



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 5WMM / pdb_00005wmm
Title : Crystal structure of an adenylation domain interrupted by a methylation domain (AMA4) from nonribosomal peptide synthetase TioS
Authors : Pang, A.H.; Mori, S.; Garneau-Tsodikova, S.; Tsodikov, O.V.
Deposited on : 2017-07-30
Resolution : 2.90 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

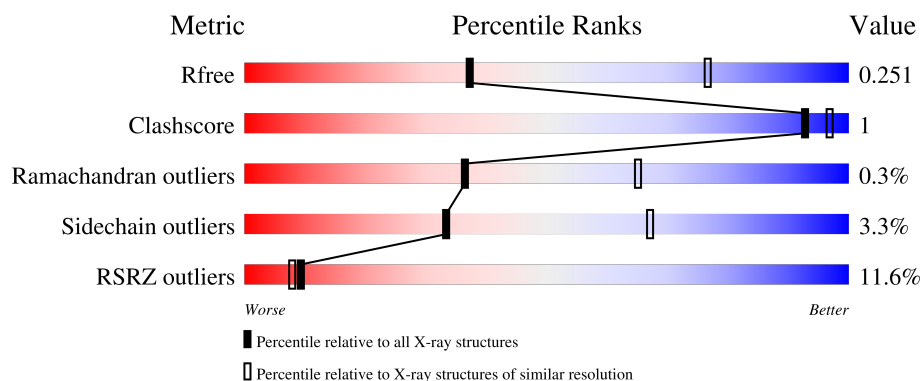
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	926	10% 89% 5% 6%
2	B	87	21% 70% • 26%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7342 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 NRPS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	870	Total	C	N	O	S	0	0	0
			6755	4256	1238	1244	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q333U7
A	-19	GLY	-	expression tag	UNP Q333U7
A	-18	SER	-	expression tag	UNP Q333U7
A	-17	SER	-	expression tag	UNP Q333U7
A	-16	HIS	-	expression tag	UNP Q333U7
A	-15	HIS	-	expression tag	UNP Q333U7
A	-14	HIS	-	expression tag	UNP Q333U7
A	-13	HIS	-	expression tag	UNP Q333U7
A	-12	HIS	-	expression tag	UNP Q333U7
A	-11	HIS	-	expression tag	UNP Q333U7
A	-10	SER	-	expression tag	UNP Q333U7
A	-9	SER	-	expression tag	UNP Q333U7
A	-8	GLY	-	expression tag	UNP Q333U7
A	-7	LEU	-	expression tag	UNP Q333U7
A	-6	VAL	-	expression tag	UNP Q333U7
A	-5	PRO	-	expression tag	UNP Q333U7
A	-4	ARG	-	expression tag	UNP Q333U7
A	-3	GLY	-	expression tag	UNP Q333U7
A	-2	SER	-	expression tag	UNP Q333U7
A	-1	HIS	-	expression tag	UNP Q333U7
A	0	MET	-	expression tag	UNP Q333U7

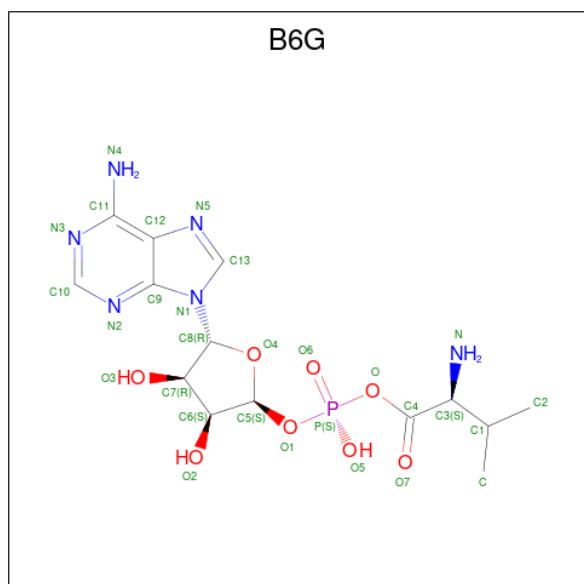
- Molecule 2 is a protein called MbtH homologue.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	64	Total	C	N	O	S	0	0	0
			522	331	86	104	1			

