



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 04:45 PM EDT

PDB ID : 3A8W
Title : Crystal Structure of PKC α kinase domain
Authors : Takimura, T.; Kamata, K.
Deposited on : 2009-10-11
Resolution : 2.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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)	:	2.39

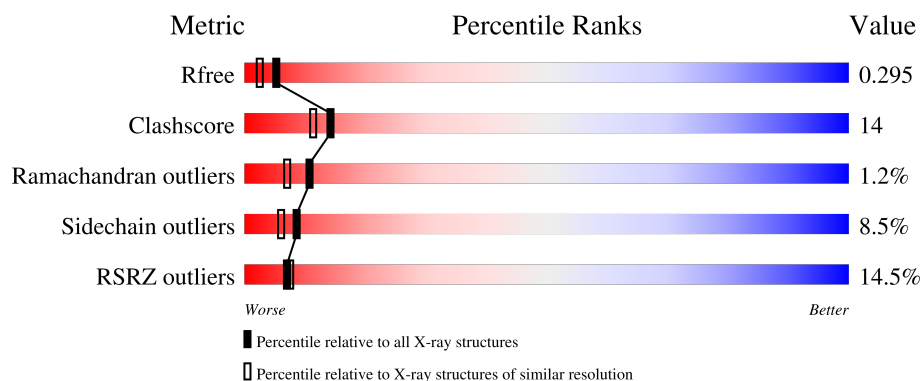
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	345	<div> <div>5%</div> <div>77%</div> <div>14%</div> <div>5%</div> </div>
1	B	345	<div> <div>23%</div> <div>60%</div> <div>30%</div> <div>6%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5598 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.

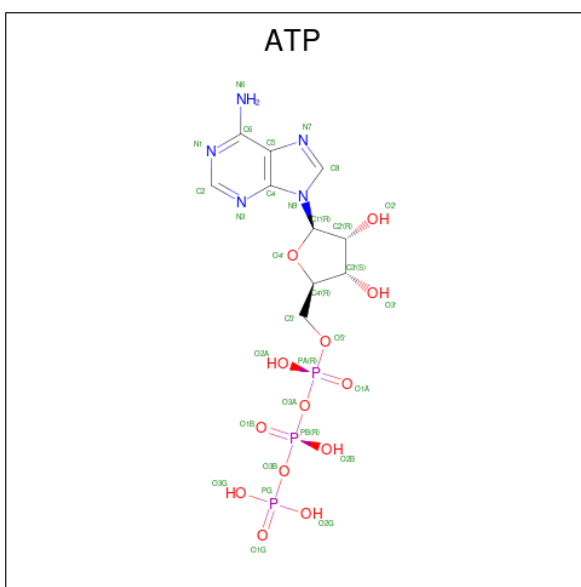
- Molecule 1 is a protein called Protein kinase C iota type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	P	S	0	0	0
			2681	1716	450	499	2	14			
1	B	329	Total	C	N	O	P	S	0	0	0
			2688	1716	448	508	2	14			

There are 10 discrepancies between the modelled and reference sequences:

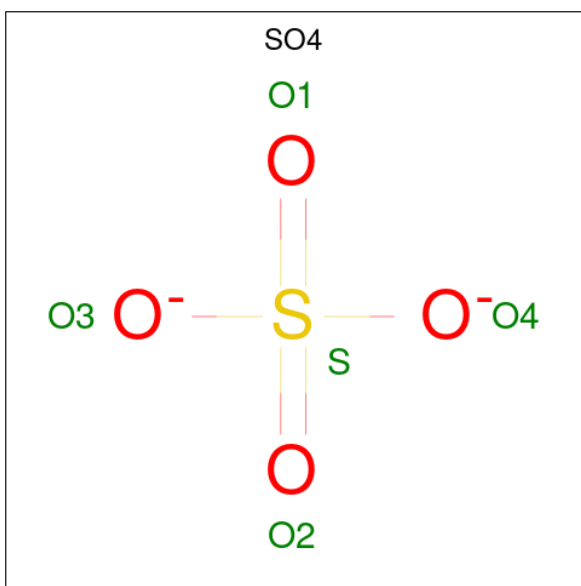
Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLY	-	expression tag	UNP P41743
A	236	ALA	-	expression tag	UNP P41743
A	237	MET	-	expression tag	UNP P41743
A	238	ASP	-	expression tag	UNP P41743
A	239	PRO	-	expression tag	UNP P41743
B	235	GLY	-	expression tag	UNP P41743
B	236	ALA	-	expression tag	UNP P41743
B	237	MET	-	expression tag	UNP P41743
B	238	ASP	-	expression tag	UNP P41743
B	239	PRO	-	expression tag	UNP P41743

