



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:29 AM UTC

PDB ID : 4EQ5 / pdb_00004eq5
Title : DNA ligase from the archaeon Thermococcus sibiricus
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Deposited on : 2012-04-18
Resolution : 2.85 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

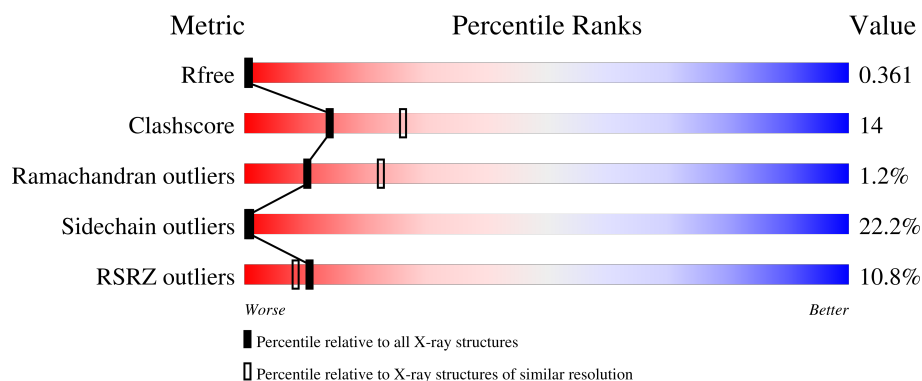
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	571	10% 51% 32% 7% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3884 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.

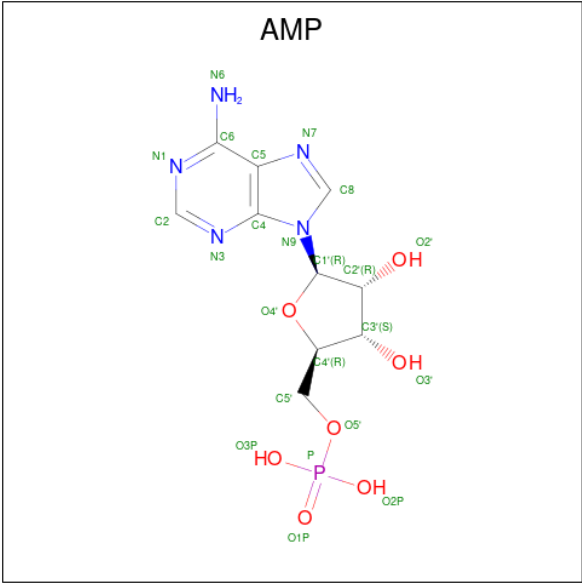
- Molecule 1 is a protein called DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3859	2484	654	710	11	35	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C6A2U9
A	2	ARG	-	expression tag	UNP C6A2U9
A	3	GLY	-	expression tag	UNP C6A2U9
A	4	SER	-	expression tag	UNP C6A2U9
A	5	HIS	-	expression tag	UNP C6A2U9
A	6	HIS	-	expression tag	UNP C6A2U9
A	7	HIS	-	expression tag	UNP C6A2U9
A	8	HIS	-	expression tag	UNP C6A2U9
A	9	HIS	-	expression tag	UNP C6A2U9
A	10	HIS	-	expression tag	UNP C6A2U9
A	11	GLY	-	expression tag	UNP C6A2U9
A	12	SER	-	expression tag	UNP C6A2U9