There are 16 discrepancies between the modelled and reference sequences:

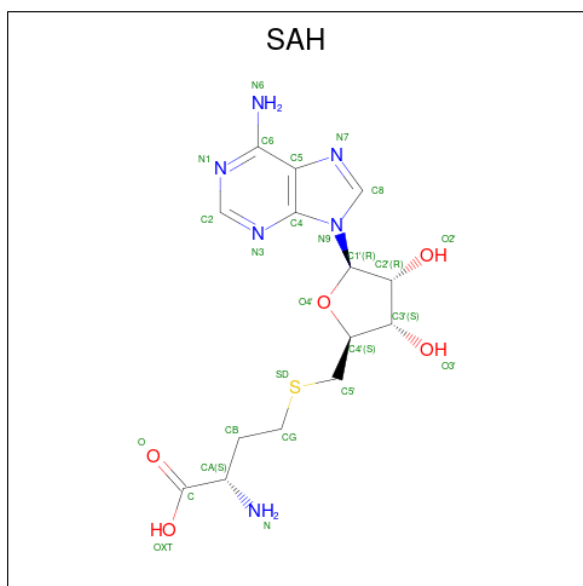
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP Q333U6
B	-14	GLY	-	expression tag	UNP Q333U6
B	-13	SER	-	expression tag	UNP Q333U6
B	-12	SER	-	expression tag	UNP Q333U6
B	-11	HIS	-	expression tag	UNP Q333U6
B	-10	HIS	-	expression tag	UNP Q333U6
B	-9	HIS	-	expression tag	UNP Q333U6
B	-8	HIS	-	expression tag	UNP Q333U6
B	-7	HIS	-	expression tag	UNP Q333U6
B	-6	HIS	-	expression tag	UNP Q333U6
B	-5	SER	-	expression tag	UNP Q333U6
B	-4	GLN	-	expression tag	UNP Q333U6
B	-3	ASP	-	expression tag	UNP Q333U6
B	-2	PRO	-	expression tag	UNP Q333U6
B	-1	ASN	-	expression tag	UNP Q333U6
B	0	SER	-	expression tag	UNP Q333U6

- Molecule 3 is (2S)-2-amino-3-methylbutanoyl (2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl hydrogen (S)-phosphate (CCD ID: B6G) (formula: $C_{14}H_{21}N_6O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	14	6	8	1		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		

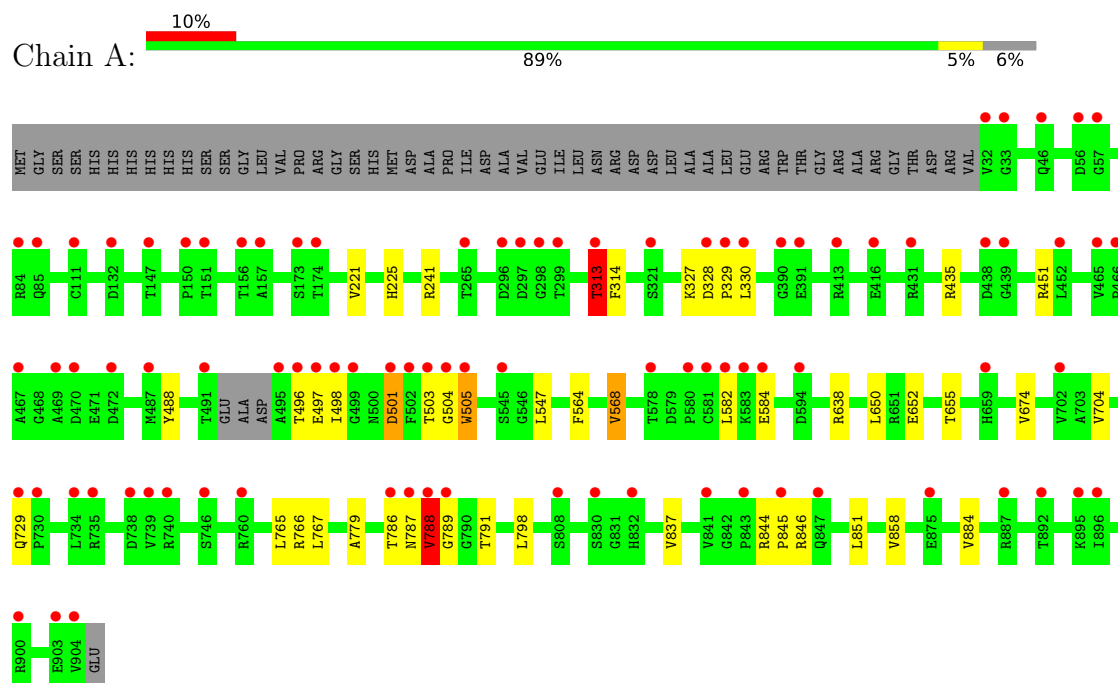
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		