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

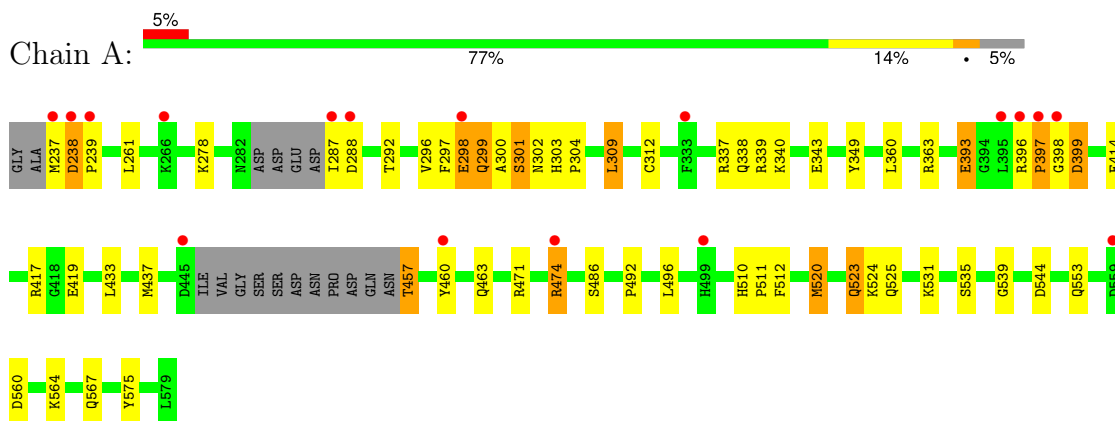
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total 87	O 87	0	0
4	B	75	Total 75	O 75	0	0

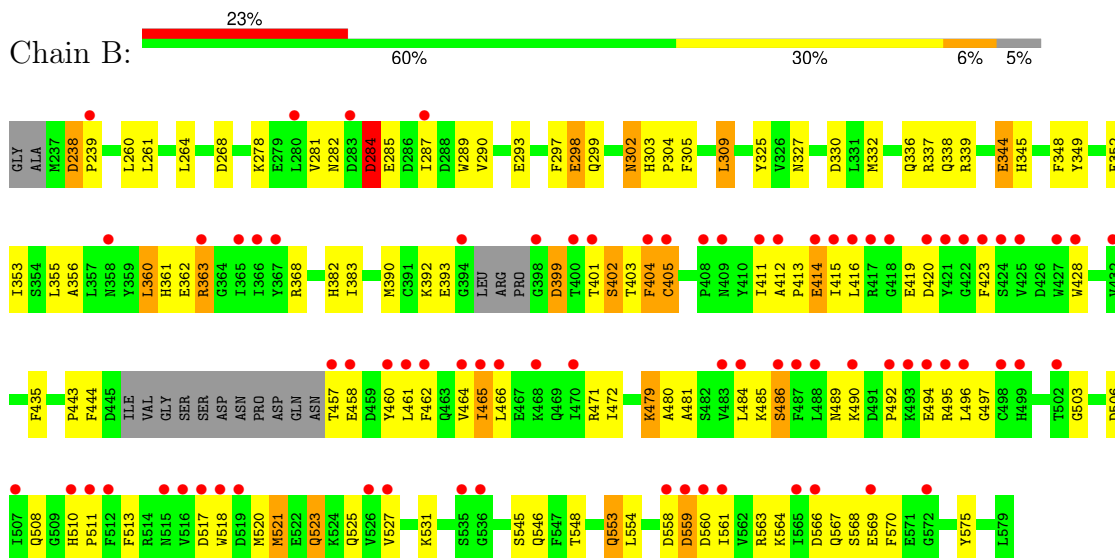
3 Residue-property plots [i](#)

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: Protein kinase C iota type



• Molecule 1: Protein kinase C iota type



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.04Å 89.14Å 206.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 2.10 40.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.92-2.10) 99.9 (40.92-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.247 , 0.301 0.245 , 0.295	Depositor DCC
R_{free} test set	2332 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5598	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4, TPO, ATP

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	0.46	1/2722 (0.0%)	0.56	0/3670
1	B	0.49	0/2728	0.61	0/3678
All	All	0.47	1/5450 (0.0%)	0.59	0/7348

