



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:27 AM UTC

PDB ID : 4EQL / pdb\_00004eql  
Title : Crystal Structure of GH3.12 in complex with AMP and salicylate  
Authors : Westfall, C.; Zubieta, C.; Nanao, M.; Herrmann, J.; Jez, J.  
Deposited on : 2012-04-19  
Resolution : 1.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

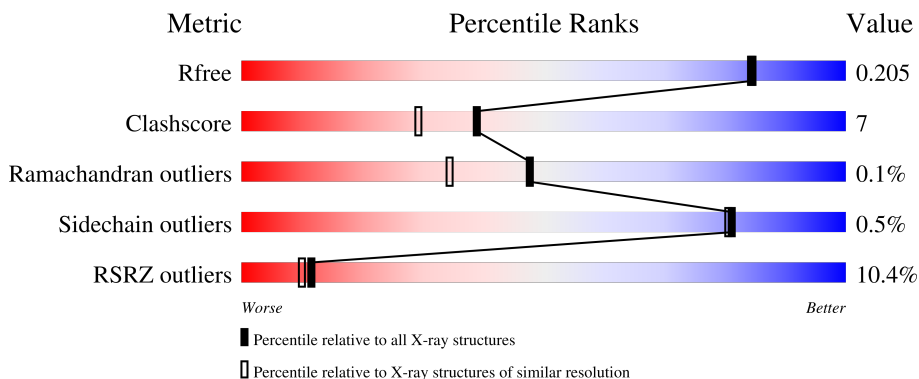
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	581	
1	B	581	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9066 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 4-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3966	2525	642	773	26	0	10	0
1	B	479	3863	2464	626	747	26	0	9	0

There are 12 discrepancies between the modelled and reference sequences:

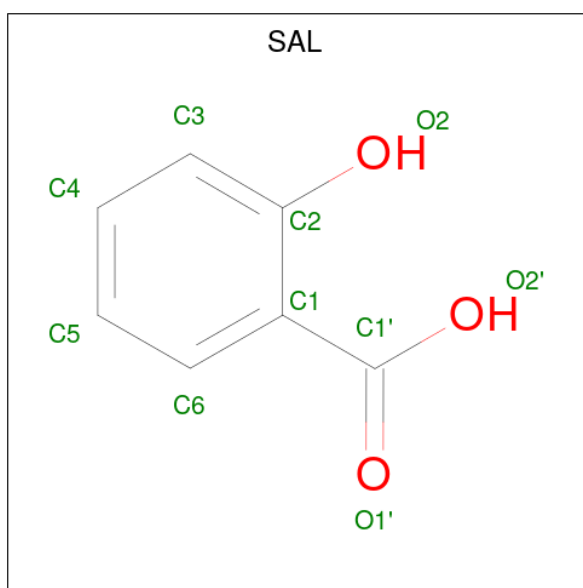
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9LYU4
A	-4	SER	-	expression tag	UNP Q9LYU4
A	-3	HIS	-	expression tag	UNP Q9LYU4
A	-2	MET	-	expression tag	UNP Q9LYU4
A	-1	ALA	-	expression tag	UNP Q9LYU4
A	0	SER	-	expression tag	UNP Q9LYU4
B	-5	GLY	-	expression tag	UNP Q9LYU4
B	-4	SER	-	expression tag	UNP Q9LYU4
B	-3	HIS	-	expression tag	UNP Q9LYU4
B	-2	MET	-	expression tag	UNP Q9LYU4
B	-1	ALA	-	expression tag	UNP Q9LYU4
B	0	SER	-	expression tag	UNP Q9LYU4

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	594	Total 594	O 594	0	0
4	B	577	Total 577	O 577	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.42Å 66.58Å 101.00Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	50.28 – 1.80 50.28 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.28-1.80) 98.8 (50.28-1.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.80Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.177 , 0.205 0.176 , 0.205	Depositor DCC
$R_{free}$ test set	5313 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, SAL

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	0.48	0/4078	0.72	1/5529 (0.0%)
1	B	0.56	3/3972 (0.1%)	0.73	0/5380
All	All	0.52	3/8050 (0.0%)	0.73	1/10909 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	LEU	C-N	-9.21	1.21	1.33
1	B	281	SER	C-O	-5.53	1.17	1.23
1	B	279	GLN	CA-C	-5.42	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	VAL	CB-CA-C	-5.42	103.49	112.26

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	3966	0	3901	54	2
1	B	3863	0	3823	61	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	12	2	0
2	B	23	0	12	1	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
4	A	594	0	0	18	0
4	B	577	0	0	24	0
All	All	9066	0	7758	107	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 7.