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

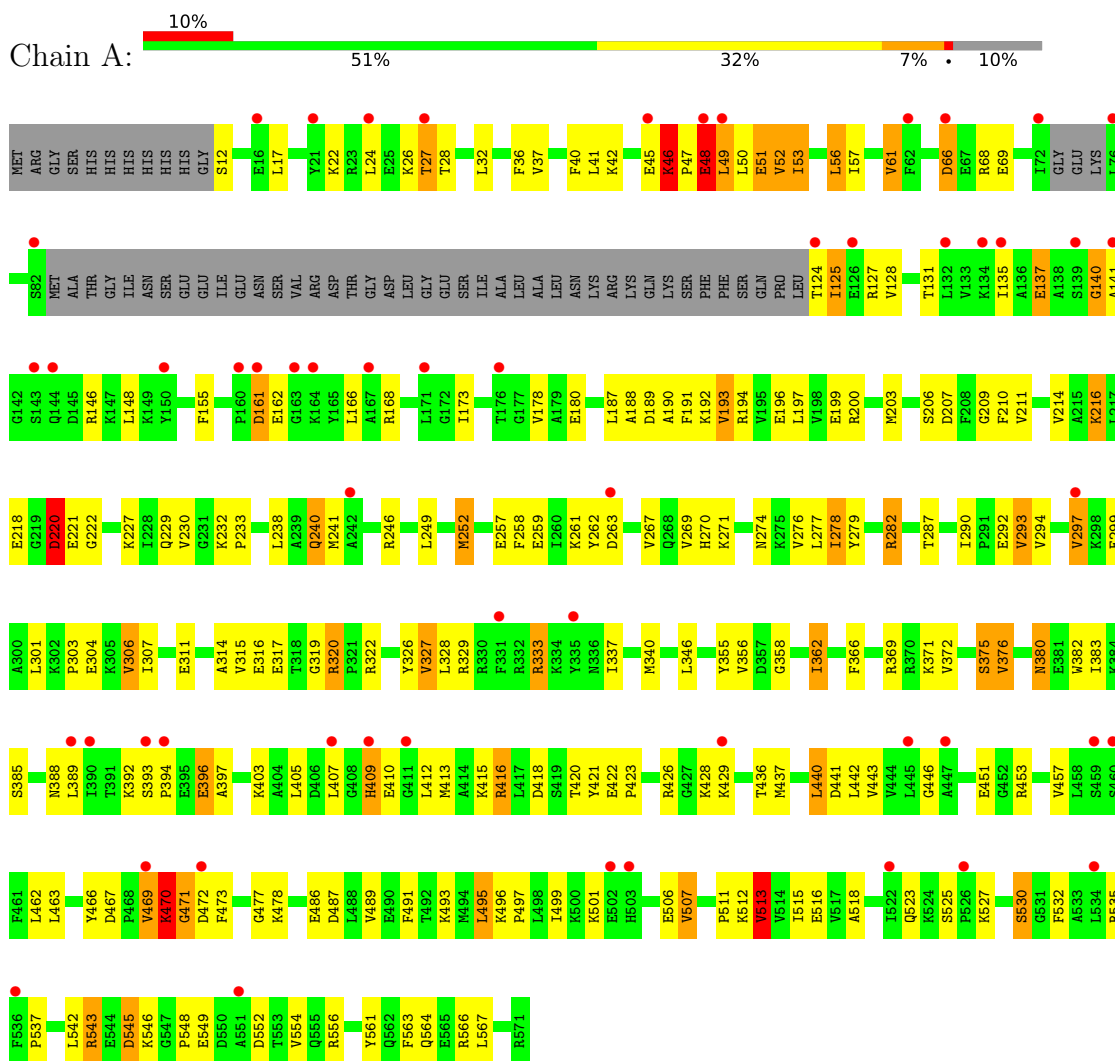
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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: DNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.59Å 87.54Å 126.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.30 – 2.85 29.30 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.30-2.85) 98.8 (29.30-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.273 , 0.357 0.270 , 0.361	Depositor DCC
R_{free} test set	939 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3884	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: 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	0.66	0/3924	1.16	27/5309 (0.5%)