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	CYS	CB-SG	-5.54	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	399	ASP	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	2681	0	2613	52	0
1	B	2688	0	2599	103	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	B	5	0	0	0	0
4	A	87	0	0	1	0
4	B	75	0	0	2	0
All	All	5598	0	5236	149	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 (149) 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:287:ILE:HD12	1:A:288:ASP:H	1.07	1.18
1:A:396:ARG:HB3	1:A:397:PRO:HD3	1.18	1.12
1:A:237:MET:CE	1:B:298:GLU:HB2	1.88	1.03
1:A:237:MET:HE1	1:B:298:GLU:HB2	1.38	1.02
1:A:397:PRO:HD2	1:A:399:ASP:HB2	1.39	1.01
1:B:523:GLN:HB2	1:B:525:GLN:OE1	1.62	0.97
1:B:559:ASP:O	1:B:563:ARG:HB2	1.65	0.96
1:B:414:GLU:HG2	1:B:492:PRO:CG	1.97	0.95
1:B:414:GLU:HG2	1:B:492:PRO:HG3	1.49	0.92
1:A:287:ILE:CD1	1:A:288:ASP:H	1.86	0.87
1:A:287:ILE:HD12	1:A:288:ASP:N	1.89	0.86
1:B:472:ILE:HG21	1:B:481:ALA:HB2	1.58	0.85
1:A:396:ARG:HB3	1:A:397:PRO:CD	2.05	0.85
1:B:401:THR:O	1:B:420:ASP:HB2	1.78	0.83
1:B:414:GLU:CG	1:B:492:PRO:HG3	2.09	0.82
1:B:299:GLN:HG2	1:B:363:ARG:HG2	1.63	0.80
1:A:398:GLY:O	1:A:399:ASP:O	1.99	0.80
1:B:405:CYS:HB3	4:B:874:HOH:O	1.82	0.79
1:B:297:PHE:HB3	1:B:309:LEU:HG	1.65	0.78
1:A:396:ARG:CB	1:A:397:PRO:HD3	2.07	0.77
1:B:349:TYR:O	1:B:353:ILE:HG13	1.84	0.77
1:B:489:ASN:ND2	1:B:494:GLU:HB3	2.04	0.73
1:B:278:LYS:HZ3	1:B:567:GLN:HE22	1.38	0.72
1:B:303:HIS:CG	1:B:304:PRO:HD2	2.25	0.71
1:B:414:GLU:HG2	1:B:492:PRO:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:HD11	1:B:521:MET:HG2	1.74	0.70
1:A:292:THR:HG23	1:A:393:GLU:HG2	1.73	0.69
1:B:497:GLY:HA2	1:B:503:GLY:O	1.94	0.68
1:A:520:MET:HG3	1:A:525:GLN:HB2	1.77	0.67
1:A:300:ALA:O	1:A:301:SER:O	2.12	0.66
1:A:457:THR:O	1:A:460:TYR:N	2.28	0.66
1:B:416:LEU:HB2	1:B:466:LEU:HD21	1.78	0.66
1:B:508:GLN:HG2	1:B:518:TRP:CE2	2.31	0.66
1:B:472:ILE:HG21	1:B:481:ALA:CB	2.26	0.66
1:A:298:GLU:HG3	1:A:299:GLN:N	2.11	0.65
1:A:417:ARG:HD2	1:A:419:GLU:OE2	1.97	0.64
1:A:278:LYS:HZ2	1:A:567:GLN:HE22	1.44	0.64
1:A:560:ASP:O	1:A:564:LYS:HD2	1.97	0.64
1:B:361:HIS:CE1	1:B:423:PHE:HB3	2.34	0.62
1:A:301:SER:O	1:A:302:ASN:HB3	1.97	0.62
1:A:474:ARG:HE	1:A:474:ARG:H	1.48	0.62
1:B:403:TPO:O	1:B:404:PHE:HB3	2.01	0.61
1:B:352:GLU:OE2	1:B:382:HIS:ND1	2.23	0.61
1:A:238:ASP:OD2	1:A:239:PRO:HD2	2.00	0.61
1:B:238:ASP:HB2	1:B:239:PRO:CD	2.31	0.61
