



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:47 am BST

PDB ID : 4AZV / pdb\_00004azv  
Title : Co-crystal structure of WbdD and kinase inhibitor GW435821x.  
Authors : Hagelueken, G.; Huang, H.; Naismith, J.H.  
Deposited on : 2012-06-26  
Resolution : 3.29 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

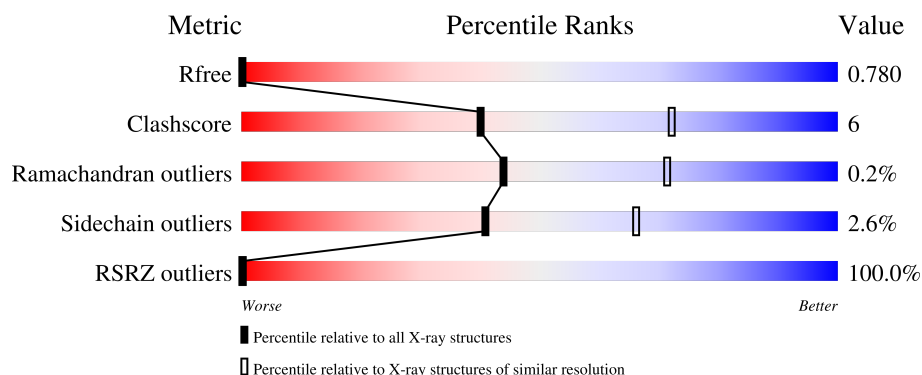
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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  $\geq 3$ , 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	569	

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
3	SO4	A	1475	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1476	-	-	-	X
3	SO4	A	1477	-	-	X	X
3	SO4	A	1478	-	-	X	-
4	CL	A	1479	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7251 atoms, of which 3563 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.

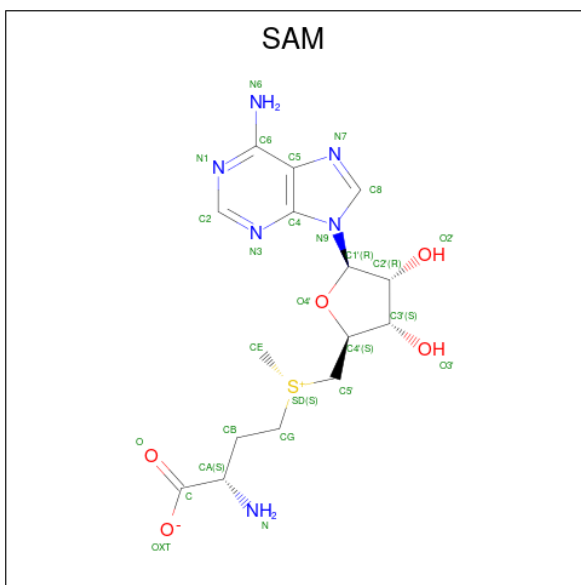
- Molecule 1 is a protein called WBDD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	442	7185	2346	3545	619	665	10	0	7	0

There are 18 discrepancies between the modelled and reference sequences:

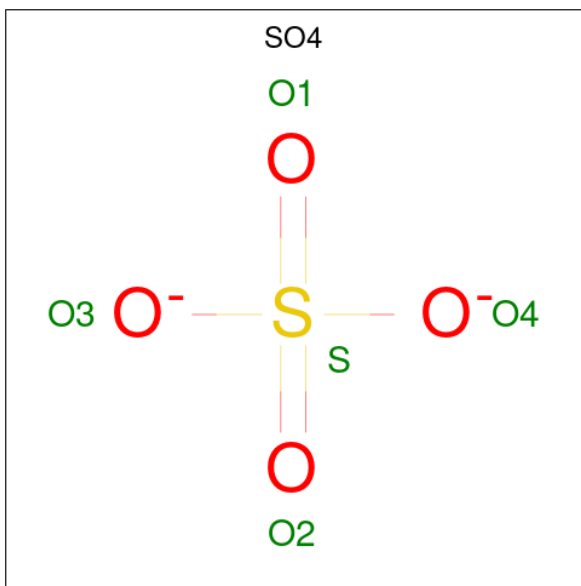
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q47592
A	-11	HIS	-	expression tag	UNP Q47592
A	-10	HIS	-	expression tag	UNP Q47592
A	-9	HIS	-	expression tag	UNP Q47592
A	-8	HIS	-	expression tag	UNP Q47592
A	-7	HIS	-	expression tag	UNP Q47592
A	-6	HIS	-	expression tag	UNP Q47592
A	-5	GLU	-	expression tag	UNP Q47592
A	-4	ASN	-	expression tag	UNP Q47592
A	-3	LEU	-	expression tag	UNP Q47592
A	-2	TYR	-	expression tag	UNP Q47592
A	-1	PHE	-	expression tag	UNP Q47592
A	0	GLN	-	expression tag	UNP Q47592
A	1	GLY	-	expression tag	UNP Q47592
A	168	PHE	LEU	conflict	UNP Q47592
A	273	TYR	HIS	conflict	UNP Q47592
A	440	VAL	ALA	conflict	UNP Q47592
A	480	VAL	GLY	conflict	UNP Q47592

- 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	H	N	O	S	0	0
			45	15	18	6	5	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.32Å 159.32Å 159.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.66 – 3.29 112.66 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (112.66-3.29) 97.0 (112.66-3.29)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.13 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.223 , 0.265 0.782 , 0.780	Depositor DCC
$R_{free}$ test set	266 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.207 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.48	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, SAM, SO4

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	0.40	0/3759	0.63	0/5108

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	460	GLY	Peptide

### 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	3640	3545	3530	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	18	22	5	0
3	A	20	0	0	20	4
4	A	1	0	0	0	0
All	All	3688	3563	3552	47	4

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 6.

All (47) 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:168:PHE:HB3	3:A:1477:SO4:O3	1.60	1.00
1:A:169:TYR:O	1:A:172:VAL:HG22	1.67	0.92
1:A:168:PHE:HA	3:A:1477:SO4:O1	1.72	0.89
1:A:168:PHE:CB	3:A:1477:SO4:O3	2.22	0.82
1:A:169:TYR:HD1	3:A:1477:SO4:S	2.06	0.79
1:A:168:PHE:HB3	3:A:1477:SO4:S	2.24	0.78
1:A:169:TYR:HD1	3:A:1477:SO4:O2	1.69	0.75
1:A:168:PHE:CA	3:A:1477:SO4:S	2.77	0.73
1:A:168:PHE:HA	3:A:1477:SO4:S	2.29	0.71
1:A:328:ARG:HB2	3:A:1478:SO4:O1	1.90	0.71
1:A:33:CYS:HA	3:A:1475:SO4:O2	1.91	0.70
1:A:169:TYR:CD1	3:A:1477:SO4:O2	2.52	0.61
1:A:168:PHE:CB	3:A:1477:SO4:S	2.87	0.61
1:A:33:CYS:N	3:A:1475:SO4:O2	2.35	0.59
1:A:169:TYR:CD1	3:A:1477:SO4:S	2.94	0.58
1:A:78:ILE:C	1:A:78:ILE:HD12	2.25	0.57
1:A:169:TYR:HB3	3:A:1477:SO4:O4	2.04	0.57
1:A:252:LYS:HE3	1:A:308:MET:CE	2.35	0.56
1:A:328:ARG:NH2	3:A:1478:SO4:O4	2.38	0.56
1:A:37:LEU:O	1:A:41:THR:HG23	2.06	0.55
1:A:33:CYS:CA	3:A:1475:SO4:O2	2.56	0.54
1:A:109[A]:ARG:HA	2:A:1474:SAM:N1	2.24	0.53
1:A:252:LYS:HE3	1:A:308:MET:HE2	1.91	0.52
1:A:169:TYR:CD1	3:A:1477:SO4:O3	2.65	0.48
1:A:168:PHE:CA	3:A:1477:SO4:O1	2.55	0.47
1:A:109[B]:ARG:HA	2:A:1474:SAM:N1	2.28	0.47
1:A:416:PHE:N	1:A:464:GLN:OE1	2.47	0.47
1:A:246:GLY:HA3	1:A:249:TYR:CE2	2.50	0.47
1:A:348:TRP:CE3	1:A:382:TRP:CZ3	3.04	0.45
1:A:48:SER:HA	1:A:55:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:205:MET:HA	2.17	0.44
1:A:110:ILE:HG13	2:A:1474:SAM:C2	2.48	0.44
1:A:155:GLN:OE1	1:A:212:ARG:HD2	2.17	0.43
1:A:169:TYR:CB	3:A:1477:SO4:O4	2.66	0.43
1:A:467:ILE:HA	1:A:470:GLU:HB2	2.01	0.43
1:A:467:ILE:O	1:A:471:THR:N	2.46	0.42
1:A:391:PHE:HZ	1:A:429:VAL:HG11	1.84	0.42
1:A:426:LEU:HD12	1:A:430:TRP:CD1	2.54	0.42
1:A:32:ASP:O	1:A:33:CYS:HB2	2.20	0.42
1:A:348:TRP:CE3	1:A:382:TRP:CH2	3.08	0.42
1:A:348:TRP:CZ3	1:A:382:TRP:HZ3	2.38	0.41
1:A:433:PRO:HG2	1:A:436:ARG:HD3	2.02	0.41
1:A:460:GLY:HA3	1:A:461:ALA:HA	1.87	0.41
1:A:108:GLY:O	2:A:1474:SAM:H2	2.21	0.41
1:A:462:THR:O	1:A:463:GLU:C	2.59	0.41
1:A:426:LEU:HD12	1:A:430:TRP:HD1	1.85	0.40
1:A:82:ASP:OD1	2:A:1474:SAM:O2'	2.38	0.40