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	10

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LYS	CA-C-N	11.77	131.53	119.64
1	A	46	LYS	C-N-CA	11.77	131.53	119.64
1	A	52	VAL	CA-C-N	7.42	127.55	120.43
1	A	52	VAL	C-N-CA	7.42	127.55	120.43
1	A	393	SER	CA-C-N	6.90	126.53	119.56
1	A	393	SER	C-N-CA	6.90	126.53	119.56
1	A	140	GLY	N-CA-C	6.82	121.13	110.96
1	A	66	ASP	N-CA-C	6.80	119.53	111.71
1	A	320	ARG	CA-C-N	6.52	126.75	119.90
1	A	320	ARG	C-N-CA	6.52	126.75	119.90
1	A	48	GLU	N-CA-C	-6.49	105.66	112.93
1	A	52	VAL	N-CA-C	6.37	122.58	109.34
1	A	527	LYS	N-CA-C	-6.28	105.66	113.38
1	A	525	SER	CA-C-N	-6.14	113.62	121.91
1	A	525	SER	C-N-CA	-6.14	113.62	121.91
1	A	61	VAL	N-CA-C	-6.12	105.72	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LYS	N-CA-C	5.91	117.58	109.18
1	A	155	PHE	N-CA-C	5.81	119.47	112.38
1	A	141	ALA	N-CA-C	5.74	119.09	111.75
1	A	372	VAL	CB-CA-C	-5.63	104.76	111.97
1	A	513	VAL	N-CA-C	5.59	115.90	107.80
1	A	53	ILE	CB-CA-C	-5.56	108.42	113.70
1	A	467	ASP	CA-C-N	5.43	124.89	119.24
1	A	467	ASP	C-N-CA	5.43	124.89	119.24
1	A	47	PRO	N-CA-C	-5.21	106.94	114.18
1	A	319	GLY	N-CA-C	-5.12	108.17	115.64
1	A	53	ILE	N-CA-C	5.07	119.01	112.67

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLU	Peptide
1	A	140	GLY	Peptide
1	A	220	ASP	Peptide
1	A	45	GLU	Peptide
1	A	46	LYS	Peptide
1	A	469	VAL	Peptide
1	A	470	LYS	Peptide
1	A	471	GLY	Peptide
1	A	48	GLU	Peptide
1	A	51	GLU	Peptide

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	3859	0	3712	108	0
2	A	23	0	12	1	0
3	A	2	0	0	0	0
All	All	3884	0	3724	108	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 14.