All (107) 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:571:LYS:N	4:A:1223:HOH:O	1.88	1.05
1:A:39:LYS:HA	1:A:44[B]:GLN:HE21	1.28	0.96
1:B:275:GLU:OE1	4:B:1031:HOH:O	1.91	0.87
1:B:574:SER:O	1:B:575:ILE:HB	1.75	0.86
1:B:100:GLY:HA3	4:B:1219:HOH:O	1.77	0.85
1:B:87[B]:ARG:NH1	4:B:1098:HOH:O	2.12	0.83
1:B:128[B]:THR:CG2	1:B:177:TRP:CZ2	2.65	0.79
1:B:570:ALA:N	4:B:1172:HOH:O	2.16	0.78
1:A:49:ASP:HB3	4:A:1063:HOH:O	1.83	0.77
1:B:128[B]:THR:HG23	1:B:177:TRP:CZ2	2.20	0.77
1:A:44[B]:GLN:NE2	4:A:1160:HOH:O	2.18	0.76
1:A:132:LYS:HE3	4:A:1088:HOH:O	1.91	0.70
1:B:288:ARG:NH1	4:B:760:HOH:O	2.23	0.70
1:B:87[B]:ARG:HG3	1:B:87[B]:ARG:HH11	1.57	0.69
1:A:310:MET:HE2	1:A:310:MET:HA	1.75	0.68
1:B:99:SER:HB2	4:B:1211:HOH:O	1.95	0.67
1:B:87[B]:ARG:CZ	4:B:1098:HOH:O	2.41	0.67
1:B:360:PRO:O	1:B:361:MET:HE2	1.96	0.65
1:A:132:LYS:HB3	4:A:1015:HOH:O	1.99	0.63
1:A:280:ASN:ND2	4:A:814:HOH:O	2.32	0.63
1:A:488:GLU:HB2	1:B:152:PRO:HA	1.81	0.63
1:B:87[B]:ARG:NH1	1:B:87[B]:ARG:HG3	2.15	0.62
1:B:130:HIS:HE1	4:B:728:HOH:O	1.83	0.62
1:B:68:ILE:HD11	1:B:394:MET:HE1	1.81	0.62
1:A:499:LEU:HD21	1:B:510:LYS:CD	2.31	0.61
1:A:387:ASN:HB2	4:A:1197:HOH:O	2.01	0.60
1:A:438:VAL:HG12	1:A:438:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HG2	1:B:388:PHE:CG	2.38	0.59
1:B:53:LYS:HE2	1:B:57:LYS:HE2	1.84	0.59
1:A:39:LYS:HA	1:A:44[B]:GLN:NE2	2.08	0.59
1:A:81[B]:SER:HB2	1:A:89:ILE:HD12	1.86	0.58
1:A:39:LYS:HD3	1:A:44[B]:GLN:NE2	2.20	0.57
1:A:510:LYS:CD	1:B:499:LEU:HD21	2.33	0.57
1:B:329:GLU:OE2	4:B:1003:HOH:O	2.16	0.57
1:A:111:LYS:HE2	4:A:1134:HOH:O	2.04	0.57
1:A:135:GLU:HG3	4:A:842:HOH:O	2.05	0.57
1:B:49:ASP:HA	4:B:1087:HOH:O	2.03	0.56
1:B:99:SER:CB	4:B:1211:HOH:O	2.51	0.56
1:A:499:LEU:HD21	1:B:510:LYS:HD3	1.87	0.56
1:A:111:LYS:HG2	1:A:388:PHE:CG	2.41	0.55
1:A:130:HIS:HE1	4:A:793:HOH:O	1.90	0.55
1:A:233:TRP:HE1	1:B:247:ASN:ND2	2.04	0.55
1:B:128[B]:THR:HG23	1:B:177:TRP:HZ2	1.71	0.55
1:A:360:PRO:O	1:A:361:MET:HE2	2.08	0.54
1:B:288:ARG:NH1	4:B:1029:HOH:O	2.36	0.54
1:B:100:GLY:O	4:B:1219:HOH:O	2.19	0.53
1:A:175:SER:HB3	4:A:937:HOH:O	2.09	0.53
1:A:417:ARG:HD3	1:A:428:LYS:HD3	1.91	0.52
1:B:504:SER:C	4:B:1216:HOH:O	2.52	0.52
1:A:8:ASN:CG	1:A:9:GLU:H	2.17	0.52
1:A:494:LEU:HD13	1:A:572:PHE:CE2	2.46	0.50
1:A:44[B]:GLN:NE2	4:A:1139:HOH:O	2.45	0.50
1:A:492:GLU:HG3	4:B:1148:HOH:O	2.10	0.50
1:B:31:GLU:HG3	1:B:51:PHE:CD2	2.47	0.50
1:B:9:GLU:N	4:B:918:HOH:O	2.44	0.49