1:B:298:GLU:HG3	1:B:299:GLN:N	2.16	0.60
1:A:237:MET:HE3	1:B:298:GLU:HB2	1.80	0.60
1:B:457:THR:HG22	1:B:460:TYR:H	1.66	0.60
1:A:414:GLU:HG3	1:A:492:PRO:HG3	1.82	0.60
1:B:518:TRP:O	1:B:521:MET:HB3	2.02	0.60
1:B:305:PHE:HB2	1:B:356:ALA:HB2	1.83	0.60
1:A:237:MET:HE1	1:B:298:GLU:CB	2.23	0.59
1:B:460:TYR:O	1:B:464:VAL:HG23	2.04	0.58
1:B:355:LEU:CD1	1:B:521:MET:HG2	2.34	0.58
1:B:278:LYS:NZ	1:B:567:GLN:HE22	2.00	0.57
1:A:278:LYS:NZ	1:A:567:GLN:HE22	2.03	0.57
1:A:553:GLN:OE1	4:A:866:HOH:O	2.17	0.57
1:B:413:PRO:HA	1:B:416:LEU:HD12	1.87	0.57
1:B:305:PHE:CZ	1:B:352:GLU:HG2	2.40	0.56
1:B:348:PHE:CE1	1:B:521:MET:HE1	2.41	0.56
1:A:474:ARG:H	1:A:474:ARG:NE	2.02	0.56
1:B:489:ASN:HD21	1:B:494:GLU:HB3	1.68	0.56
1:B:332:MET:HE2	1:B:336:GLN:HG3	1.88	0.56
1:A:303:HIS:CG	1:A:304:PRO:HD2	2.40	0.56
1:B:303:HIS:CD2	1:B:304:PRO:HD2	2.42	0.55
1:B:413:PRO:O	1:B:416:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:HIS:ND1	1:B:304:PRO:HD2	2.22	0.54
1:A:535:SER:O	1:A:539:GLY:HA2	2.08	0.53
1:B:344:GLU:H	1:B:344:GLU:CD	2.11	0.53
1:B:278:LYS:HE2	1:B:570:PHE:CD1	2.43	0.53
1:B:503:GLY:O	1:B:506:ASP:HB2	2.08	0.53
1:B:303:HIS:CE1	1:B:304:PRO:HD2	2.43	0.53
1:B:510:HIS:CG	1:B:511:PRO:HD2	2.43	0.53
1:B:435:PHE:CE2	1:B:443:PRO:HA	2.45	0.52
1:B:368:ARG:CZ	1:B:392:LYS:HB2	2.40	0.51
1:B:403:TPO:O1P	1:B:403:TPO:N	2.43	0.51
1:B:490:LYS:O	1:B:492:PRO:HD3	2.10	0.51
1:A:349:TYR:CD2	1:A:437:MET:HE1	2.46	0.51
1:B:309:LEU:HD13	1:B:575:TYR:CD2	2.46	0.51
1:B:287:ILE:HG21	1:B:569:GLU:HB3	1.93	0.51
1:A:349:TYR:HD2	1:A:437:MET:HE1	1.76	0.50
1:B:281:VAL:HG22	1:B:281:VAL:O	2.12	0.50
1:B:545:SER:HA	1:B:548:THR:OG1	2.12	0.50
1:A:292:THR:O	1:A:296:VAL:HG23	2.12	0.50
1:B:462:PHE:HA	1:B:465:ILE:HG13	1.93	0.50
1:A:486:SER:OG	1:A:496:LEU:HB2	2.12	0.49
1:B:414:GLU:CG	1:B:492:PRO:CG	2.75	0.49
1:A:301:SER:O	1:A:302:ASN:CB	2.60	0.49
1:B:289:TRP:CH2	1:B:293:GLU:HG3	2.48	0.49
1:B:461:LEU:O	1:B:465:ILE:HG13	2.12	0.49
1:A:338:GLN:O	1:A:339:ARG:HB2	2.13	0.48
1:B:428:TRP:HE3	1:B:495:ARG:HH21	1.52	0.48
1:B:508:GLN:HG2	1:B:518:TRP:CD2	2.48	0.48
1:B:492:PRO:HA	1:B:495:ARG:HH11	1.78	0.48
1:B:560:ASP:O	1:B:564:LYS:HB2	2.14	0.48
1:B:444:PHE:CZ	1:B:465:ILE:HG23	2.49	0.48
1:A:523:GLN:O	1:A:524:LYS:HB2	2.13	0.47
1:A:460:TYR:O	1:A:463:GLN:N	2.48	0.47
1:B:428:TRP:CE3	1:B:495:ARG:NH2	2.67	0.47
1:B:558:ASP:OD2	1:B:561:ILE:HG13	2.15	0.47
1:B:510:HIS:O	1:B:513:PHE:N	2.35	0.47
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.79	0.47