All (108) 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:269:VAL:HG22	1:A:278:ILE:HD12	1.59	0.84
1:A:252:MET:HE2	1:A:416:ARG:HG2	1.67	0.77
1:A:53:ILE:HD11	1:A:125:ILE:HD13	1.71	0.71
1:A:552:ASP:HB3	1:A:556:ARG:HG2	1.70	0.71
1:A:238:LEU:HB2	1:A:426:ARG:HG2	1.73	0.70
1:A:168:ARG:O	1:A:173:ILE:N	2.26	0.68
1:A:337:ILE:HD12	1:A:337:ILE:H	1.59	0.65
1:A:252:MET:HG3	1:A:416:ARG:HD3	1.79	0.65
1:A:240:GLN:HG2	1:A:428:LYS:HE2	1.79	0.64
1:A:366:PHE:HD1	1:A:369:ARG:HH21	1.45	0.63
1:A:303:PRO:HB2	1:A:306:VAL:HG22	1.81	0.62
1:A:41:LEU:HD13	1:A:187:LEU:HD23	1.82	0.62
1:A:471:GLY:O	1:A:473:PHE:N	2.25	0.62
1:A:278:ILE:HG13	1:A:279:TYR:N	2.15	0.60
1:A:355:TYR:OH	1:A:358:GLY:HA2	2.01	0.60
1:A:426:ARG:NH2	2:A:601:AMP:O1P	2.33	0.59
1:A:37:VAL:HG13	1:A:57:ILE:HD13	1.83	0.59
1:A:42:LYS:HE2	1:A:190:ALA:HA	1.83	0.59
1:A:512:LYS:HA	1:A:548:PRO:HG3	1.86	0.58
1:A:124:THR:HG23	1:A:127:ARG:H	1.67	0.57
1:A:276:VAL:O	1:A:277:LEU:HD23	2.05	0.57
1:A:261:LYS:HB2	1:A:413:MET:HG2	1.87	0.57
1:A:188:ALA:HA	1:A:193:VAL:HG23	1.86	0.57
1:A:314:ALA:H	1:A:327:VAL:HG22	1.71	0.56
1:A:146:ARG:O	1:A:148:LEU:N	2.39	0.55
1:A:440:LEU:O	1:A:516:GLU:HA	2.07	0.55
1:A:530:SER:HB2	1:A:532:PHE:HB2	1.88	0.54
1:A:210:PHE:O	1:A:214:VAL:HG23	2.07	0.54
1:A:257:GLU:HG2	1:A:415:LYS:HB2	1.89	0.53
1:A:297:VAL:HG22	1:A:301:LEU:HD12	1.91	0.53
1:A:328:LEU:HD22	1:A:545:ASP:HB3	1.91	0.52
1:A:290:ILE:HB	1:A:293:VAL:HG23	1.91	0.52
1:A:369:ARG:NH1	1:A:421:TYR:HB2	2.24	0.52
1:A:48:GLU:O	1:A:50:LEU:N	2.43	0.52
1:A:333:ARG:HA	1:A:340:MET:HE1	1.92	0.52
1:A:271:LYS:NZ	1:A:304:GLU:HA	2.24	0.52
1:A:316:GLU:HG3	1:A:322:ARG:HD3	1.92	0.51
1:A:282:ARG:HG2	1:A:545:ASP:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG11	1:A:511:PRO:HB2	1.93	0.51
1:A:380:ASN:N	1:A:380:ASN:OD1	2.42	0.51
1:A:499:ILE:HG23	1:A:507:VAL:HG13	1.91	0.51
1:A:24:LEU:HD23	1:A:36:PHE:HD2	1.76	0.50
1:A:314:ALA:HA	1:A:346:LEU:HD23	1.93	0.50
1:A:396:GLU:H	1:A:396:GLU:CD	2.19	0.50
1:A:124:THR:O	1:A:128:VAL:HG23	2.11	0.50
1:A:326:TYR:O	1:A:329:ARG:HB2	2.12	0.50
1:A:131:THR:O	1:A:135:ILE:HG22	2.11	0.50
1:A:380:ASN:HB2	1:A:382:TRP:H	1.75	0.50
1:A:196:GLU:O	1:A:199:GLU:HB3	2.11	0.49
1:A:462:LEU:HD12	1:A:477:GLY:O	2.11	0.49
1:A:191:PHE:CE2	1:A:216:LYS:HB2	2.48	0.49
1:A:262:TYR:HB2	1:A:311:GLU:HG2	1.95	0.49
1:A:543:ARG:HD3	1:A:546:LYS:HD2	1.94	0.49
1:A:24:LEU:HD21	1:A:36:PHE:HB2	1.95	0.49
1:A:491:PHE:O	1:A:495:LEU:HB2	2.12	0.49
1:A:27:THR:HG21	1:A:36:PHE:HE2	1.78	0.48