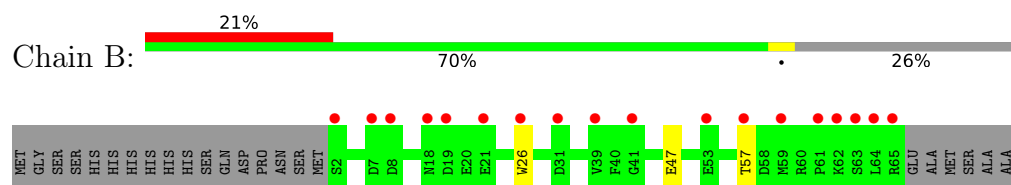
3 Residue-property plots [i](#)

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: NRPS



• Molecule 2: MbtH homologue



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.71Å 136.71Å 228.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.90) 99.3 (40.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.236 , 0.253 0.235 , 0.251	Depositor DCC
R_{free} test set	2855 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B6G, CA, CL, 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	0.58	0/6919	0.83	1/9445 (0.0%)
2	B	0.58	0/539	0.82	0/736
All	All	0.58	0/7458	0.83	1/10181 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	GLN	N-CA-C	5.66	121.32	113.45

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	6755	0	6693	21	0
2	B	522	0	466	0	0
3	A	29	0	0	0	0
4	A	26	0	19	0	0
5	A	3	0	0	0	0
6	A	3	0	0	0	0
7	A	4	0	0	0	0
All	All	7342	0	7178	21	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 1.

All (21) 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:655:THR:HG22	1:A:674:VAL:HG21	1.86	0.57
1:A:505:TRP:HA	1:A:505:TRP:CE3	2.42	0.54
1:A:327:LYS:HB3	1:A:329:PRO:HD2	1.90	0.53
1:A:497:GLU:HG3	1:A:498:ILE:H	1.74	0.53
1:A:858:VAL:HG13	1:A:884:VAL:HG11	1.92	0.52
1:A:496:THR:OG1	1:A:497:GLU:N	2.43	0.51
1:A:505:TRP:HA	1:A:505:TRP:HE3	1.77	0.49
1:A:779:ALA:CB	1:A:786:THR:HG21	2.42	0.49
1:A:498:ILE:O	1:A:498:ILE:HG23	2.12	0.49
1:A:788:VAL:HG13	1:A:789:GLY:O	2.14	0.47
1:A:488:TYR:CD2	1:A:568:VAL:HG22	2.50	0.47
1:A:328:ASP:N	1:A:329:PRO:CD	2.78	0.47
1:A:501:ASP:O	1:A:547:LEU:HD21	2.15	0.46
1:A:221:VAL:O	1:A:225:HIS:ND1	2.51	0.44
1:A:844:ARG:N	1:A:845:PRO:HD3	2.33	0.43
1:A:497:GLU:HG3	1:A:498:ILE:N	2.35	0.41
1:A:497:GLU:CG	1:A:498:ILE:H	2.34	0.41
1:A:766:ARG:NH2	1:A:837:VAL:O	2.54	0.41
1:A:313:THR:OG1	1:A:314:PHE:N	2.54	0.40
1:A:327:LYS:CB	1:A:329:PRO:HD2	2.51	0.40
1:A:503:THR:HG23	1:A:504:GLY:N	2.37	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	866/926 (94%)	828 (96%)	36 (4%)	2 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	62/87 (71%)	57 (92%)	4 (6%)	1 (2%)	7	27
All	All	928/1013 (92%)	885 (95%)	40 (4%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	788	VAL
1	A	313	THR
2	B	57	THR