1:A:309:LEU:HD13	1:A:575:TYR:CD2	2.50	0.47
1:B:461:LEU:O	1:B:465:ILE:CG1	2.63	0.46
1:A:297:PHE:HB3	1:A:309:LEU:HB2	1.97	0.45
1:A:297:PHE:O	1:A:301:SER:OG	2.28	0.45
1:A:343:GLU:CG	1:A:512:PHE:HE1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLN:HE21	1:A:523:GLN:HA	1.82	0.45
1:B:330:ASP:OD2	1:B:330:ASP:C	2.55	0.45
1:B:553:GLN:HG2	1:B:554:LEU:N	2.31	0.45
1:B:338:GLN:NE2	4:B:777:HOH:O	2.43	0.45
1:A:523:GLN:HE21	1:A:523:GLN:CA	2.29	0.45
1:B:492:PRO:HA	1:B:495:ARG:NH1	2.32	0.44
1:B:559:ASP:OD1	1:B:559:ASP:N	2.51	0.44
1:B:412:ALA:O	1:B:416:LEU:HG	2.18	0.44
1:B:497:GLY:O	1:B:503:GLY:HA3	2.17	0.44
1:B:284:ASP:HB2	1:B:285:GLU:H	1.58	0.44
1:B:353:ILE:HG12	1:B:383:ILE:HD13	2.00	0.44
1:B:486:SER:HB3	1:B:496:LEU:HB2	1.99	0.43
1:B:238:ASP:HB2	1:B:239:PRO:HD2	2.00	0.43
1:B:393:GLU:O	1:B:393:GLU:HG2	2.17	0.43
1:A:567:GLN:HE21	1:A:567:GLN:HA	1.82	0.43
1:B:282:ASN:ND2	1:B:282:ASN:C	2.72	0.43
1:A:460:TYR:O	1:A:463:GLN:HB2	2.19	0.43
1:B:281:VAL:CG2	1:B:290:VAL:HG23	2.49	0.43
1:B:479:LYS:HE3	1:B:479:LYS:HB2	1.44	0.43
1:B:558:ASP:OD1	1:B:558:ASP:C	2.57	0.43
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.91	0.42
1:B:462:PHE:N	1:B:462:PHE:CD1	2.88	0.42
1:B:484:LEU:HD23	1:B:484:LEU:HA	1.81	0.42
1:B:402:SER:O	1:B:403:TPO:C	2.67	0.42
1:B:412:ALA:H	1:B:415:ILE:HD12	1.83	0.42
1:A:396:ARG:CB	1:A:397:PRO:CD	2.83	0.42
1:B:413:PRO:HD2	1:B:414:GLU:OE2	2.19	0.42
1:A:237:MET:HE2	1:B:575:TYR:CE1	2.55	0.42
1:A:510:HIS:HA	1:A:511:PRO:HD3	1.95	0.42
1:B:489:ASN:OD1	1:B:489:ASN:C	2.59	0.42
1:B:480:ALA:O	1:B:484:LEU:HB2	2.20	0.41
1:B:527:VAL:O	1:B:527:VAL:HG13	2.19	0.41
1:A:237:MET:CE	1:B:298:GLU:CB	2.79	0.41
1:B:325:TYR:CZ	1:B:327:ASN:HB3	2.55	0.41
1:B:401:THR:O	1:B:420:ASP:CB	2.60	0.41
1:B:281:VAL:HG21	1:B:290:VAL:CG2	2.50	0.41
1:B:566:ASP:OD2	1:B:568:SER:OG	2.38	0.41
1:A:338:GLN:C	1:A:340:LYS:H	2.24	0.41
1:B:553:GLN:HE21	1:B:553:GLN:HB3	1.68	0.41
1:B:517:ASP:CG	1:B:520:MET:HG3	2.41	0.40
1:B:435:PHE:CD1	1:B:443:PRO:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:CG1	1:A:288:ASP:H	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/345 (93%)	293 (92%)	24 (8%)	3 (1%)	14	11
1	B	321/345 (93%)	293 (91%)	23 (7%)	5 (2%)	8	4
All	All	641/690 (93%)	586 (91%)	47 (7%)	8 (1%)	11	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	SER
1	A	397	PRO
1	A	399	ASP
1	B	284	ASP
1	B	302	ASN
1	B	399	ASP
1	B	390	MET
1	B	404	PHE