All (4) 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:1477:SO4:O1	3:A:1477:SO4:O2[10_555]	2.02	0.18
3:A:1477:SO4:O4	3:A:1477:SO4:O4[7_555]	2.07	0.13
3:A:1477:SO4:O2	3:A:1477:SO4:O4[7_555]	2.13	0.07
3:A:1477:SO4:O1	3:A:1477:SO4:O1[7_555]	2.14	0.06

## 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	441/569 (78%)	427 (97%)	13 (3%)	1 (0%)	44 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	GLY

### 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	390/486 (80%)	380 (97%)	10 (3%)	41	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	PHE
1	A	193	GLU
1	A	381	SER
1	A	395	ASN
1	A	416	PHE
1	A	426	LEU
1	A	441	LEU
1	A	459	ARG
1	A	462	THR
1	A	463	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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$
3	SO4	A	1476	-	4,4,4	0.44	0	6,6,6	0.26	0
3	SO4	A	1475	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	A	1478	-	4,4,4	0.35	0	6,6,6	0.47	0
2	SAM	A	1474	-	24,29,29	1.18	4 (16%)	23,42,42	1.94	4 (17%)
3	SO4	A	1477	1	4,4,4	0.97	0	6,6,6	1.59	1 (16%)

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	1474	-	-	2/12/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1474	SAM	C2-N3	3.10	1.37	1.32
2	A	1474	SAM	OXT-C	-2.31	1.23	1.30
2	A	1474	SAM	O4'-C4'	-2.05	1.40	1.45
2	A	1474	SAM	C2-N1	2.02	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1474	SAM	N3-C2-N1	-6.45	118.60	128.68
2	A	1474	SAM	OXT-C-O	-4.23	114.49	124.09
2	A	1474	SAM	C2-N1-C6	2.77	123.48	118.75
2	A	1474	SAM	OXT-C-CA	2.60	122.25	113.38
3	A	1477	SO4	O3-S-O1	2.42	121.96	109.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