1:A:53:ILE:O	1:A:56:LEU:N	2.46	0.48
1:A:327:VAL:HG13	1:A:346:LEU:HD22	1.94	0.48
1:A:337:ILE:HG13	1:A:340:MET:HE2	1.95	0.48
1:A:446:GLY:C	1:A:462:LEU:HB3	2.39	0.48
1:A:12:SER:O	1:A:124:THR:OG1	2.31	0.47
1:A:124:THR:OG1	1:A:125:ILE:N	2.47	0.47
1:A:146:ARG:C	1:A:148:LEU:H	2.22	0.47
1:A:563:PHE:O	1:A:567:LEU:HG	2.14	0.47
1:A:193:VAL:HG12	1:A:220:ASP:OD1	2.15	0.47
1:A:17:LEU:HD21	1:A:56:LEU:HB3	1.97	0.47
1:A:37:VAL:O	1:A:40:PHE:N	2.48	0.47
1:A:290:ILE:O	1:A:294:VAL:HG23	2.14	0.47
1:A:441:ASP:OD1	1:A:516:GLU:HG3	2.15	0.46
1:A:207:ASP:O	1:A:211:VAL:HG23	2.15	0.46
1:A:267:VAL:HB	1:A:278:ILE:HD11	1.97	0.46
1:A:303:PRO:HD3	1:A:376:VAL:HG13	1.98	0.46
1:A:496:LYS:HB3	1:A:497:PRO:HD3	1.98	0.45
1:A:515:ILE:HG22	1:A:542:LEU:HB3	1.98	0.45
1:A:194:ARG:HB2	1:A:197:LEU:HG	1.99	0.45
1:A:238:LEU:CB	1:A:426:ARG:HG2	2.45	0.45
1:A:303:PRO:CD	1:A:376:VAL:HG13	2.47	0.44
1:A:259:GLU:OE1	1:A:415:LYS:NZ	2.42	0.44
1:A:362:ILE:HG23	1:A:421:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG13	1:A:270:HIS:HB3	1.99	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.73	0.43
1:A:371:LYS:O	1:A:375:SER:OG	2.31	0.43
1:A:470:LYS:HE3	1:A:470:LYS:O	2.18	0.43
1:A:466:TYR:HB2	1:A:473:PHE:CE2	2.54	0.43
1:A:221:GLU:HB3	1:A:222:GLY:H	1.35	0.43
1:A:478:LYS:HB3	1:A:478:LYS:HE3	1.66	0.43
1:A:409:HIS:HB2	1:A:410:GLU:H	1.74	0.42
1:A:307:ILE:HB	1:A:355:TYR:HB3	2.01	0.42
1:A:394:PRO:O	1:A:397:ALA:HB3	2.20	0.42
1:A:518:ALA:O	1:A:537:PRO:HA	2.19	0.42
1:A:206:SER:OG	1:A:233:PRO:O	2.36	0.42
1:A:26:LYS:HA	1:A:26:LYS:HD3	1.82	0.41
1:A:189:ASP:O	1:A:192:LYS:HD3	2.20	0.41
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.83	0.41
1:A:487:ASP:O	1:A:491:PHE:HD1	2.03	0.41
1:A:259:GLU:CD	1:A:415:LYS:HZ3	2.25	0.41
1:A:203:MET:HB3	1:A:423:PRO:HB2	2.02	0.41
1:A:561:TYR:O	1:A:564:GLN:HB3	2.21	0.41
1:A:314:ALA:H	1:A:327:VAL:CG2	2.34	0.41
1:A:46:LYS:HB2	1:A:49:LEU:HA	2.01	0.41
1:A:180:GLU:OE1	1:A:549:GLU:HG2	2.20	0.41
1:A:499:ILE:HD13	1:A:507:VAL:HG21	2.02	0.41
1:A:271:LYS:HZ2	1:A:304:GLU:HA	1.84	0.41
1:A:22:LYS:NZ	1:A:161:ASP:OD2	2.52	0.40
1:A:258:PHE:O	1:A:388:ASN:HA	2.20	0.40
1:A:66:ASP:OD2	1:A:68:ARG:NH1	2.54	0.40
1:A:50:LEU:O	1:A:209:GLY:HA2	2.22	0.40
1:A:495:LEU:CD1	1:A:513:VAL:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/571 (89%)	476 (93%)	28 (6%)	6 (1%)	10	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ASP
1	A	49	LEU
1	A	52	VAL
1	A	220	ASP
1	A	51	GLU
1	A	137	GLU