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	292/306 (95%)	275 (94%)	17 (6%)	17	15
1	B	293/306 (96%)	260 (89%)	33 (11%)	4	2
All	All	585/612 (96%)	535 (92%)	50 (8%)	8	6

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	A	261	LEU
1	A	298	GLU
1	A	299	GLN
1	A	309	LEU
1	A	337	ARG
1	A	360	LEU
1	A	363	ARG
1	A	393	GLU
1	A	433	LEU
1	A	457	THR
1	A	471	ARG
1	A	474	ARG
1	A	520	MET
1	A	523	GLN
1	A	531	LYS
1	A	544	ASP
1	B	238	ASP
1	B	260	LEU
1	B	261	LEU
1	B	264	LEU
1	B	268	ASP
1	B	284	ASP
1	B	298	GLU
1	B	302	ASN
1	B	309	LEU
1	B	337	ARG
1	B	339	ARG
1	B	344	GLU
1	B	345	HIS
1	B	360	LEU
1	B	362	GLU
1	B	363	ARG
1	B	402	SER
1	B	405	CYS

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Mol	Chain	Res	Type
1	B	411	ILE
1	B	414	GLU
1	B	419	GLU
1	B	458	GLU
1	B	465	ILE
1	B	471	ARG
1	B	479	LYS
1	B	485	LYS
1	B	486	SER
1	B	521	MET
1	B	523	GLN
1	B	531	LYS
1	B	546	GLN
1	B	553	GLN
1	B	559	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	508	GLN
1	A	523	GLN
1	A	567	GLN
1	B	546	GLN
1	B	553	GLN
1	B	567	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	B	555	1	8,10,11	0.99	0	10,14,16	1.20	0
1	TPO	A	403	1	8,10,11	0.63	0	10,14,16	1.14	0
1	TPO	B	403	1	8,10,11	0.82	0	10,14,16	1.07	0
1	TPO	A	555	1	8,10,11	0.84	0	10,14,16	1.03	0

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
1	TPO	B	555	1	-	0/9/11/13	-
1	TPO	A	403	1	-	0/9/11/13	-
1	TPO	B	403	1	-	1/9/11/13	-
1	TPO	A	555	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	403	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	403	TPO	3	0

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$
3	SO4	B	611	-	4,4,4	0.22	0	6,6,6	0.25	0
2	ATP	A	601	-	28,33,33	0.92	1 (3%)	34,52,52	1.37	4 (11%)
2	ATP	B	601	-	28,33,33	1.37	3 (10%)	34,52,52	1.39	4 (11%)

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	ATP	A	601	-	-	2/18/38/38	0/3/3/3
2	ATP	B	601	-	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ATP	PA-O3A	4.70	1.64	1.59
2	B	601	ATP	PB-O3A	2.71	1.62	1.59
2	B	601	ATP	PB-O3B	2.37	1.62	1.59
2	A	601	ATP	PA-O3A	2.02	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	N3-C2-N1	-4.75	122.22	128.67
2	A	601	ATP	N3-C2-N1	-4.30	122.83	128.67
2	A	601	ATP	O3B-PB-O1B	-3.12	101.32	110.70
2	A	601	ATP	C4-C5-N7	-2.87	106.30	109.34
2	B	601	ATP	O3G-PG-O2G	2.36	116.64	107.80
2	B	601	ATP	N6-C6-N1	2.31	123.26	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	O3B-PB-O1B	-2.28	103.86	110.70
2	A	601	ATP	O2A-PA-O3A	2.00	112.68	107.27

There are no chirality outliers.

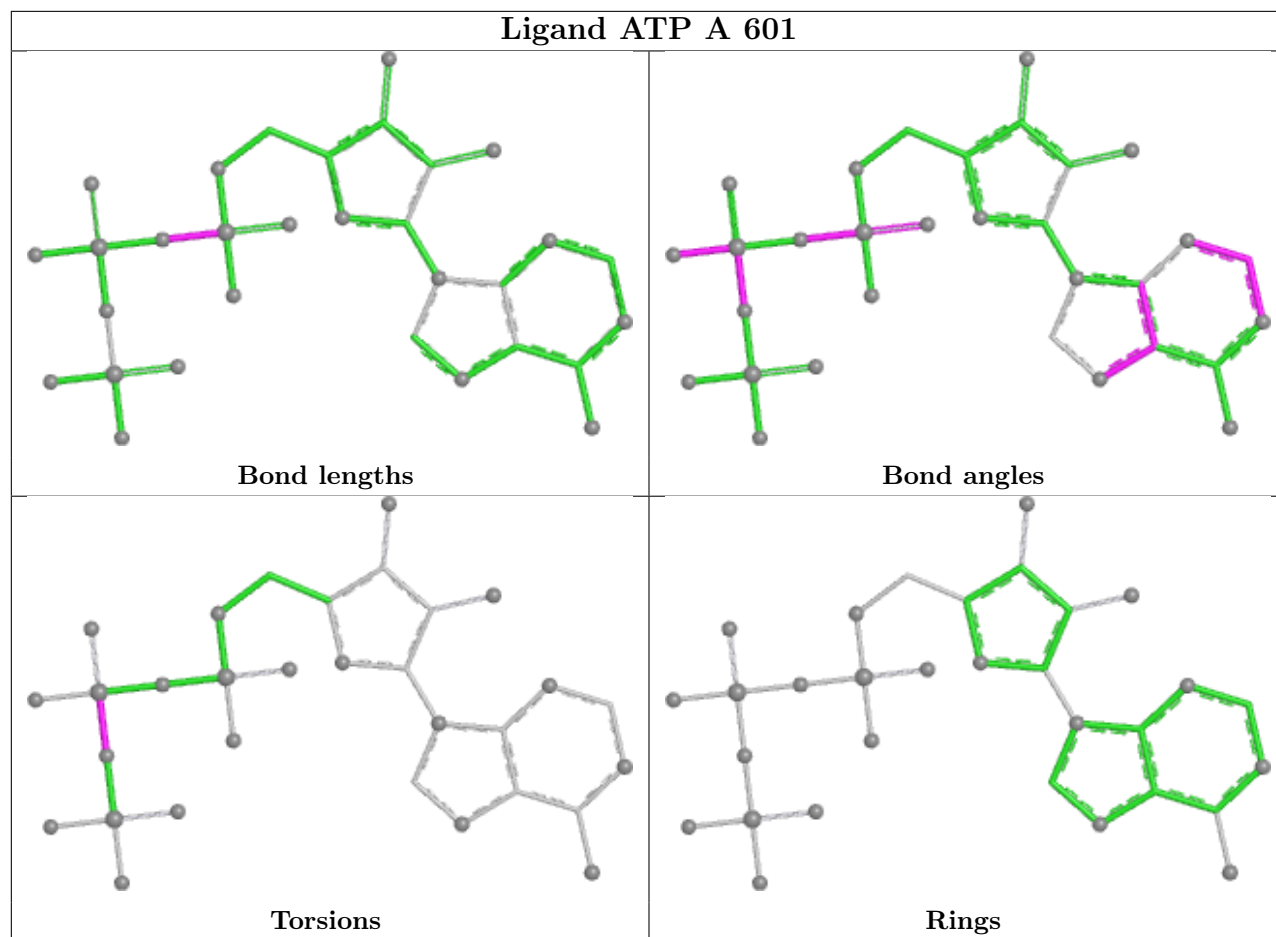
All (4) torsion outliers are listed below:

