



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:51 PM UTC

PDB ID : 6OMS / pdb_00006oms
Title : Arabidopsis GH3.12 with Chorismate
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Deposited on : 2019-04-19
Resolution : 1.94 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

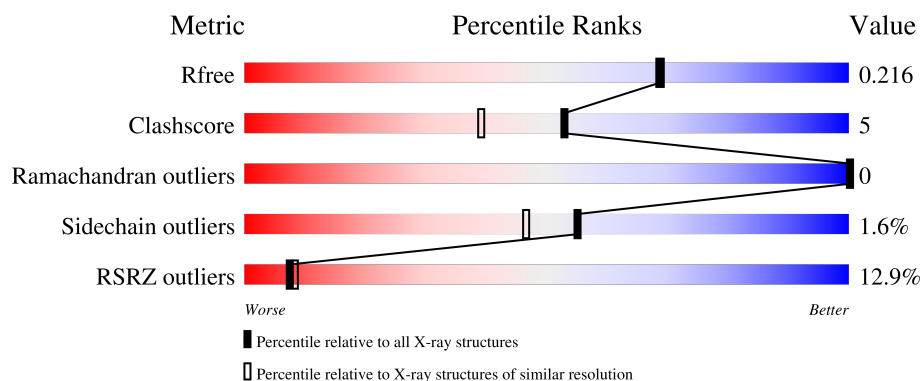
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	575	10% 77% 8% 15%
1	B	575	12% 77% 8% 14%

2 Entry composition [i](#)

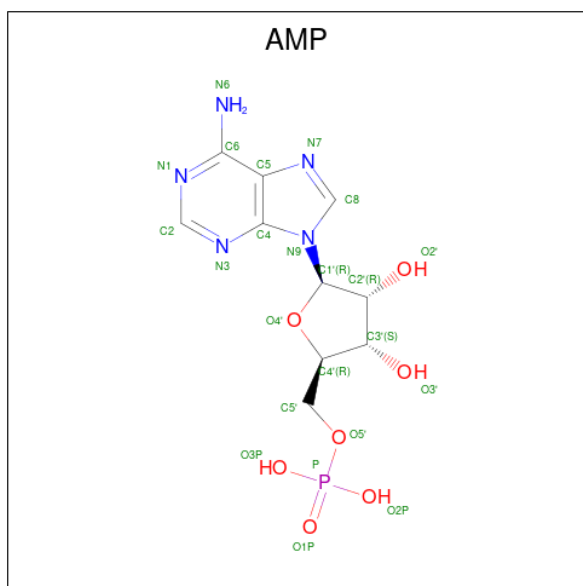
There are 4 unique types of molecules in this entry. The entry contains 8642 atoms, of which 8 are hydrogens and 0 are deuteriums.

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.

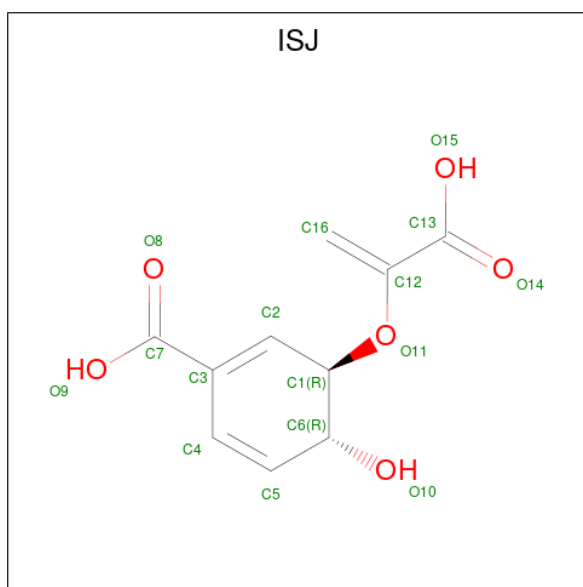
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	5	0
			3911	2494	635	756	26			
1	B	492	Total	C	N	O	S	0	9	0
			3969	2529	646	768	26			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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 (3R,4R)-3-[(1-carboxyethenyl)oxy]-4-hydroxycyclohexa-1,5-diene-1-carboxylic acid (CCD ID: ISJ) (formula: $C_{10}H_{10}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			24	10	8	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	361	Total	O	0	0
			361	361		
4	B	331	Total	O	0	0
			331	331		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.44Å 67.00Å 100.96Å 90.00° 106.36° 90.00°	Depositor
Resolution (Å)	48.59 – 1.94 48.59 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.59-1.94) 99.1 (48.59-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.186 , 0.216 0.188 , 0.216	Depositor DCC
R_{free} test set	4319 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: ISJ, AMP