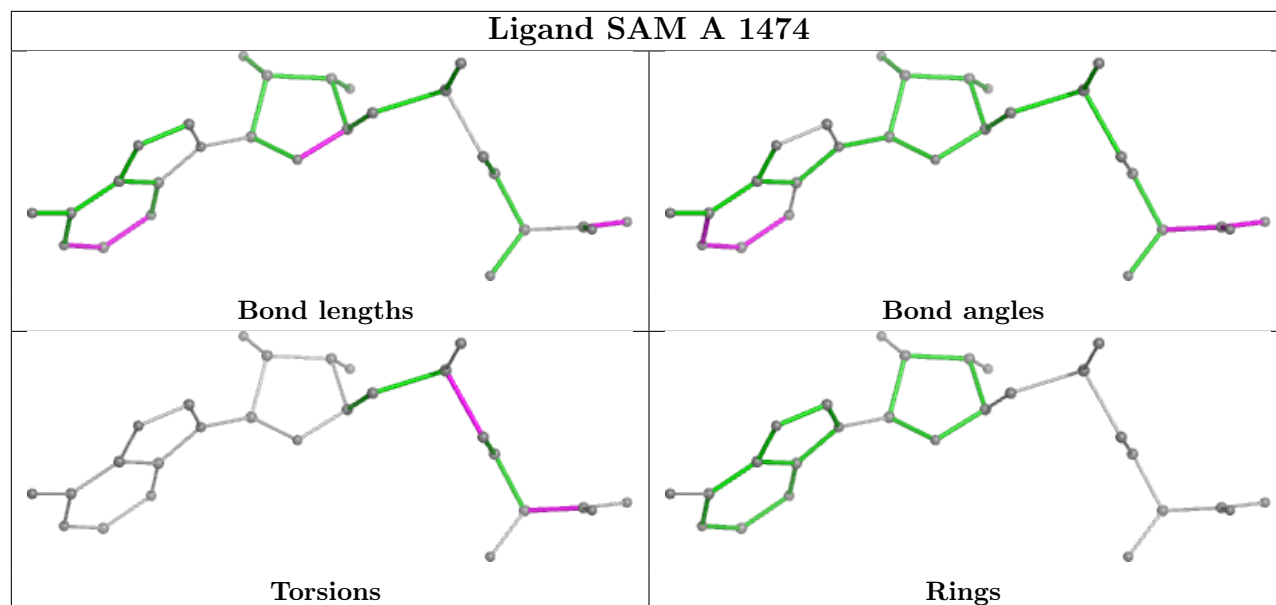
Mol	Chain	Res	Type	Atoms
2	A	1474	SAM	CB-CG-SD-C5'
2	A	1474	SAM	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1475	SO4	3	0
3	A	1478	SO4	2	0
2	A	1474	SAM	5	0
3	A	1477	SO4	15	4

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/569 (77%)	6.75	442 (100%) 0 0	52, 101, 145, 213	7 (1%)