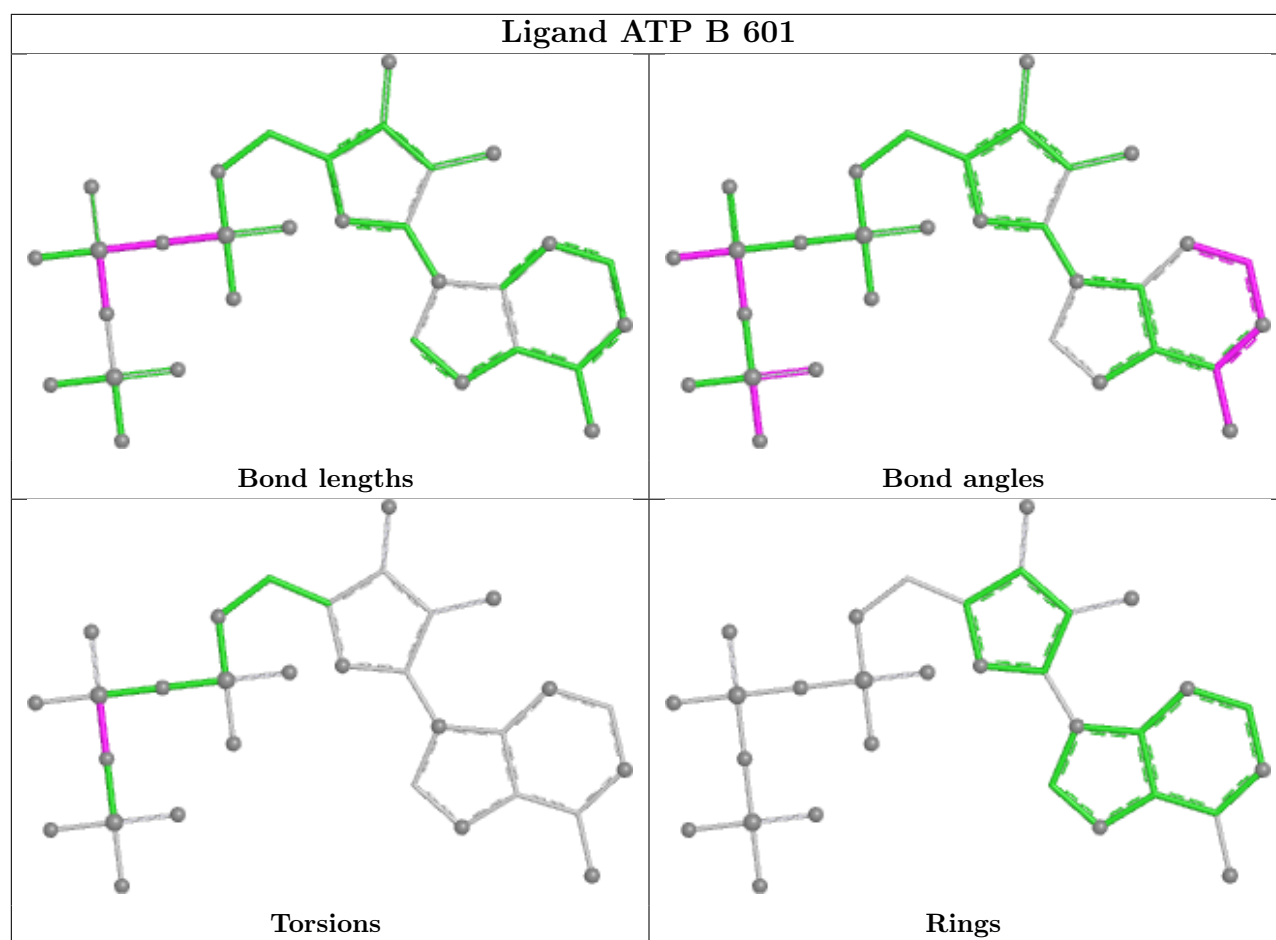
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	PG-O3B-PB-O1B
2	B	601	ATP	PG-O3B-PB-O2B
2	A	601	ATP	PG-O3B-PB-O2B
2	B	601	ATP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [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	326/345 (94%)	0.40	17 (5%) 34 36	14, 30, 49, 62	0
1	B	327/345 (94%)	1.09	78 (23%) 2 2	8, 33, 55, 70	0
All	All	653/690 (94%)	0.75	95 (14%) 7 7	8, 31, 53, 70	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	PHE	5.5
1	A	287	ILE	5.5
1	B	420	ASP	5.5
1	B	470	ILE	4.7
1	B	423	PHE	4.2
1	A	238	ASP	4.1
1	B	561	ILE	4.1
1	B	415	ILE	4.0
1	B	421	TYR	3.9
1	B	461	LEU	3.8
1	B	464	VAL	3.7
1	B	408	PRO	3.6
1	B	496	LEU	3.6
1	B	526	VAL	3.6
1	B	411	ILE	3.5
1	B	488	LEU	3.5
1	B	460	TYR	3.4
1	B	417	ARG	3.4
1	B	565	ILE	3.4
1	B	424	SER	3.3
1	B	492	PRO	3.3
1	B	536	GLY	3.3
1	B	493	LYS	3.2
1	B	465	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	466	LEU	3.2
1	B	366	ILE	3.2
1	B	560	ASP	3.2
1	B	468	LYS	3.1
1	B	457	THR	3.1
1	B	502	THR	3.1
1	B	458	GLU	3.1
1	A	397	PRO	3.0
1	B	515	ASN	3.0
1	B	394	GLY	3.0
1	B	412	ALA	3.0
1	B	418	GLY	2.9
1	B	462	PHE	2.9