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	705/750 (94%)	682 (97%)	23 (3%)	33	67
2	B	56/75 (75%)	54 (96%)	2 (4%)	31	65
All	All	761/825 (92%)	736 (97%)	25 (3%)	33	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	313	THR
1	A	330	LEU
1	A	435	ARG
1	A	451	ARG
1	A	501	ASP
1	A	505	TRP
1	A	564	PHE
1	A	568	VAL
1	A	582	LEU
1	A	584	GLU
1	A	638	ARG
1	A	650	LEU

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Mol	Chain	Res	Type
1	A	652	GLU
1	A	704	VAL
1	A	765	LEU
1	A	767	LEU
1	A	787	ASN
1	A	788	VAL
1	A	791	THR
1	A	798	LEU
1	A	846	ARG
1	A	851	LEU
2	B	26	TRP
2	B	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	186	ASN
1	A	513	ASN
1	A	591	GLN
1	A	646	ASN
1	A	727	HIS
1	A	772	ASN
1	A	787	ASN
1	A	876	HIS
1	A	898	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
4	SAH	A	1002	-	27,28,28	1.55	5 (18%)	36,40,40	2.00	10 (27%)
3	B6G	A	1001	-	27,31,31	1.52	4 (14%)	41,47,47	2.31	12 (29%)

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
4	SAH	A	1002	-	-	0/15/31/31	0/3/3/3
3	B6G	A	1001	-	-	7/19/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	B6G	C12-C9	5.18	1.48	1.39
4	A	1002	SAH	C5-C4	4.99	1.48	1.39
4	A	1002	SAH	C5-C6	2.94	1.49	1.41
3	A	1001	B6G	C12-C11	2.86	1.49	1.41
3	A	1001	B6G	C12-N5	-2.63	1.34	1.39
4	A	1002	SAH	C8-N7	2.46	1.36	1.31
4	A	1002	SAH	C5-N7	-2.39	1.34	1.39
4	A	1002	SAH	OXT-C	-2.25	1.23	1.30
3	A	1001	B6G	C13-N5	2.23	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	B6G	C12-C9-N2	-6.40	117.91	126.72
4	A	1002	SAH	C5-C4-N3	-5.73	118.83	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	B6G	O1-C5-C6	5.42	115.44	106.65
3	A	1001	B6G	N2-C9-N1	4.97	135.62	127.17
4	A	1002	SAH	N3-C4-N9	4.51	134.84	127.17
3	A	1001	B6G	C1-C3-C4	4.38	118.03	111.11
3	A	1001	B6G	C10-N2-C9	3.89	121.34	111.83
4	A	1002	SAH	C2-N3-C4	3.70	120.87	111.83
4	A	1002	SAH	C4-C5-N7	-3.61	106.46	110.58
3	A	1001	B6G	C9-C12-N5	-3.45	106.63	110.58
3	A	1001	B6G	N2-C10-N3	-3.40	123.44	128.58
4	A	1002	SAH	N3-C2-N1	-3.32	123.55	128.58
3	A	1001	B6G	C5-O4-C8	3.30	111.94	106.05
3	A	1001	B6G	O-P-O1	3.09	110.94	103.35
4	A	1002	SAH	OXT-C-O	-2.97	117.35	124.08
4	A	1002	SAH	C5-N7-C8	2.69	107.67	103.45
4	A	1002	SAH	C4-N9-C8	2.67	108.54	105.74
3	A	1001	B6G	C6-C7-C8	2.66	106.50	101.46
3	A	1001	B6G	C12-N5-C13	2.62	107.57	103.45
4	A	1002	SAH	C6-C5-N7	2.22	136.37	132.09
3	A	1001	B6G	C5-C6-C7	2.08	104.87	102.29
4	A	1002	SAH	N9-C8-N7	-2.07	111.00	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