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	361/490 (74%)	281 (78%)	80 (22%)	1	0

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	THR
1	A	56	LEU
1	A	61	VAL
1	A	69	GLU
1	A	125	ILE
1	A	161	ASP
1	A	162	GLU
1	A	166	LEU
1	A	178	VAL
1	A	193	VAL
1	A	200	ARG
1	A	216	LYS
1	A	218	GLU
1	A	229	GLN

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Mol	Chain	Res	Type
1	A	232	LYS
1	A	240	GLN
1	A	241	MET
1	A	246	ARG
1	A	249	LEU
1	A	252	MET
1	A	263	ASP
1	A	274	ASN
1	A	278	ILE
1	A	282	ARG
1	A	287	THR
1	A	292	GLU
1	A	293	VAL
1	A	297	VAL
1	A	299	GLU
1	A	306	VAL
1	A	315	VAL
1	A	317	GLU
1	A	320	ARG
1	A	327	VAL
1	A	333	ARG
1	A	356	VAL
1	A	362	ILE
1	A	375	SER
1	A	376	VAL
1	A	380	ASN
1	A	383	ILE
1	A	385	SER
1	A	389	LEU
1	A	392	LYS
1	A	396	GLU
1	A	403	LYS
1	A	407	LEU
1	A	409	HIS
1	A	412	LEU
1	A	416	ARG
1	A	418	ASP
1	A	420	THR
1	A	422	GLU
1	A	429	LYS
1	A	436	THR
1	A	437	MET

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Mol	Chain	Res	Type
1	A	440	LEU
1	A	442	LEU
1	A	451	GLU
1	A	453	ARG
1	A	457	VAL
1	A	463	LEU
1	A	469	VAL
1	A	470	LYS
1	A	486	GLU
1	A	489	VAL
1	A	493	LYS
1	A	495	LEU
1	A	501	LYS
1	A	506	GLU
1	A	507	VAL
1	A	513	VAL
1	A	523	GLN
1	A	530	SER
1	A	535	ARG
1	A	543	ARG
1	A	545	ASP
1	A	554	VAL
1	A	566	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	555	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	1.50	4 (16%)	37,38,38	1.94	8 (21%)

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	-	-	7/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	AMP	C5-C4	5.17	1.48	1.39
2	A	601	AMP	C5-C6	2.86	1.48	1.41
2	A	601	AMP	C5-N7	-2.44	1.34	1.39
2	A	601	AMP	C8-N7	2.33	1.36	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	C5-C4-N3	-6.23	118.14	126.72
2	A	601	AMP	N3-C4-N9	4.81	135.35	127.17
2	A	601	AMP	C4-C5-N7	-3.86	106.17	110.58
2	A	601	AMP	C2-N3-C4	3.60	120.62	111.83
2	A	601	AMP	N3-C2-N1	-2.91	124.18	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	C5-N7-C8	2.76	107.78	103.45
2	A	601	AMP	O3P-P-O5'	-2.24	100.83	106.67
2	A	601	AMP	C4-N9-C8	2.15	108.00	105.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