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	0.30	0/4009	0.49	0/5431
1	B	0.30	0/4079	0.49	0/5525
All	All	0.30	0/8088	0.49	0/10956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3911	0	3859	45	2
1	B	3969	0	3924	42	2
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	B	16	8	8	3	0
4	A	361	0	0	6	0
4	B	331	0	0	4	0
All	All	8634	8	7815	78	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 5.

All (78) 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:145:THR:HG21	1:A:166:LYS:HE3	1.31	1.09
1:A:43:LEU:HD13	1:A:48:ILE:HD11	1.40	1.00
1:A:510:LYS:HD3	1:B:499:LEU:HD21	1.51	0.90
1:A:515:LYS:HB2	1:B:575:ILE:HD11	1.59	0.82
1:A:145:THR:HG21	1:A:166:LYS:CE	2.09	0.82
1:A:145:THR:CG2	1:A:166:LYS:HE3	2.12	0.79
1:B:511:ARG:HG3	1:B:515:LYS:HD3	1.65	0.79
1:A:575:ILE:HG13	1:B:515:LYS:HG3	1.67	0.76
1:A:438:VAL:HA	1:A:501:MET:HE2	1.68	0.73
1:B:11:PHE:HB2	1:B:125[B]:GLN:NE2	2.05	0.72
1:B:217:ILE:HD13	3:B:602:ISJ:C3	2.20	0.72
1:A:124:MET:O	1:A:128[B]:THR:HG23	1.92	0.70
1:A:515:LYS:HB2	1:B:575:ILE:CD1	2.24	0.68
1:B:217:ILE:HD13	3:B:602:ISJ:C2	2.24	0.67
1:A:48:ILE:HG13	1:A:48:ILE:O	1.99	0.63
1:B:141:MET:HE2	3:B:602:ISJ:H16	1.81	0.63
1:B:341:LYS:HD3	4:B:937:HOH:O	2.00	0.60
1:B:53:LYS:HE2	1:B:57:LYS:HE2	1.82	0.60
1:A:310:MET:HG3	4:A:761:HOH:O	2.02	0.59
1:B:440:GLN:OE1	1:B:504:SER:HB3	2.01	0.59
1:A:279:GLN:N	1:A:279:GLN:OE1	2.37	0.56
1:A:523:GLU:CD	1:A:525:ARG:HE	2.13	0.56
1:A:43:LEU:CD1	1:A:48:ILE:HD11	2.26	0.56
1:A:373:GLU:HG3	1:A:373:GLU:O	2.05	0.55
1:A:575:ILE:HG13	1:B:515:LYS:CG	2.35	0.55
1:B:98:THR:HG23	1:B:102:ALA:O	2.07	0.54
1:A:574:SER:O	1:A:575:ILE:HB	2.06	0.54
1:A:128[B]:THR:HG22	1:A:177:TRP:CZ2	2.43	0.54
1:A:43:LEU:HD13	1:A:48:ILE:CD1	2.28	0.52
1:B:111:LYS:HG2	1:B:388:PHE:CG	2.45	0.51
1:B:574:SER:O	1:B:575:ILE:HB	2.10	0.51
1:A:510:LYS:CD	1:B:499:LEU:HD21	2.33	0.51
1:A:503:GLU:HG2	1:B:503:GLU:HG2	1.94	0.50
1:B:361:MET:HE3	1:B:382:GLU:HB2	1.94	0.50
1:B:440:GLN:OE1	1:B:504:SER:CB	2.60	0.49
1:A:166:LYS:HD3	4:A:703:HOH:O	2.11	0.49
1:A:511:ARG:NH1	1:A:516:ASP:OD2	2.45	0.49
1:A:575:ILE:CG1	1:B:515:LYS:HD2	2.43	0.49
1:A:166:LYS:CD	4:A:703:HOH:O	2.60	0.49