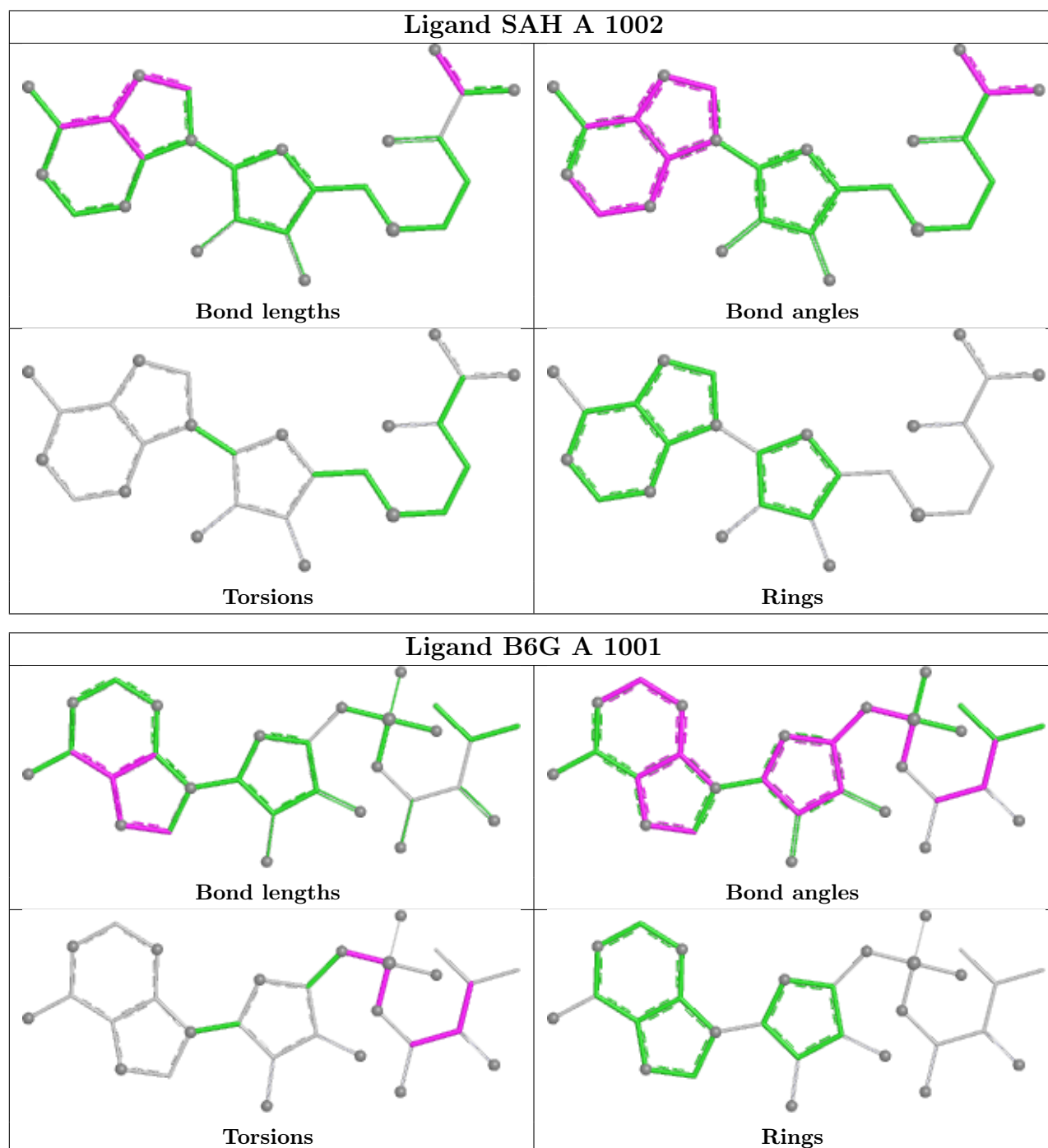
Mol	Chain	Res	Type	Atoms
3	A	1001	B6G	C5-O1-P-O
3	A	1001	B6G	N-C3-C4-O7
3	A	1001	B6G	N-C3-C4-O
3	A	1001	B6G	C2-C1-C3-C4
3	A	1001	B6G	C4-O-P-O6
3	A	1001	B6G	C2-C1-C3-N
3	A	1001	B6G	C-C1-C3-C4

