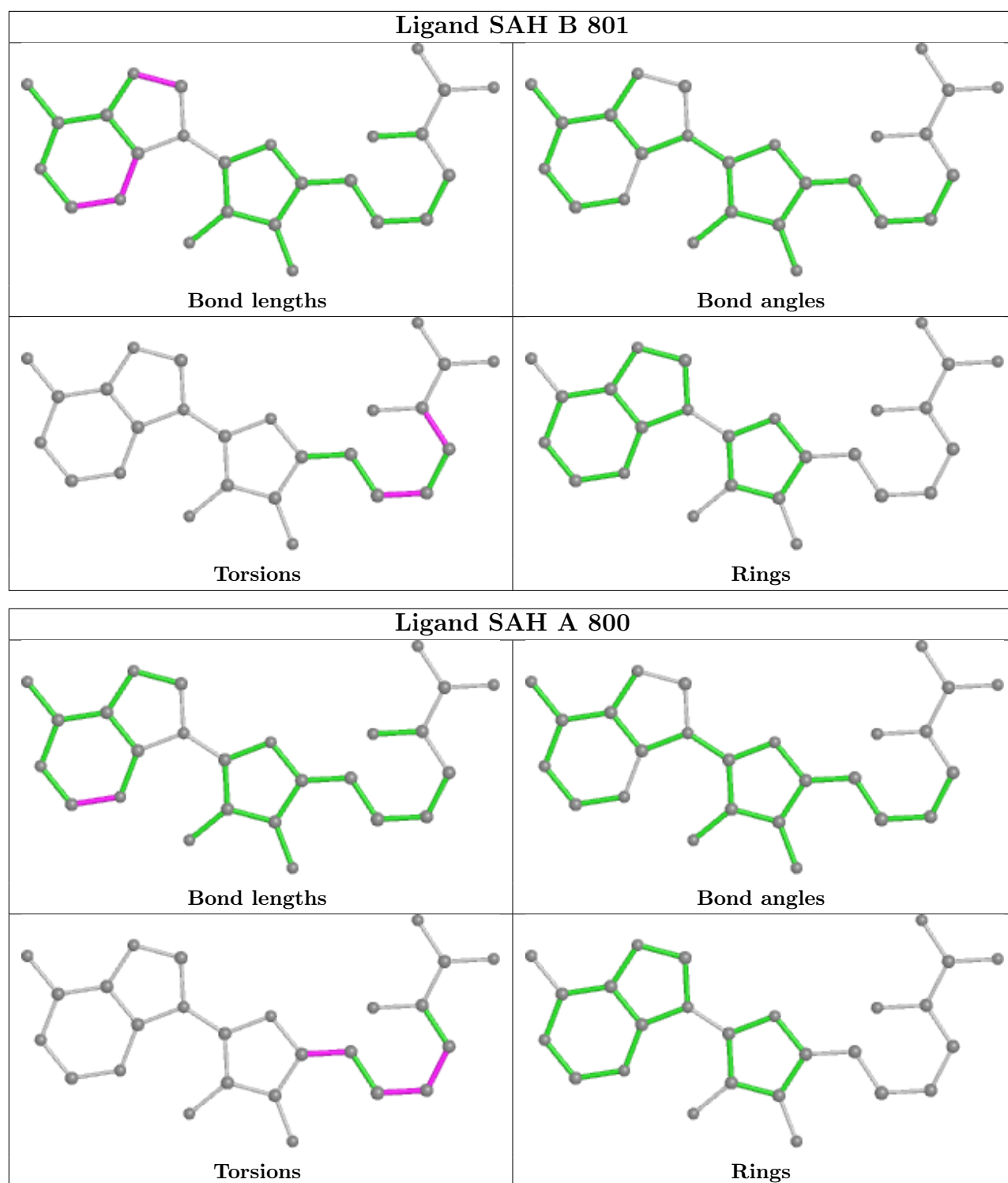
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	SAH	1	0
3	C	902	MLZ	1	0
3	C	900	MLZ	2	0
2	B	801	SAH	1	0