1:A:399:ILE:HD12	1:A:416:ARG:CZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ARG:CG	1:B:515:LYS:HD3	2.38	0.49
1:B:148:GLU:H	1:B:148:GLU:CD	2.22	0.47
1:A:439:SER:O	1:A:440:GLN:HG2	2.14	0.47
1:B:119:ILE:HG13	1:B:331:THR:HG21	1.96	0.47
1:A:303:SER:O	1:A:306:GLN:HG2	2.15	0.47
1:B:575:ILE:HG22	1:B:575:ILE:O	2.14	0.46
1:B:135:GLU:HG3	4:B:846:HOH:O	2.15	0.46
1:A:111:LYS:HG2	1:A:388:PHE:CG	2.51	0.46
1:B:499:LEU:HG	1:B:503:GLU:OE2	2.16	0.46
1:B:511:ARG:O	1:B:515:LYS:HB2	2.16	0.46
1:A:128[B]:THR:CG2	1:A:177:TRP:HZ2	2.29	0.45
1:B:148:GLU:HG3	1:B:158:ARG:HE	1.81	0.45
1:B:420:VAL:HA	1:B:430:ASN:HA	1.98	0.45
1:A:363:GLY:O	1:A:366:LYS:HE3	2.17	0.45
1:B:11:PHE:HB2	1:B:125[B]:GLN:HE22	1.79	0.45
1:A:288:ARG:HD2	4:A:707:HOH:O	2.17	0.44
1:A:166:LYS:NZ	4:A:703:HOH:O	2.41	0.44
1:B:498:CYS:SG	1:B:524:ILE:HD12	2.56	0.44
1:A:111:LYS:HG2	1:A:388:PHE:CB	2.48	0.43
1:A:128[B]:THR:CG2	1:A:177:TRP:CZ2	3.02	0.43
1:B:399:ILE:HD11	1:B:418:GLU:OE2	2.19	0.43
1:A:124:MET:HE3	1:A:125:GLN:HE21	1.84	0.43
1:A:81:SER:HB2	1:A:89[A]:ILE:HG12	2.00	0.42
1:A:52:ASP:OD1	1:A:54:GLU:HG2	2.19	0.42
1:B:575:ILE:O	1:B:575:ILE:CG2	2.66	0.42
1:A:575:ILE:HG21	1:B:515:LYS:HD2	2.02	0.42
1:B:300:VAL:HG22	1:B:322:SER:HB2	2.01	0.42
1:B:470:VAL:HG11	1:B:501:MET:HE1	2.01	0.42
1:B:494:LEU:HD22	1:B:572:PHE:CE2	2.54	0.42
1:A:43:LEU:HB3	1:A:48:ILE:HD11	2.02	0.42
1:A:422:LEU:HD13	1:A:468:TYR:CD2	2.55	0.41
1:B:464:PHE:CD1	1:B:465:PRO:HA	2.56	0.41
1:B:166:LYS:CE	4:B:766:HOH:O	2.69	0.41
1:B:516:ASP:HA	4:B:981:HOH:O	2.19	0.41
1:A:132:LYS:HG2	4:A:933:HOH:O	2.20	0.40
1:A:50:ARG:HG2	1:A:51:PHE:H	1.85	0.40
1:A:575:ILE:HA	1:A:575:ILE:HD12	1.72	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:209:ASP:OD2	1:B:50[B]:ARG:NH2[1_455]	1.93	0.27
1:A:209:ASP:OD2	1:B:50[A]:ARG:NH2[1_455]	1.93	0.27

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	484/575 (84%)	476 (98%)	8 (2%)	0	100	100
1	B	493/575 (86%)	482 (98%)	11 (2%)	0	100	100
All	All	977/1150 (85%)	958 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	451/523 (86%)	444 (98%)	7 (2%)	55	46
1	B	459/523 (88%)	452 (98%)	7 (2%)	57	49
All	All	910/1046 (87%)	896 (98%)	14 (2%)	55	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	149	SER