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 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

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, 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	870/926 (93%)	0.69	90 (10%)	12 10	41, 82, 124, 157	0
2	B	64/87 (73%)	1.24	18 (28%)	1 1	68, 83, 108, 132	0
All	All	934/1013 (92%)	0.73	108 (11%)	9 8	41, 82, 122, 157	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	LEU	7.3
1	A	467	ALA	5.9
1	A	503	THR	5.8
1	A	466	PRO	5.7
1	A	498	ILE	5.5
1	A	495	ALA	5.3
1	A	329	PRO	5.3
2	B	65	ARG	5.1
1	A	491	THR	5.0
1	A	505	TRP	4.9
1	A	32	VAL	4.6
1	A	452	LEU	4.3
1	A	439	GLY	4.1
1	A	499	GLY	4.1
1	A	132	ASP	4.0
1	A	788	VAL	4.0
1	A	845	PRO	3.9
1	A	299	THR	3.8
1	A	330	LEU	3.7
1	A	496	THR	3.6
1	A	469	ALA	3.6
1	A	465	VAL	3.5
1	A	896	ILE	3.5
2	B	62	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	843	PRO	3.1
1	A	150	PRO	3.1
1	A	892	THR	3.1
2	B	63	SER	3.1
1	A	298	GLY	3.0
1	A	504	GLY	3.0
1	A	786	THR	3.0
2	B	57	THR	3.0
1	A	738	ASP	3.0
2	B	61	PRO	3.0
1	A	85	GLN	3.0
1	A	497	GLU	2.9
1	A	438	ASP	2.9
1	A	734	LEU	2.9
2	B	19	ASP	2.9
1	A	580	PRO	2.8
2	B	18	ASN	2.8
1	A	321	SER	2.8
1	A	56	ASP	2.8
1	A	157	ALA	2.7
2	B	41	GLY	2.7
1	A	735	ARG	2.7
1	A	502	PHE	2.7
1	A	582	LEU	2.7
2	B	26	TRP	2.7
1	A	174	THR	2.7
1	A	313	THR	2.7
1	A	578	THR	2.7
2	B	21	GLU	2.6
1	A	297	ASP	2.6
1	A	584	GLU	2.6
1	A	296	ASP	2.6
1	A	903	GLU	2.5
1	A	904	VAL	2.5
1	A	413	ARG	2.5
1	A	501	ASP	2.5
1	A	33	GLY	2.5
1	A	328	ASP	2.4
1	A	57	GLY	2.4
2	B	2	SER	2.4
1	A	808	SER	2.4
1	A	391	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	416	GLU	2.4
1	A	594	ASP	2.4
2	B	31	ASP	2.4
1	A	830	SER	2.4
1	A	659	HIS	2.4
1	A	887	ARG	2.3
2	B	39	VAL	2.3
1	A	875	GLU	2.3
1	A	173	SER	2.3
1	A	265	THR	2.3
1	A	760	ARG	2.3
2	B	8	ASP	2.3
1	A	472	ASP	2.3
1	A	847	GLN	2.3
1	A	739	VAL	2.3
1	A	729	GLN	2.2
1	A	470	ASP	2.2
1	A	545	SER	2.2
1	A	740	ARG	2.2
1	A	390	GLY	2.2
1	A	832	HIS	2.2
2	B	7	ASP	2.2
1	A	111	CYS	2.2
1	A	147	THR	2.2
1	A	151	THR	2.2
1	A	46	GLN	2.1
1	A	789	GLY	2.1
1	A	581	CYS	2.1
1	A	487	MET	2.1
2	B	53	GLU	2.1
1	A	583	LYS	2.1
1	A	787	ASN	2.1
1	A	895	LYS	2.1
1	A	84	ARG	2.1
2	B	59	MET	2.1
1	A	841	VAL	2.1
1	A	431	ARG	2.1
1	A	730	PRO	2.0
1	A	900	ARG	2.0
1	A	156	THR	2.0
1	A	746	SER	2.0
1	A	702	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