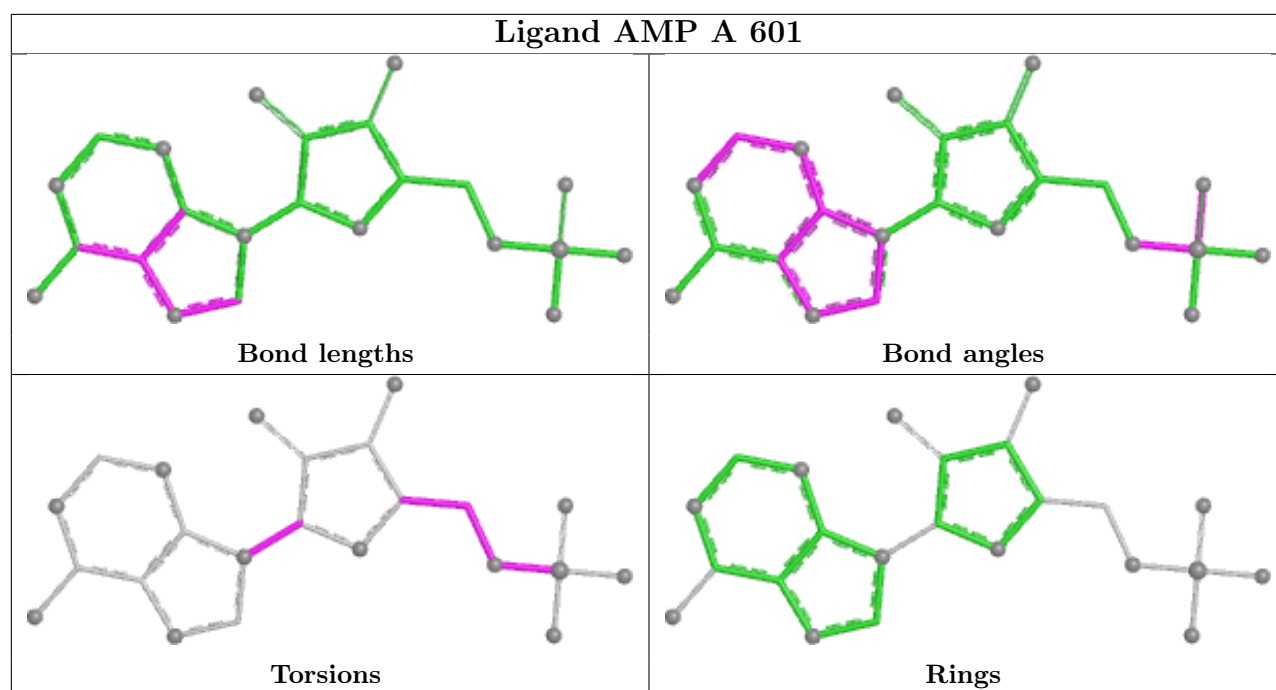
Mol	Chain	Res	Type	Atoms
2	A	601	AMP	C5'-O5'-P-O2P
2	A	601	AMP	C5'-O5'-P-O3P
2	A	601	AMP	C4'-C5'-O5'-P
2	A	601	AMP	C5'-O5'-P-O1P
2	A	601	AMP	O4'-C1'-N9-C4
2	A	601	AMP	O4'-C1'-N9-C8
2	A	601	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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, 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	509/571 (89%)	0.77	55 (10%) 11 8	32, 72, 141, 219	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	GLU	4.7
1	A	522	ILE	4.1
1	A	176	THR	3.9
1	A	143	SER	3.7
1	A	472	ASP	3.5
1	A	447	ALA	3.5
1	A	49	LEU	3.4
1	A	72	ILE	3.2
1	A	460	SER	3.1
1	A	409	HIS	3.0
1	A	502	GLU	3.0
1	A	21	TYR	2.9
1	A	411	GLY	2.9
1	A	124	THR	2.8
1	A	394	PRO	2.7
1	A	445	LEU	2.7
1	A	160	PRO	2.7
1	A	263	ASP	2.7
1	A	459	SER	2.7
1	A	536	PHE	2.6
1	A	135	ILE	2.6
1	A	503	HIS	2.5
1	A	167	ALA	2.5
1	A	24	LEU	2.4
1	A	534	LEU	2.4
1	A	62	PHE	2.4
1	A	126	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	82	SER	2.3
1	A	171	LEU	2.3
1	A	407	LEU	2.3
1	A	526	PRO	2.3
1	A	469	VAL	2.3
1	A	163	GLY	2.3
1	A	242	ALA	2.3
1	A	134	LYS	2.3
1	A	393	SER	2.2
1	A	389	LEU	2.2
1	A	141	ALA	2.2
1	A	429	LYS	2.2
1	A	139	SER	2.2
1	A	144	GLN	2.1
1	A	297	VAL	2.1
1	A	66	ASP	2.1
1	A	76	LEU	2.1
1	A	132	LEU	2.1
1	A	331	PHE	2.1
1	A	551	ALA	2.1
1	A	16	GLU	2.1
1	A	45	GLU	2.1
1	A	335	TYR	2.1
1	A	390	ILE	2.1
1	A	27	THR	2.1
1	A	164	LYS	2.0
1	A	161	ASP	2.0
1	A	150	TYR	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.