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 ⓘ

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	430/444 (96%)	0.60	52 (12%) 4 5	46, 70, 120, 130	0
1	B	441/444 (99%)	0.40	40 (9%) 9 11	41, 64, 101, 123	0
1	C	439/444 (98%)	0.27	21 (4%) 30 37	45, 66, 97, 113	0
All	All	1310/1332 (98%)	0.42	113 (8%) 10 12	41, 67, 108, 130	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	TYR	7.3
1	C	487	PHE	6.2
1	B	229	ASN	5.9
1	A	239	ASP	5.8
1	B	228	ARG	5.8

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](#)

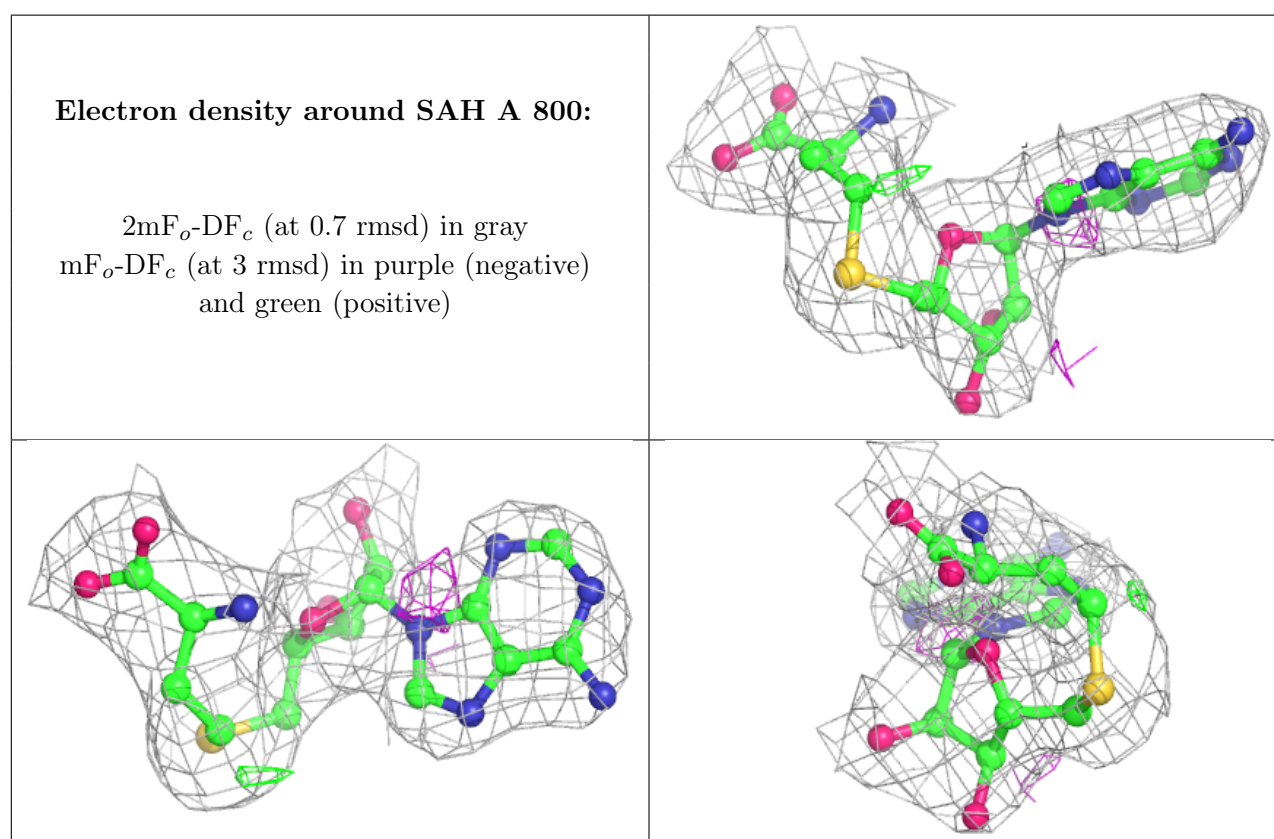
There are no monosaccharides in this entry.

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.