1:A:100:GLY:N	4:A:1292:HOH:O	2.28	0.49
1:B:224:ARG:HG3	1:B:464:PHE:CZ	2.47	0.49
1:A:39:LYS:HD3	1:A:44[B]:GLN:HE22	1.76	0.49
2:B:601:AMP:O3P	4:B:886:HOH:O	2.20	0.49
1:B:494:LEU:HD13	1:B:572:PHE:CE2	2.48	0.48
1:A:53:LYS:HE2	1:A:57:LYS:HE2	1.95	0.48
1:B:279:GLN:HG3	4:B:760:HOH:O	2.13	0.48
1:B:224:ARG:HG3	1:B:464:PHE:HZ	1.78	0.48
1:A:488:GLU:HG3	1:B:154:GLY:HA2	1.96	0.47
1:B:574:SER:HA	4:B:1260:HOH:O	2.14	0.47
1:B:87[B]:ARG:NH2	4:B:1098:HOH:O	2.47	0.47
1:A:417:ARG:NH2	4:A:1004:HOH:O	2.47	0.46
1:A:470:VAL:HG21	1:A:501:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE2	1:A:129:LYS:HE2	2.15	0.46
1:A:230:LYS:HE3	1:A:282:TRP:CD1	2.51	0.46
1:B:470:VAL:HG11	1:B:501:MET:HE1	1.98	0.46
1:B:111:LYS:HG2	1:B:388:PHE:CB	2.46	0.46
1:B:276:ILE:O	1:B:279:GLN:HG2	2.16	0.45
1:B:571:LYS:NZ	4:B:1225:HOH:O	2.48	0.45
1:B:111:LYS:HE2	4:B:1027:HOH:O	2.15	0.45
1:B:522:LEU:C	1:B:522:LEU:HD23	2.41	0.45
1:A:428:LYS:HE2	2:A:601:AMP:H4'	1.99	0.45
1:B:361:MET:HG3	1:B:399:ILE:HD12	1.98	0.44
1:A:40:THR:O	1:A:44[B]:GLN:HG2	2.18	0.44
1:A:69:LYS:N	1:A:70:PRO:CD	2.81	0.44
2:A:601:AMP:O2P	4:A:1267:HOH:O	2.21	0.44
1:B:128[B]:THR:HG21	1:B:177:TRP:CZ2	2.51	0.43
1:B:497:CYS:O	1:B:501:MET:HG3	2.17	0.43
1:A:175:SER:CB	4:A:937:HOH:O	2.66	0.43
1:A:233:TRP:HE1	1:B:247:ASN:HD22	1.66	0.43
1:A:438:VAL:O	1:A:438:VAL:CG1	2.63	0.42
1:A:510:LYS:NZ	1:B:499:LEU:HD21	2.34	0.42
1:B:241:ARG:HD3	4:B:1014:HOH:O	2.19	0.42
1:B:575:ILE:HD12	1:B:575:ILE:HA	1.92	0.42
1:B:274:GLU:O	1:B:278:ASN:HB2	2.20	0.42
1:A:310:MET:HE3	4:A:1183:HOH:O	2.19	0.42
1:B:53:LYS:HE3	1:B:355:TYR:OH	2.19	0.42
1:B:574:SER:O	1:B:575:ILE:CB	2.55	0.42
1:A:168:ASP:OD1	1:A:171:LYS:HE3	2.19	0.42
1:B:173:ARG:HB2	1:B:174:PRO:HD2	2.01	0.42
1:B:360:PRO:HG2	1:B:367:ASN:O	2.19	0.42
1:A:147:GLN:HG3	1:A:148:GLU:N	2.35	0.41
1:A:488:GLU:HB2	1:B:151:THR:O	2.20	0.41
1:B:69:LYS:N	1:B:70:PRO:CD	2.83	0.41
1:A:418:GLU:O	1:A:419:ASN:HB2	2.19	0.41
1:A:8:ASN:CG	1:A:9:GLU:N	2.78	0.41
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.93	0.41
1:B:100:GLY:CA	4:B:1219:HOH:O	2.50	0.41
1:A:247:ASN:ND2	1:B:233:TRP:HE1	2.19	0.41
1:A:213:ARG:NH1	1:A:297:GLU:OE1	2.45	0.40
1:B:173:ARG:HB2	1:B:174:PRO:CD	2.52	0.40
1:A:55:LEU:HD23	4:A:1056:HOH:O	2.22	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)
1:A:275:GLU:CD	1:B:280:ASN:OD1[2_545]	1.79	0.41
1:A:275:GLU:OE1	1:B:280:ASN:OD1[2_545]	1.88	0.32