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	316	ASN
1	A	463	THR
1	A	499	LEU
1	A	575	ILE
1	B	9	GLU
1	B	54	GLU
1	B	146	LYS
1	B	148	GLU
1	B	370	VAL
1	B	396	VAL
1	B	575	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	125	GLN
1	A	231	ASN
1	A	239	ASN
1	A	367	ASN
1	A	411	GLN
1	A	430	ASN
1	B	193	ASN
1	B	239	ASN
1	B	247	ASN
1	B	316	ASN
1	B	411	GLN

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

3 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	B	601	-	25,25,25	1.38	5 (20%)	37,38,38	1.71	10 (27%)
2	AMP	A	601	-	25,25,25	1.36	5 (20%)	37,38,38	1.81	8 (21%)
3	ISJ	B	602	-	16,16,16	2.44	7 (43%)	13,22,22	2.45	9 (69%)

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	B	601	-	-	5/10/26/26	0/3/3/3
2	AMP	A	601	-	-	5/10/26/26	0/3/3/3
3	ISJ	B	602	-	-	4/10/25/25	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ISJ	C1-C2	4.57	1.56	1.50
2	B	601	AMP	C5-C4	4.56	1.47	1.39
2	A	601	AMP	C5-C4	4.46	1.47	1.39
3	B	602	ISJ	O11-C1	-4.44	1.39	1.46
3	B	602	ISJ	C4-C3	3.95	1.51	1.43
3	B	602	ISJ	C3-C7	3.05	1.54	1.48
2	B	601	AMP	C8-N7	2.51	1.36	1.31
2	B	601	AMP	C4-N9	-2.48	1.32	1.37
2	A	601	AMP	C5-C6	2.43	1.47	1.41
3	B	602	ISJ	C4-C5	-2.38	1.28	1.33
3	B	602	ISJ	C12-C13	2.30	1.51	1.49
2	A	601	AMP	C8-N7	2.21	1.35	1.31
2	A	601	AMP	C4-N9	-2.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	AMP	C5-N7	-2.18	1.35	1.39
2	B	601	AMP	C5-C6	2.15	1.47	1.41
3	B	602	ISJ	O10-C6	-2.14	1.39	1.43
2	B	601	AMP	C5-N7	-2.12	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	C5-C4-N3	-4.91	119.95	126.72
3	B	602	ISJ	O9-C7-C3	4.54	125.75	113.72
2	A	601	AMP	N3-C4-N9	4.49	134.80	127.17
2	B	601	AMP	C5-C4-N3	-4.46	120.57	126.72
2	B	601	AMP	N3-C4-N9	3.67	133.41	127.17
2	A	601	AMP	C4-N9-C8	3.66	109.58	105.74
2	B	601	AMP	N3-C2-N1	-3.27	123.63	128.58
2	A	601	AMP	C2-N3-C4	3.22	119.69	111.83
2	B	601	AMP	C2-N3-C4	3.14	119.51	111.83
2	A	601	AMP	N3-C2-N1	-3.14	123.83	128.58
3	B	602	ISJ	C6-C5-C4	-2.93	117.29	123.08
3	B	602	ISJ	C5-C4-C3	-2.81	118.61	122.38
2	B	601	AMP	C4-N9-C8	2.73	108.60	105.74
3	B	602	ISJ	O15-C13-C12	2.68	118.48	113.91
3	B	602	ISJ	O8-C7-C3	-2.63	115.46	121.92
2	A	601	AMP	C4-C5-N7	-2.51	107.72	110.58
3	B	602	ISJ	O11-C12-C13	2.51	121.83	115.59
2	B	601	AMP	O3P-P-O2P	2.38	116.74	107.80
2	B	601	AMP	C4-C5-N7	-2.37	107.88	110.58
2	A	601	AMP	N9-C8-N7	-2.36	110.59	113.94
3	B	602	ISJ	C1-O11-C12	2.29	120.58	117.03
3	B	602	ISJ	C16-C12-C13	-2.24	118.58	122.73
2	B	601	AMP	O2P-P-O5'	-2.24	100.83	106.67
2	B	601	AMP	O3P-P-O5'	-2.19	100.96	106.67
3	B	602	ISJ	O9-C7-O8	-2.17	118.73	123.90
2	A	601	AMP	C5-N7-C8	2.16	106.85	103.45
2	B	601	AMP	C2-N1-C6	2.11	122.20	118.73

There are no chirality outliers.