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	16.7
1	A	452	LEU	13.3
1	A	100	ASP	12.7
1	A	34	ASN	12.6
1	A	43	GLN	12.1
1	A	327	ASP	12.0
1	A	195	ASP	12.0
1	A	274	GLU	11.9
1	A	469	GLN	11.7
1	A	69	LEU	11.7
1	A	316	LEU	11.6
1	A	284	GLN	11.5
1	A	433	PRO	11.3
1	A	244	PHE	11.3
1	A	107	VAL	11.3
1	A	259	PRO	11.3
1	A	352	VAL	11.2
1	A	200	PRO	11.1
1	A	229	PRO	11.0
1	A	427	TYR	10.9
1	A	375	THR	10.9
1	A	15	ILE	10.8
1	A	294	VAL	10.7
1	A	161	LEU	10.6
1	A	296	ALA	10.5
1	A	386	LEU	10.5
1	A	44	TYR	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	87	ASN	10.4
1	A	55	LEU	10.4
1	A	208	VAL	10.4
1	A	198	LEU	10.3
1	A	315	LEU	10.2
1	A	302	GLN	10.1
1	A	292	PRO	10.1
1	A	456	GLU	10.1
1	A	128	LEU	10.1
1	A	37	LEU	10.0
1	A	323	GLY	10.0
1	A	342	LEU	10.0
1	A	64	GLN	9.9
1	A	156	ALA	9.8
1	A	228	GLN	9.7
1	A	371	GLY	9.7
1	A	99	PRO	9.7
1	A	426	LEU	9.7
1	A	153	VAL	9.7
1	A	217	ASP	9.7
1	A	26	ASP	9.6
1	A	182	ILE	9.5
1	A	124	LEU	9.5
1	A	265	ALA	9.5
1	A	102	ALA	9.5
1	A	103	ALA	9.4
1	A	113	VAL	9.3
1	A	175	PRO	9.3
1	A	70	SER	9.3
1	A	60	LEU	9.3
1	A	9	VAL	9.3
1	A	270	ARG	9.2
1	A	230	TYR	9.2
1	A	32	ASP	9.2
1	A	299	GLU	9.1
1	A	214	LEU	9.1
1	A	453	PRO	9.1
1	A	159	LEU	9.1
1	A	305	TRP	9.0
1	A	347	PHE	8.9
1	A	442	LEU	8.9
1	A	464	GLN	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	8.9
1	A	370	PHE	8.9
1	A	19	ILE	8.8
1	A	180	GLU	8.8
1	A	465	TRP	8.8
1	A	278[A]	GLU	8.8
1	A	372	SER	8.8
1	A	377	PRO	8.8
1	A	248	ASP	8.8
1	A	170	TRP	8.8
1	A	212	ARG	8.7
1	A	309	GLU	8.6
1	A	204	PRO	8.6
1	A	196	THR	8.5
1	A	116	ALA	8.5
1	A	8	LEU	8.5
1	A	422	TRP	8.5
1	A	109[A]	ARG	8.4
1	A	227	ASN	8.4
1	A	202	PRO	8.4
1	A	28	ASP	8.4
1	A	59	ASP	8.3
1	A	167	PRO	8.3
1	A	31	ARG	8.3
1	A	143	VAL	8.3
1	A	220	GLN	8.3
1	A	467	ILE	8.3
1	A	345	GLN	8.2
1	A	145	ARG	8.1
1	A	183	GLU	8.1
1	A	216	ASN	8.1
1	A	176	ASP	8.1
1	A	295	LEU	8.1
1	A	105	PHE	8.1
1	A	165	GLU	8.0
1	A	317	SER	8.0
1	A	417	ASN	8.0
1	A	310	LYS	8.0
1	A	76	ALA	8.0
1	A	384	THR	7.9
1	A	382	TRP	7.9
1	A	147	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	330	LYS	7.9
1	A	221	PRO	7.9
1	A	398	PHE	7.9
1	A	430	TRP	7.9
1	A	226	GLN	7.9
1	A	89	ASN	7.9
1	A	260	HIS	7.9
1	A	328	ARG	7.8
1	A	30	ALA	7.8
1	A	346	GLY	7.8
1	A	61	GLY	7.8
1	A	137	LEU	7.7
1	A	215	ILE	7.7
1	A	257	ASP	7.7
1	A	41	THR	7.7
1	A	449	LYS	7.7
1	A	6	ASN	7.7
1	A	395	ASN	7.7
1	A	188	TYR	7.7
1	A	472	VAL	7.6
1	A	348	TRP	7.6
1	A	110	ILE	7.6
1	A	130	VAL	7.6
1	A	118	GLU	7.5
1	A	258	MET	7.5
1	A	121	GLU	7.5
1	A	364[A]	HIS	7.5
1	A	24	GLU	7.5
1	A	75	GLY	7.5
1	A	144	LYS	7.5
1	A	337	ARG	7.5
1	A	218	PHE	7.5
1	A	349	HIS	7.5