### 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	496/581 (85%)	488 (98%)	8 (2%)	0	100	100
1	B	480/581 (83%)	470 (98%)	9 (2%)	1 (0%)	43	31
All	All	976/1162 (84%)	958 (98%)	17 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASN

#### 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	458/527 (87%)	457 (100%)	1 (0%)	87	87
1	B	448/527 (85%)	445 (99%)	3 (1%)	76	73
All	All	906/1054 (86%)	902 (100%)	4 (0%)	81	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	B	278	ASN
1	B	279	GLN
1	B	575	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	130	HIS
1	A	244	HIS
1	A	255	GLN
1	A	278	ASN
1	A	367	ASN
1	A	411	GLN
1	B	130	HIS
1	B	193	ASN
1	B	244	HIS
1	B	247	ASN
1	B	278	ASN
1	B	367	ASN
1	B	411	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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	AMP	A	601	-	25,25,25	1.35	4 (16%)	37,38,38	1.97	11 (29%)
3	SAL	B	602	-	10,10,10	0.76	0	13,13,13	1.03	1 (7%)
2	AMP	B	601	-	25,25,25	1.33	4 (16%)	37,38,38	1.83	8 (21%)
3	SAL	A	602	-	10,10,10	0.72	0	13,13,13	0.94	1 (7%)

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	AMP	A	601	-	-	5/10/26/26	0/3/3/3
3	SAL	B	602	-	-	0/4/4/4	0/1/1/1
2	AMP	B	601	-	-	5/10/26/26	0/3/3/3
3	SAL	A	602	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	AMP	C5-C4	4.22	1.46	1.39
2	B	601	AMP	C5-C4	4.21	1.46	1.39
2	A	601	AMP	C4-N9	-2.81	1.31	1.37
2	B	601	AMP	C5-C6	2.66	1.48	1.41
2	A	601	AMP	C8-N7	2.57	1.36	1.31
2	B	601	AMP	C8-N7	2.28	1.36	1.31
2	A	601	AMP	C5-C6	2.21	1.47	1.41
2	B	601	AMP	C4-N9	-2.08	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	AMP	C5-C4-N3	-5.02	119.80	126.72
2	B	601	AMP	N3-C4-N9	4.37	134.61	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	C4-N9-C8	4.16	110.11	105.74
2	A	601	AMP	N3-C2-N1	-3.95	122.61	128.58
2	B	601	AMP	C4-N9-C8	3.78	109.71	105.74
2	A	601	AMP	C5-C4-N3	-3.67	121.67	126.72
2	B	601	AMP	C2-N3-C4	3.24	119.74	111.83
2	A	601	AMP	N3-C4-N9	3.22	132.65	127.17
2	A	601	AMP	C2-N3-C4	3.10	119.40	111.83
2	A	601	AMP	C4-N9-C1'	-3.09	119.40	126.63
2	B	601	AMP	N3-C2-N1	-3.07	123.93	128.58
2	B	601	AMP	C4-C5-N7	-2.90	107.27	110.58
2	A	601	AMP	O3P-P-O5'	-2.89	99.14	106.67
2	A	601	AMP	C4-C5-N7	-2.70	107.50	110.58
2	A	601	AMP	C6-C5-N7	2.69	137.27	132.09
2	B	601	AMP	N9-C8-N7	-2.64	110.20	113.94
2	A	601	AMP	C2-N1-C6	2.59	122.99	118.73
2	A	601	AMP	N9-C8-N7	-2.52	110.37	113.94
2	B	601	AMP	C5-N7-C8	2.38	107.19	103.45
3	B	602	SAL	O2'-C1'-C1	2.07	121.16	115.28
3	A	602	SAL	O2'-C1'-O1'	-2.04	118.97	123.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