All (14) 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

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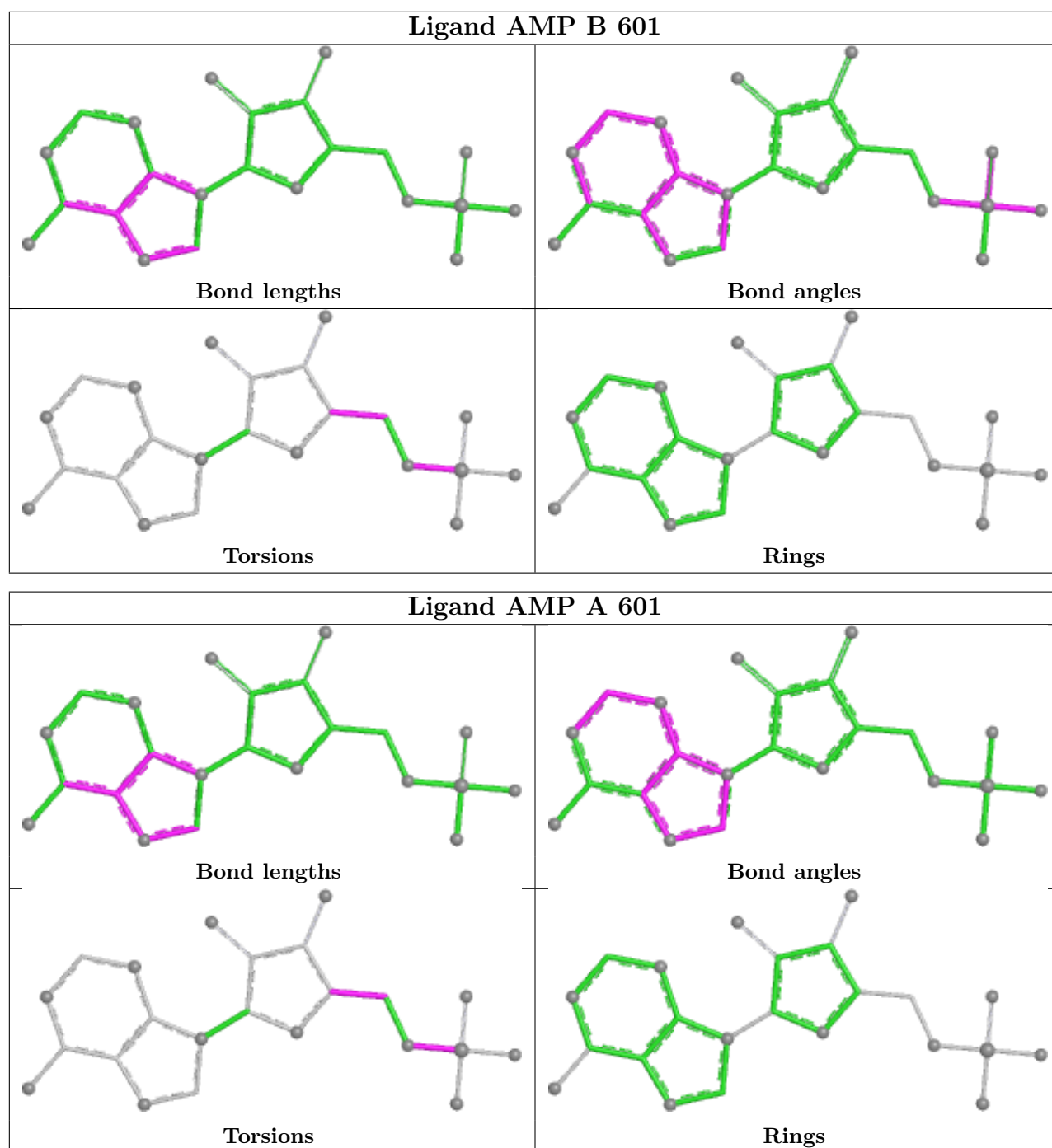
Mol	Chain	Res	Type	Atoms
2	B	601	AMP	C5'-O5'-P-O1P
2	B	601	AMP	C5'-O5'-P-O2P
2	B	601	AMP	C5'-O5'-P-O3P
2	B	601	AMP	C3'-C4'-C5'-O5'
3	B	602	ISJ	O11-C12-C13-O15
3	B	602	ISJ	C16-C12-C13-O14
3	B	602	ISJ	C16-C12-C13-O15
2	A	601	AMP	C3'-C4'-C5'-O5'
2	B	601	AMP	O4'-C4'-C5'-O5'
2	A	601	AMP	O4'-C4'-C5'-O5'
2	A	601	AMP	C5'-O5'-P-O1P
3	B	602	ISJ	O11-C12-C13-O14