1	A	367	LEU	7.4
1	A	436	ARG	7.4
1	A	250	VAL	7.4
1	A	160	GLU	7.4
1	A	186	ALA	7.4
1	A	326	ILE	7.4
1	A	136	HIS	7.3
1	A	225	TRP	7.3
1	A	253	PHE	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	ALA	7.3
1	A	131	PHE	7.3
1	A	190	LEU	7.3
1	A	441	LEU	7.3
1	A	54	PRO	7.2
1	A	446	PHE	7.2
1	A	461	ALA	7.2
1	A	14	GLU	7.2
1	A	86	GLU	7.2
1	A	470	GLU	7.2
1	A	381	SER	7.2
1	A	473	LEU	7.2
1	A	256	TYR	7.2
1	A	435	GLU	7.2
1	A	300	ASN	7.2
1	A	451	LYS	7.2
1	A	276	HIS	7.2
1	A	166	GLU	7.1
1	A	16	TYR	7.1
1	A	4	ASP	7.1
1	A	353	ARG	7.1
1	A	264	THR	7.1
1	A	459	ARG	7.1
1	A	157	VAL	7.0
1	A	199	SER	7.0
1	A	458	GLN	7.0
1	A	286	PRO	7.0
1	A	11	GLU	7.0
1	A	421	PRO	7.0
1	A	219	ASN	7.0
1	A	46	ASN	7.0
1	A	51	LEU	6.9
1	A	119	GLU	6.9
1	A	57	VAL	6.9
1	A	254	PHE	6.9
1	A	416	PHE	6.9
1	A	162	ALA	6.9
1	A	209	SER	6.9
1	A	287	ALA	6.9
1	A	141	ASP	6.9
1	A	318	ASP	6.9
1	A	425	TRP	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	241	ARG	6.8
1	A	273	TYR	6.8
1	A	40	ILE	6.8
1	A	262	ILE	6.8
1	A	50	ALA	6.8
1	A	289	PHE	6.8
1	A	206	TYR	6.8
1	A	320	LEU	6.8
1	A	210	ASN	6.8
1	A	58	LEU	6.8
1	A	396	GLU	6.8
1	A	185	CYS	6.7
1	A	397	LEU	6.7
1	A	269	GLN	6.7
1	A	366	ARG	6.7
1	A	288	GLY	6.7
1	A	252	LYS	6.7
1	A	73	SER	6.7
1	A	91	CYS	6.7
1	A	49	ARG	6.7
1	A	471	THR	6.7
1	A	385	ASN	6.7
1	A	65	GLY	6.6
1	A	437	TRP	6.6
1	A	42[A]	GLU	6.6
1	A	112	GLU	6.6
1	A	207	LEU	6.6
1	A	267	GLU	6.6
1	A	263	LEU	6.5
1	A	148	SER	6.5
1	A	297	HIS	6.5
1	A	243	TYR	6.5
1	A	360	ASP	6.5
1	A	5	LEU	6.5
1	A	266	GLU	6.5
1	A	171	GLY	6.4
1	A	201	VAL	6.4
1	A	140	ILE	6.4
1	A	432	GLU	6.4
1	A	56	ASN	6.4
1	A	17	GLN	6.4
1	A	341	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	77	THR	6.4
1	A	344	LYS	6.4
1	A	336	LEU	6.3
1	A	68	SER	6.3
1	A	369	ASP	6.3
1	A	443	LEU	6.3
1	A	376	THR	6.2
1	A	332	LEU	6.2
1	A	127	GLY	6.2
1	A	138	HIS	6.1
1	A	35	GLN	6.1
1	A	23	PRO	6.1
1	A	340	ALA	6.1
1	A	203	ARG	6.1
1	A	368	ILE	6.1
1	A	82	ASP	6.1
1	A	308	MET	6.1
1	A	117	LEU	6.1
1	A	293	ALA	6.1
1	A	290	ASP	6.0
1	A	22	HIS	6.0
1	A	325	GLU	6.0
1	A	447	GLU	6.0
1	A	197	HIS	6.0
1	A	434	VAL	6.0
1	A	18	THR	6.0
1	A	312	PRO	6.0
1	A	224	HIS	6.0
1	A	134	ILE	5.9
1	A	350	ASP	6.0
1	A	97	GLU	5.9
1	A	10	SER	5.9
1	A	155	GLN	5.9
1	A	383	PRO	5.9
1	A	133	HIS	5.9
1	A	20	PHE	5.9
1	A	338	SER	5.9
1	A	223[A]	GLN	5.9
1	A	361	ALA	5.8
1	A	181	LEU	5.8
1	A	187	PHE	5.8
1	A	93	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	164	LYS	5.8
1	A	111	GLU	5.8
1	A	192	GLY	5.8
1	A	104[A]	GLU	5.8
1	A	193	GLU	5.8
1	A	169	TYR	5.8
1	A	457	GLN	5.8
1	A	36	ARG	5.7
1	A	324	GLU	5.7
1	A	45	ASP	5.7
1	A	356	ASN	5.7
1	A	387	VAL	5.7