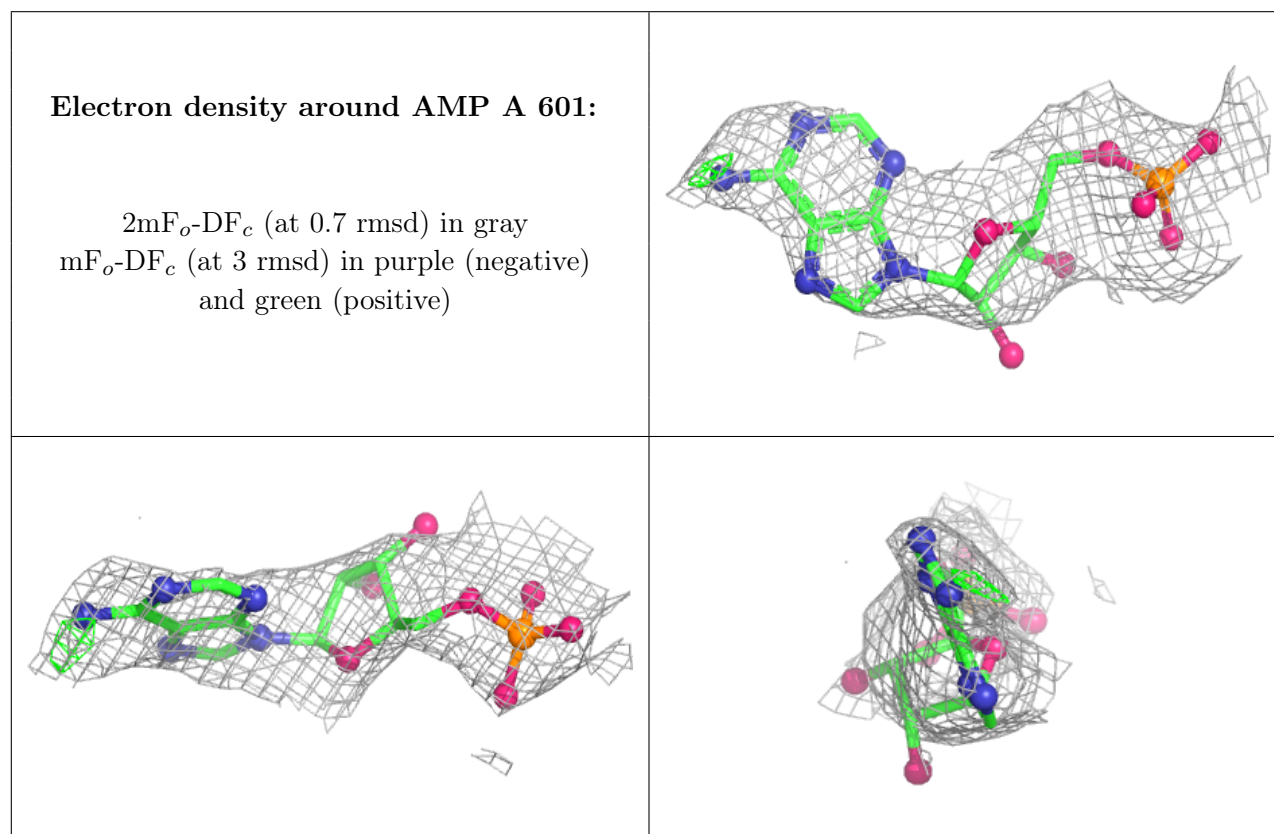
6.4 Ligands [i](#)

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
2	AMP	A	601	23/23	0.81	0.20	116,116,116,116	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.