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ISJ	3	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, 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	487/575 (84%)	0.23	59 (12%)  	7, 17, 60, 73	5 (1%)
1	B	492/575 (85%)	0.27	67 (13%)  	7, 17, 56, 68	9 (1%)
All	All	979/1150 (85%)	0.25	126 (12%)  	7, 17, 58, 73	14 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	THR	6.4
1	A	575	ILE	6.2
1	A	48	ILE	6.0
1	B	435	PHE	6.0
1	B	575	ILE	5.9
1	A	435	PHE	5.3
1	B	464	PHE	5.0
1	A	456	THR	5.0
1	B	465	PRO	4.8
1	B	472	LEU	4.8
1	B	100	GLY	4.5
1	B	457	SER	4.4
1	B	494	LEU	4.3
1	A	463	THR	4.2
1	A	494	LEU	4.2
1	B	440	GLN	4.1
1	A	472	LEU	3.9
1	B	569	VAL	3.9
1	A	465	PRO	3.9
1	A	424	ILE	3.8
1	A	47	LEU	3.7
1	B	499	LEU	3.7
1	B	102	ALA	3.7
1	A	464	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	3.6
1	A	570	ALA	3.5
1	A	524	ILE	3.5
1	B	470	VAL	3.5
1	B	442	LYS	3.5
1	B	458	TYR	3.5
1	B	568	VAL	3.5
1	B	511	ARG	3.4
1	B	508	VAL	3.4
1	A	459	ALA	3.3
1	A	471	TYR	3.3
1	B	147	GLN	3.2
1	B	524	ILE	3.2
1	B	471	TYR	3.2
1	A	100	GLY	3.1
1	A	434	LEU	3.1
1	B	516	ASP	3.1
1	B	468	TYR	3.1
1	A	499	LEU	3.1
1	B	8	ASN	3.1
1	B	459	ALA	3.1
1	B	519	ILE	3.1
1	A	458	TYR	3.1
1	B	434	LEU	3.1
1	B	522	LEU	3.1
1	A	422	LEU	3.0
1	A	420	VAL	3.0
1	B	424	ILE	3.0
1	B	509	TYR	3.0
1	B	514	PHE	3.0
1	B	423	SER	2.9
1	A	515	LYS	2.9
1	B	521	PRO	2.9
1	B	570	ALA	2.9
1	B	496	THR	2.9
1	B	280	ASN	2.9
1	B	500	VAL	2.8
1	B	572	PHE	2.8
1	A	505	LEU	2.8
1	B	461	THR	2.8
1	B	101	GLY	2.8
1	A	429	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	461	THR	2.8
1	A	469	VAL	2.8
1	B	422	LEU	2.7
1	A	310	MET	2.7
1	A	519	ILE	2.7
1	A	97	GLY	2.7
1	A	514	PHE	2.7
1	B	429	THR	2.7
1	A	282	TRP	2.6
1	B	426	SER	2.6
1	A	508	VAL	2.6
1	A	101	GLY	2.6
1	A	495	SER	2.6
1	B	462	SER	2.6
1	B	466	GLY	2.5
1	B	463	THR	2.5
1	A	102	ALA	2.5
1	B	441	ALA	2.5
1	A	438	VAL	2.5
1	A	497	CYS	2.5
1	B	573	PHE	2.5
1	A	573	PHE	2.4
1	B	317	ASP	2.4
1	A	525	ARG	2.4
1	A	437	ALA	2.4
1	B	498	CYS	2.4
1	A	439	SER	2.3
1	A	500	VAL	2.3
1	A	522	LEU	2.3
1	A	98	THR	2.3
1	A	572	PHE	2.3
1	A	466	GLY	2.3
1	B	517	GLY	2.3
1	B	54	GLU	2.3
1	B	428	LYS	2.3
1	B	438	VAL	2.3
1	B	98	THR	2.3
1	B	505	LEU	2.3
1	A	520	GLY	2.2
1	A	521	PRO	2.2
1	B	427	ASP	2.2
1	B	433	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	SER	2.2
1	A	468	TYR	2.2
1	B	571	LYS	2.2
1	A	418	GLU	2.2
1	A	440	GLN	2.2
1	A	426	SER	2.2
1	B	432	GLU	2.2
1	A	431	GLU	2.1
1	B	418	GLU	2.1
1	B	431	GLU	2.1
1	A	10	THR	2.1
1	A	470	VAL	2.1
1	A	462	SER	2.1
1	B	436	LYS	2.1
1	A	49	ASP	2.1
1	B	512	CYS	2.0
1	A	428	LYS	2.0
1	B	469	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.