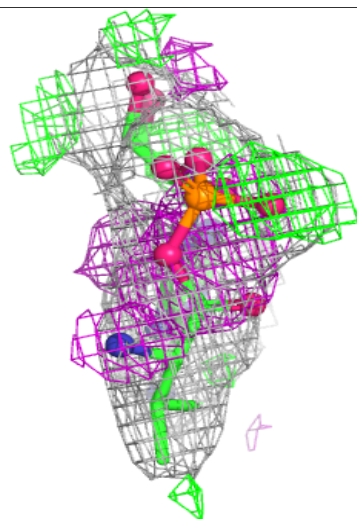
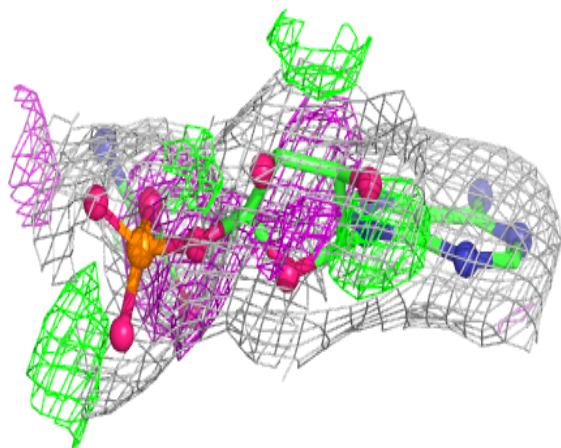
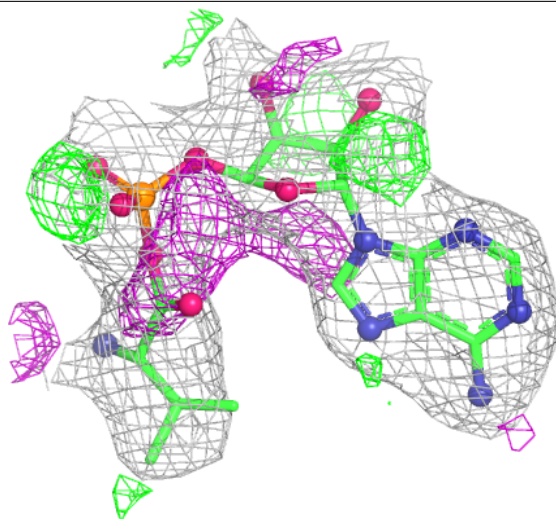
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