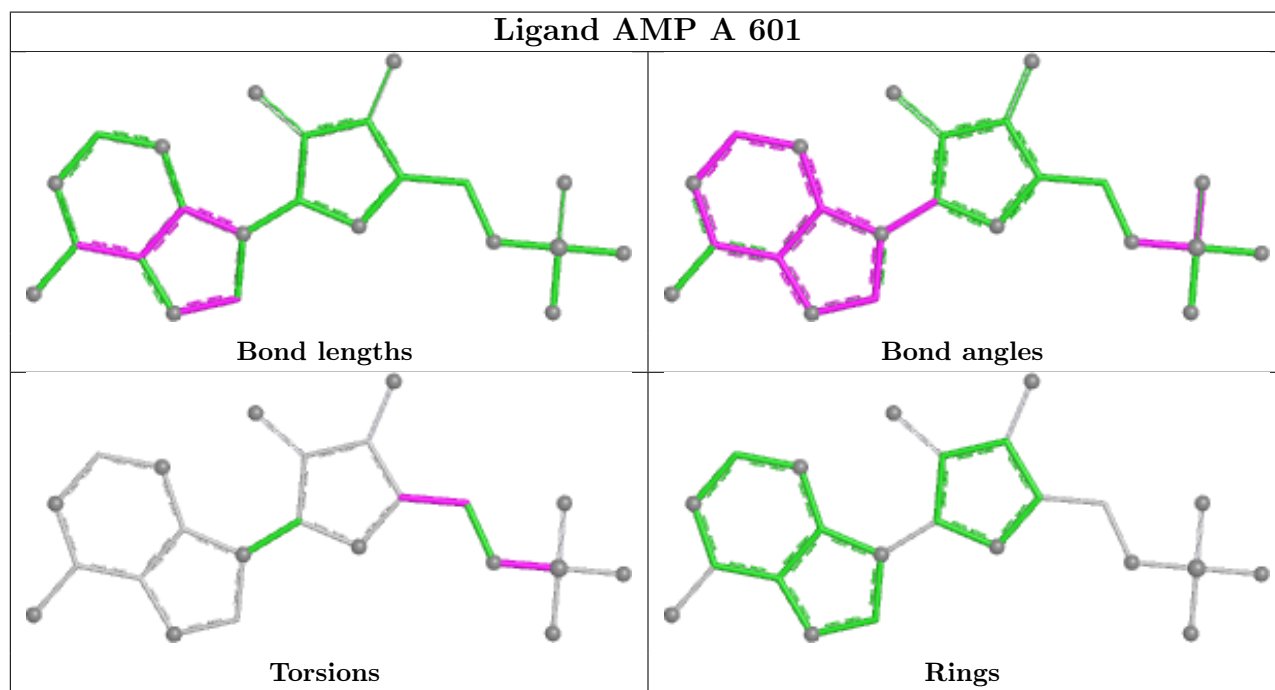
Mol	Chain	Res	Type	Atoms
2	A	601	AMP	C5'-O5'-P-O2P
2	A	601	AMP	C5'-O5'-P-O3P
2	A	601	AMP	O4'-C4'-C5'-O5'
2	B	601	AMP	C5'-O5'-P-O1P
2	B	601	AMP	C5'-O5'-P-O2P
2	B	601	AMP	C5'-O5'-P-O3P
2	B	601	AMP	C3'-C4'-C5'-O5'
2	A	601	AMP	C3'-C4'-C5'-O5'
2	B	601	AMP	O4'-C4'-C5'-O5'
2	A	601	AMP	C5'-O5'-P-O1P