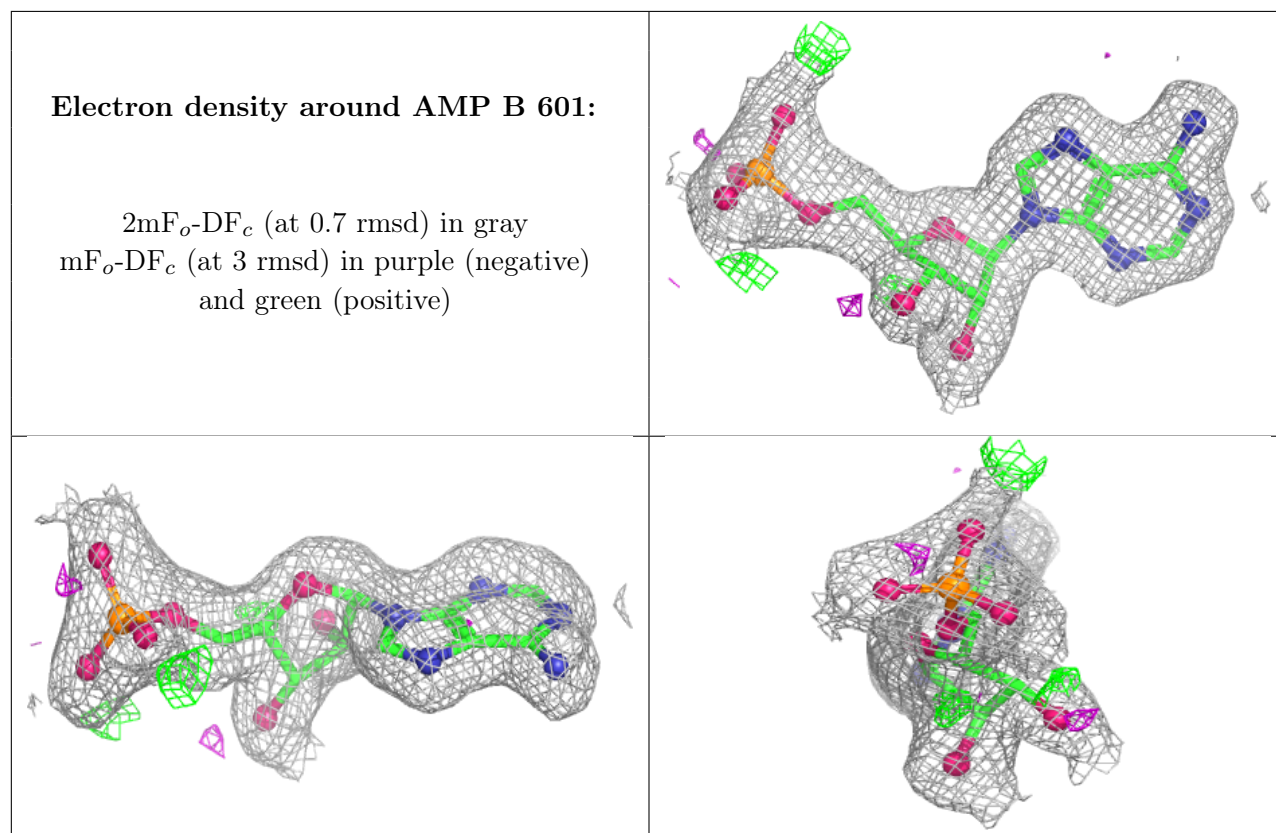
6.4 Ligands [i](#)