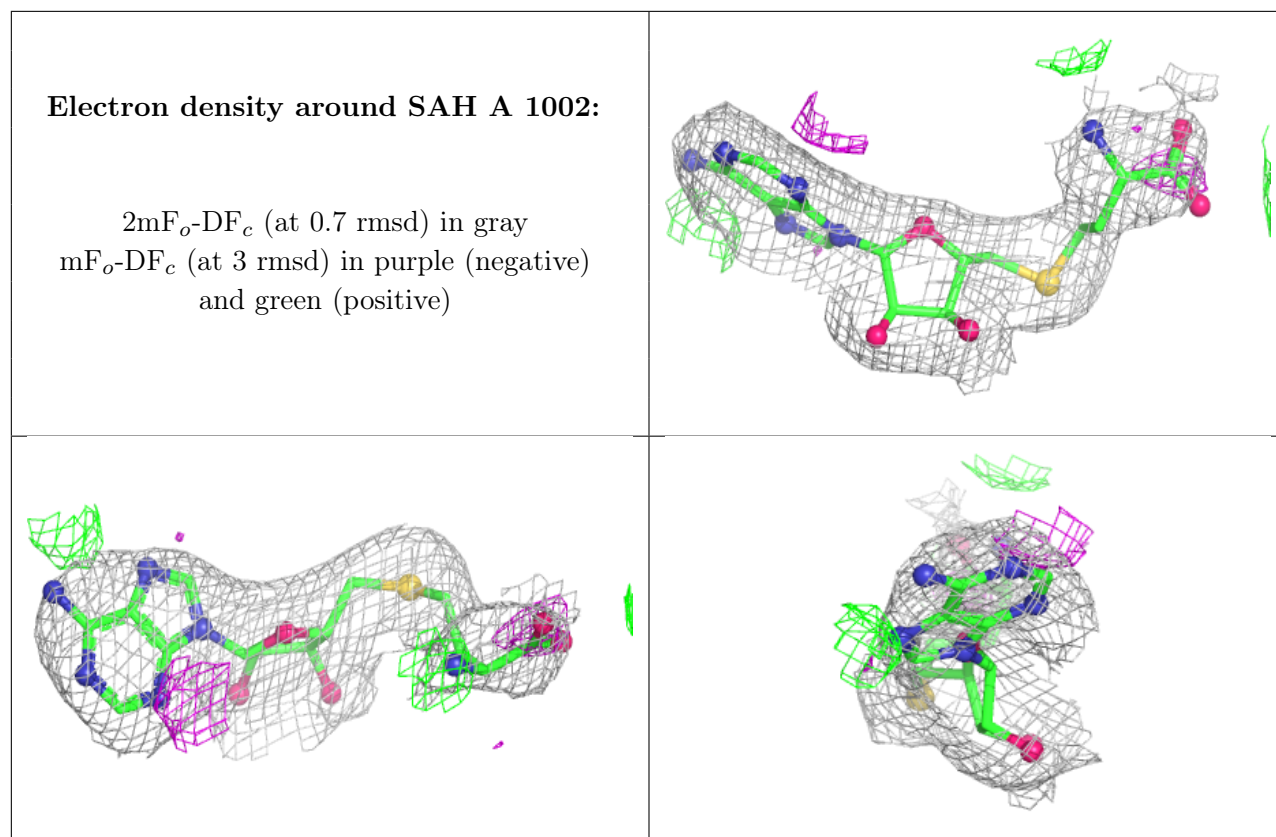
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	A	1005	1/1	0.84	0.15	97,97,97,97	0
6	CA	A	1007	1/1	0.85	0.11	117,117,117,117	0
3	B6G	A	1001	29/29	0.92	0.14	62,65,78,79	0
4	SAH	A	1002	26/26	0.95	0.12	73,76,96,99	0
5	CL	A	1004	1/1	0.95	0.14	95,95,95,95	0
6	CA	A	1006	1/1	0.96	0.13	78,78,78,78	0
6	CA	A	1008	1/1	0.96	0.11	84,84,84,84	0
5	CL	A	1003	1/1	0.98	0.10	89,89,89,89	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 B6G A 1001:

$2mF_o-DF_c$ (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.