1	A	96	GLU	5.7
1	A	285	PRO	5.7
1	A	27	GLY	5.7
1	A	363	GLN	5.7
1	A	468	ALA	5.7
1	A	255	TYR	5.7
1	A	25	TRP	5.7
1	A	239	ARG	5.6
1	A	66	PHE	5.6
1	A	12	LEU	5.6
1	A	7	THR	5.6
1	A	420	GLN	5.5
1	A	189	ARG	5.5
1	A	48	SER	5.5
1	A	268	SER	5.5
1	A	174	GLN	5.5
1	A	122	PHE	5.5
1	A	90	VAL	5.5
1	A	158	ILE	5.5
1	A	438	ASN	5.5
1	A	172	VAL	5.5
1	A	240	SER	5.4
1	A	429	VAL	5.4
1	A	277	ASN	5.4
1	A	81	ILE	5.4
1	A	74	LYS	5.4
1	A	106	ARG	5.4
1	A	335	LEU	5.4
1	A	450	ALA	5.4
1	A	129	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLU	5.3
1	A	334	SER	5.3
1	A	357	VAL	5.3
1	A	213	VAL	5.3
1	A	463	GLU	5.3
1	A	178	PRO	5.2
1	A	168	PHE	5.2
1	A	393	PHE	5.2
1	A	358	MET	5.2
1	A	431	GLN	5.2
1	A	154	THR	5.2
1	A	13	PRO	5.2
1	A	339	LEU	5.2
1	A	114	ILE	5.1
1	A	247	GLU	5.1
1	A	150	LEU	5.1
1	A	359	VAL	5.1
1	A	439	PHE	5.1
1	A	29	ALA	5.1
1	A	98	ASN	5.1
1	A	184	GLN	5.1
1	A	307	VAL	5.1
1	A	246	GLY	5.1
1	A	355	TRP	5.1
1	A	211	HIS	5.1
1	A	391	PHE	5.0
1	A	142	GLU	5.0
1	A	47	LEU	5.0
1	A	418	LEU	5.0
1	A	281	PHE	5.0
1	A	83	PHE	5.0
1	A	313	GLY	5.0
1	A	249	TYR	4.9
1	A	298	GLY	4.9
1	A	152	ASP	4.9
1	A	306	LEU	4.9
1	A	314	ARG	4.9
1	A	67	PHE	4.9
1	A	311	LEU	4.9
1	A	362	ARG	4.9
1	A	38	ASP	4.9
1	A	283	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	CYS	4.9
1	A	390	PHE	4.8
1	A	448	LYS	4.8
1	A	101	PHE	4.8
1	A	394	VAL	4.8
1	A	423	SER	4.8
1	A	351	ASP	4.8
1	A	466	ILE	4.8
1	A	275	LEU	4.7
1	A	123	ASP	4.7
1	A	120	GLY	4.7
1	A	271	ASN	4.7
1	A	53	ARG	4.6
1	A	424	ASN	4.6
1	A	132	HIS	4.6
1	A	454	SER	4.6
1	A	279	ILE	4.6
1	A	78	ILE	4.5
1	A	354	PRO	4.5
1	A	205	MET	4.5
1	A	303	SER	4.5
1	A	194	PHE	4.4
1	A	125	ALA	4.4
1	A	173	SER	4.4
1	A	282	LEU	4.4
1	A	374	VAL	4.4
1	A	455	ALA	4.4
1	A	440	VAL	4.4
1	A	135	VAL	4.3
1	A	301	ALA	4.3
1	A	88	ILE	4.3
1	A	222	PHE	4.3
1	A	419	PRO	4.3
1	A	126	ILE	4.3
1	A	389	SER	4.3
1	A	79	VAL	4.3
1	A	85	GLN	4.3
1	A	146	LEU	4.3
1	A	365	ALA	4.2
1	A	388	GLN	4.2
1	A	272[A]	LYS	4.2
1	A	331	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	242	ARG	4.1
1	A	33	CYS	4.0
1	A	191	ILE	4.0
1	A	80	GLY	3.9
1	A	63	ALA	3.9
1	A	343	GLU	3.9
1	A	163	VAL	3.9
1	A	139	GLY	3.9
1	A	322	ALA	3.9
1	A	444	ALA	3.9
1	A	84	GLN	3.8
1	A	95	ALA	3.8
1	A	428	ALA	3.8
1	A	21	GLY	3.7
1	A	52	GLY	3.7
1	A	319	MET	3.7
1	A	72	ALA	3.6
1	A	251	CYS	3.6
1	A	280	LYS	3.5
1	A	39	LEU	3.5
1	A	108	GLY	3.5
1	A	304	GLY	3.5
1	A	94	LEU	3.5
1	A	445	LEU	3.4
1	A	115	ALA	3.4
1	A	333	GLY	3.3
1	A	462	THR	3.3
1	A	151	ALA	3.3
1	A	261	GLY	3.3
1	A	373	ILE	3.3
1	A	149	ARG	3.2
1	A	321	ALA	3.2
1	A	92	ARG	3.1
1	A	245	PHE	2.9
1	A	179	ARG	2.7
1	A	71	LEU	2.7
1	A	392	VAL	2.4