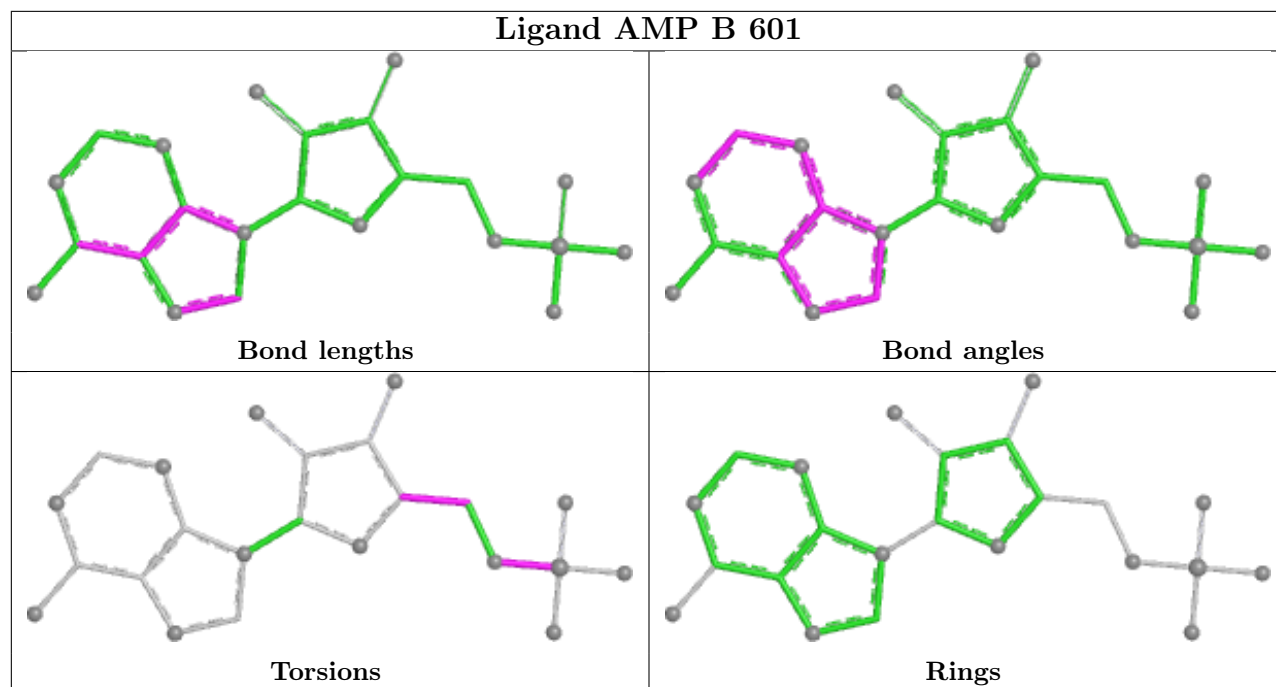
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AMP	2	0
2	B	601	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	494/581 (85%)	0.04	47 (9%) 14 12	8, 17, 66, 95	10 (2%)
1	B	479/581 (82%)	0.11	54 (11%) 10 8	8, 19, 71, 100	9 (1%)
All	All	973/1162 (83%)	0.08	101 (10%) 11 10	8, 18, 70, 100	19 (1%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	ILE	8.8
1	A	472	LEU	5.1
1	A	456	THR	5.1
1	B	280	ASN	5.0
1	B	456	THR	4.9
1	A	526	VAL	4.9
1	A	463	THR	4.8
1	B	464	PHE	4.8
1	A	464	PHE	4.7
1	B	494	LEU	4.7
1	A	458	TYR	4.5
1	B	472	LEU	4.4
1	A	490	ASP	4.4
1	A	499	LEU	4.2
1	A	465	PRO	4.1
1	A	488	GLU	4.1
1	B	431	GLU	4.0
1	B	499	LEU	4.0
1	B	572	PHE	4.0
1	A	8	ASN	4.0
1	A	489	LEU	3.9
1	B	570	ALA	3.9
1	B	100	GLY	3.8
1	B	461	THR	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	434	LEU	3.7
1	A	492	GLU	3.6
1	B	514	PHE	3.6
1	B	429	THR	3.5
1	B	47	LEU	3.5
1	B	459	ALA	3.5
1	B	505	LEU	3.5
1	B	511	ARG	3.5
1	B	515	LYS	3.4
1	A	441	ALA	3.4
1	A	495	SER	3.4
1	A	574	SER	3.3
1	A	494	LEU	3.3
1	B	282	TRP	3.3
1	B	458	TYR	3.2
1	A	459	ALA	3.2
1	B	469	VAL	3.2
1	B	524	ILE	3.2
1	A	493	ALA	3.2
1	B	495	SER	3.2
1	A	461	THR	3.2
1	B	462	SER	3.1
1	B	471	TYR	3.1
1	B	428	LYS	3.1
1	B	470	VAL	3.0
1	A	471	TYR	3.0
1	B	500	VAL	2.9
1	A	571	LYS	2.9
1	B	50	ARG	2.9
1	A	522	LEU	2.8
1	A	435	PHE	2.8
1	A	457	SER	2.8
1	A	572	PHE	2.8
1	B	497	CYS	2.8
1	A	516	ASP	2.8
1	B	573	PHE	2.7
1	B	427	ASP	2.7
1	B	468	TYR	2.7
1	B	279	GLN	2.7
1	A	423	SER	2.7
1	A	100	GLY	2.6
1	A	280	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	514	PHE	2.6
1	B	465	PRO	2.6
1	B	521	PRO	2.5
1	A	102	ALA	2.5
1	A	99	SER	2.5
1	A	438	VAL	2.5
1	B	516	ASP	2.5
1	A	511	ARG	2.5
1	A	524	ILE	2.5
1	A	424	ILE	2.4
1	A	491	GLU	2.4
1	A	509	TYR	2.4
1	B	525	ARG	2.4
1	B	9	GLU	2.4
1	A	470	VAL	2.3
1	B	522	LEU	2.3
1	B	509	TYR	2.3
1	B	463	THR	2.3
1	B	496	THR	2.3
1	A	573	PHE	2.2
1	B	419	ASN	2.2
1	B	460	ASP	2.2
1	B	508	VAL	2.2
1	B	574	SER	2.2
1	B	424	ILE	2.1
1	A	469	VAL	2.1
1	A	500	VAL	2.1
1	B	432	GLU	2.1
1	A	147	GLN	2.1
1	A	468	TYR	2.1
1	A	498	CYS	2.1
1	B	425	ASP	2.1
1	B	426	SER	2.1
1	B	498	CYS	2.1
1	B	519	ILE	2.0