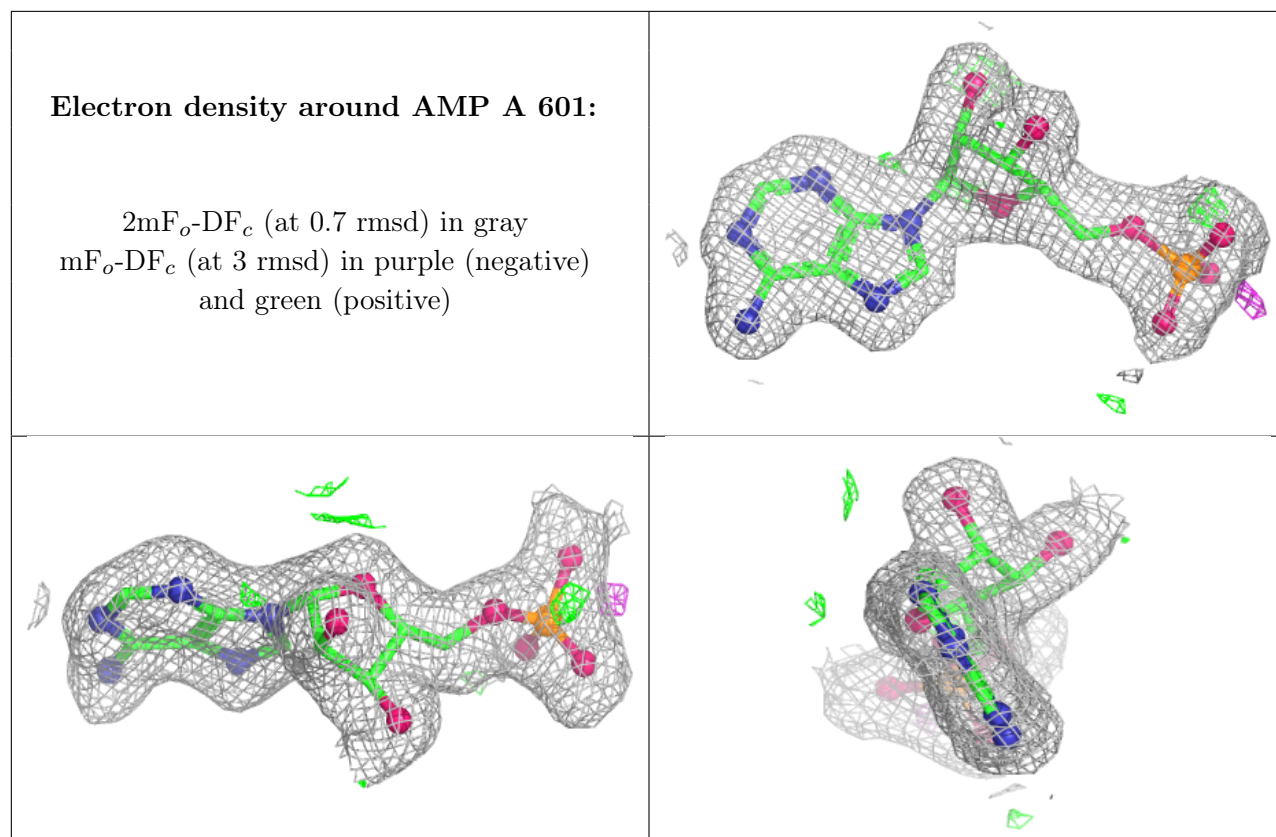
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ISJ	B	602	16/16	0.60	0.24	24,53,69,74	0
2	AMP	B	601	23/23	0.95	0.07	6,18,32,38	0
2	AMP	A	601	23/23	0.95	0.07	10,17,29,34	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.