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

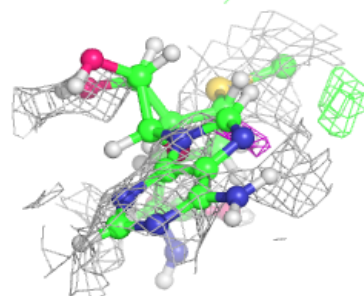
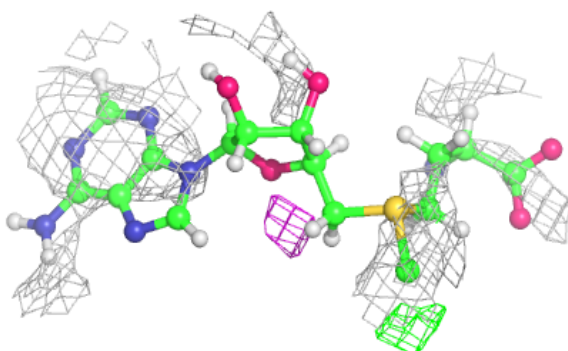
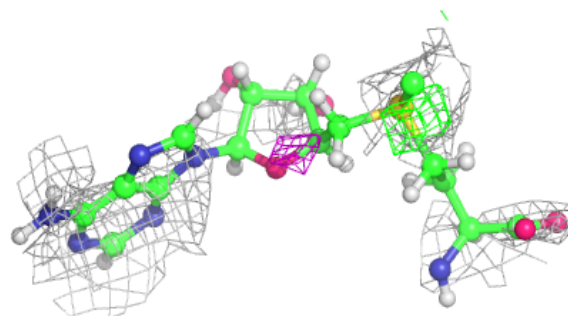
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	SO4	A	1477	5/5	0.15	0.49	85,85,85,85	0
3	SO4	A	1478	5/5	0.21	0.37	85,85,85,85	0
2	SAM	A	1474	27/27	0.25	0.39	73,78,85,97	0
3	SO4	A	1476	5/5	0.26	0.62	85,85,85,85	0
3	SO4	A	1475	5/5	0.53	0.29	85,85,85,85	0
4	CL	A	1479	1/1	0.69	0.52	85,85,85,85	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 A 1474:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.