## 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](#)

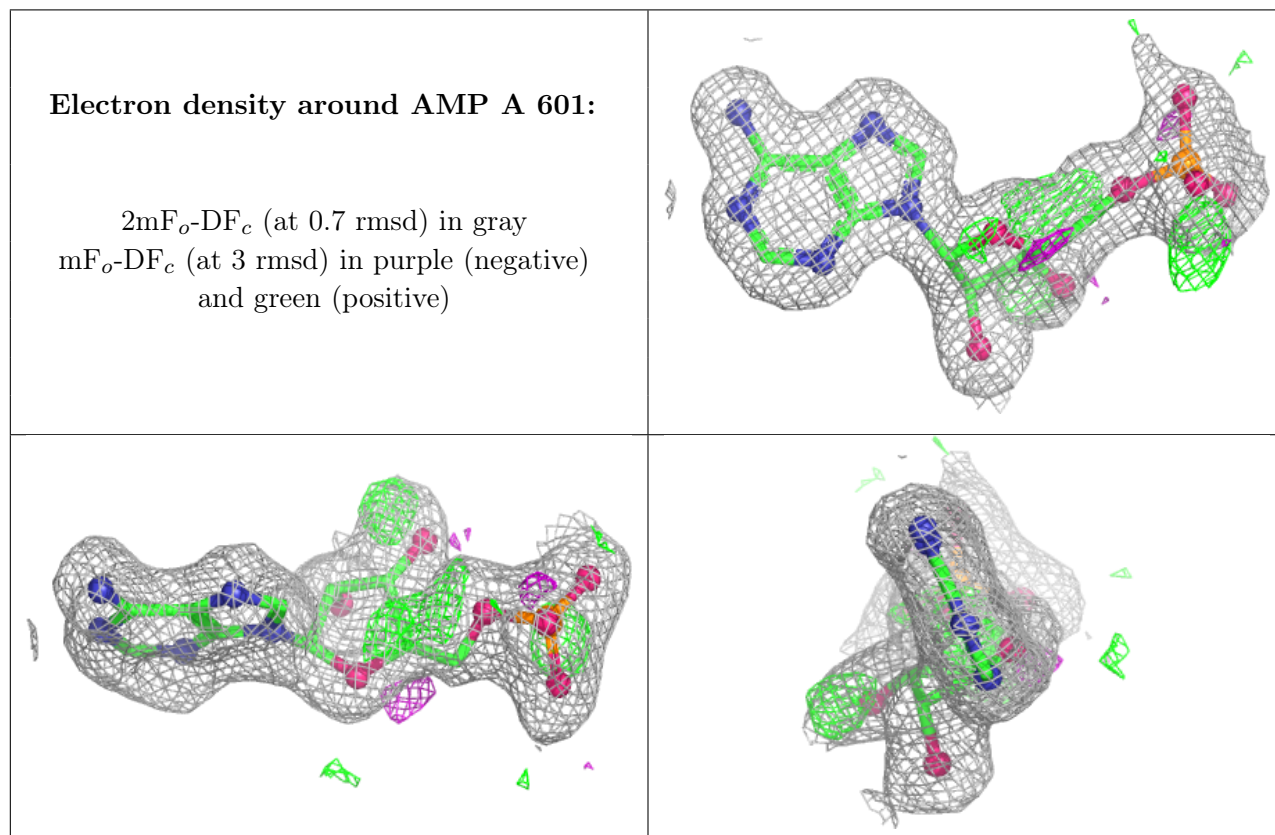
There are no oligosaccharides in this entry.