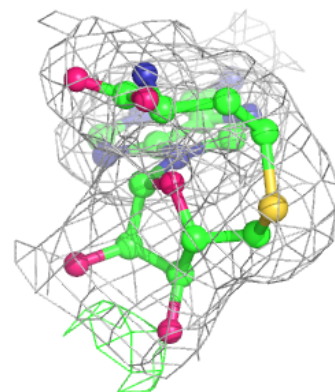
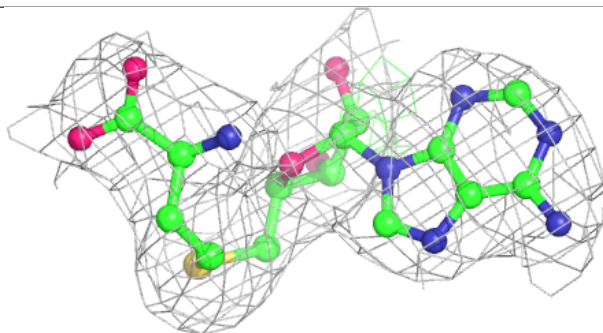
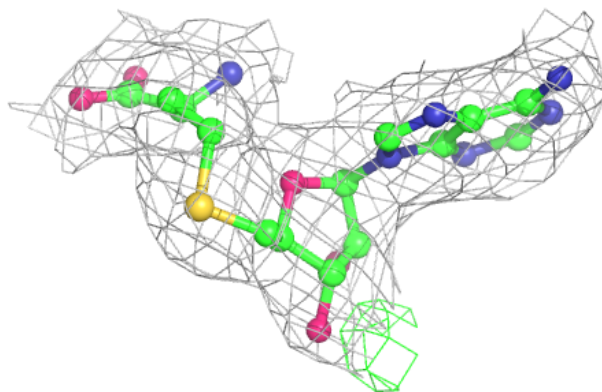
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MLZ	C	900	11/11	0.80	0.38	74,75,79,80	0
3	MLZ	C	902	11/11	0.90	0.32	46,50,54,55	0
3	MLZ	C	901	11/11	0.91	0.28	52,53,56,57	0
2	SAH	A	800	26/26	0.92	0.28	66,69,76,77	0
2	SAH	C	802	26/26	0.94	0.22	53,61,64,64	0
2	SAH	B	801	26/26	0.95	0.20	44,47,50,52	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.

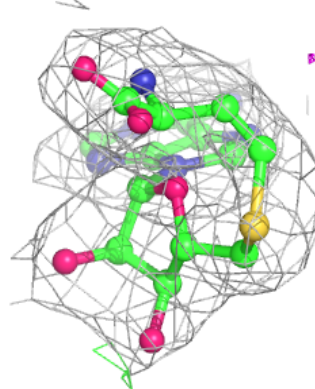
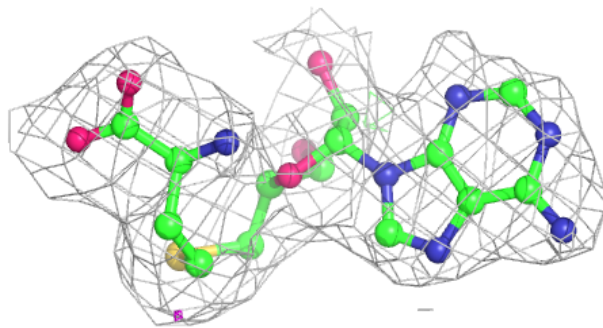
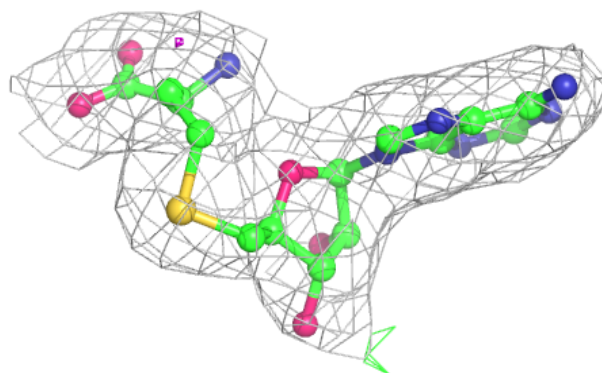


Electron density around SAH C 802:

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

**Electron density around SAH B 801:**

$2mF_o-DF_c$ (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.