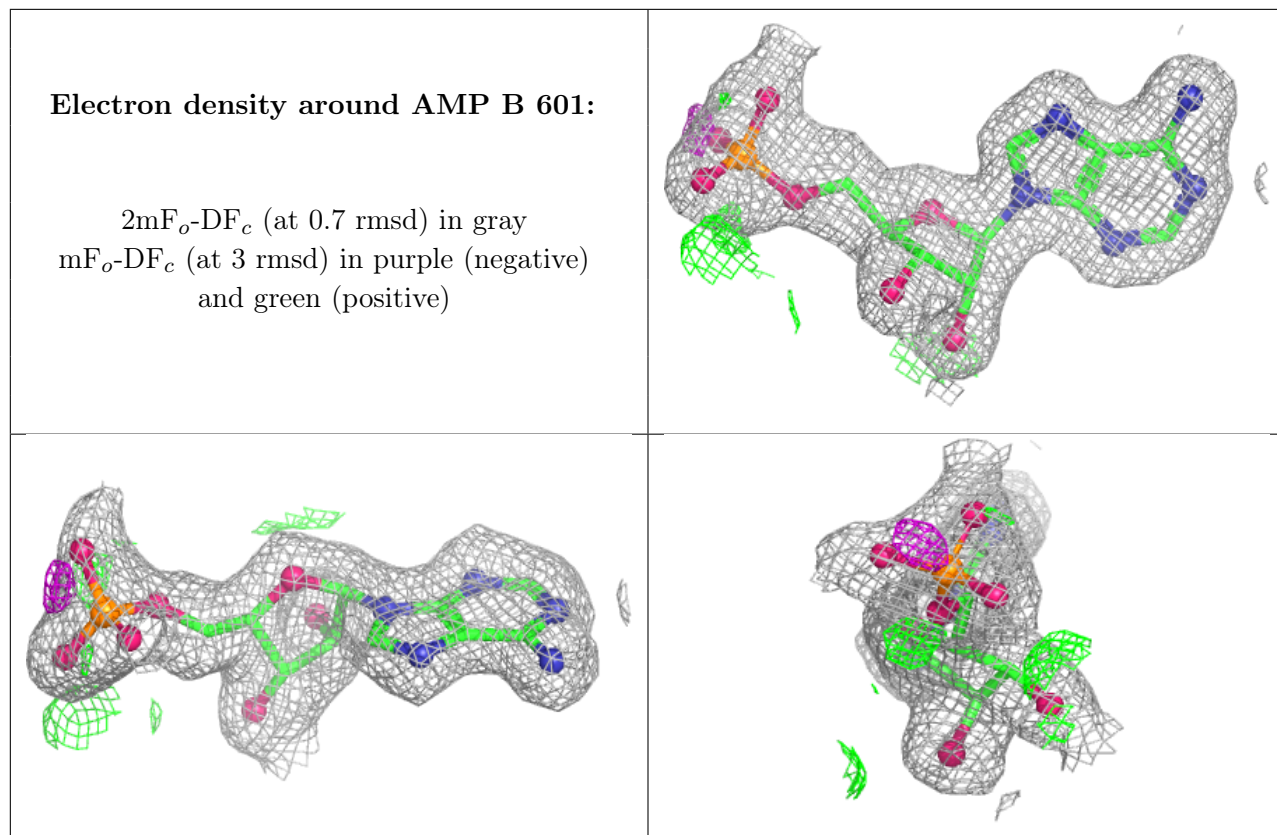
### 6.4 Ligands [i](#)

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, 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(Å <sup>2</sup> )	Q<0.9
3	SAL	B	602	10/10	0.91	0.09	19,26,30,31	0
3	SAL	A	602	10/10	0.93	0.08	17,22,24,26	0
2	AMP	A	601	23/23	0.94	0.09	8,18,32,39	0
2	AMP	B	601	23/23	0.96	0.07	9,17,34,42	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.