1	B	512	PHE	2.9
1	B	427	TRP	2.9
1	B	398	GLY	2.9
1	B	416	LEU	2.9
1	B	518	TRP	2.9
1	A	395	LEU	2.9
1	B	425	VAL	2.9
1	B	409	ASN	2.9
1	A	333	PHE	2.8
1	A	460	TYR	2.8
1	B	484	LEU	2.8
1	B	495	ARG	2.7
1	B	566	ASP	2.7
1	B	363	ARG	2.7
1	B	499	HIS	2.7
1	B	487	PHE	2.7
1	B	428	TRP	2.6
1	B	507	ILE	2.6
1	B	432	VAL	2.6
1	B	365	ILE	2.6
1	A	474	ARG	2.6
1	B	511	PRO	2.5
1	B	287	ILE	2.5
1	B	535	SER	2.5
1	A	237	MET	2.5
1	B	483	VAL	2.5
1	B	239	PRO	2.5
1	B	414	GLU	2.5
1	A	445	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	401	THR	2.5
1	A	288	ASP	2.4
1	B	367	TYR	2.4
1	B	516	VAL	2.4
1	A	398	GLY	2.4
1	B	422	GLY	2.4
1	B	559	ASP	2.4
1	B	280	LEU	2.4
1	A	396	ARG	2.4
1	B	558	ASP	2.4
1	B	498	CYS	2.3
1	B	405	CYS	2.3
1	A	239	PRO	2.3
1	B	519	ASP	2.3
1	B	569	GLU	2.3
1	A	559	ASP	2.3
1	B	517	ASP	2.3
1	B	486	SER	2.2
1	B	572	GLY	2.2
1	B	400	THR	2.2
1	B	358	ASN	2.2
1	A	499	HIS	2.1
1	B	527	VAL	2.1
1	B	494	GLU	2.1
1	A	266	LYS	2.1
1	A	298	GLU	2.0
1	B	283	ASP	2.0
1	B	510	HIS	2.0
1	B	490	LYS	2.0

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

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(\AA^2)	Q<0.9
1	TPO	B	403	11/12	0.64	0.19	53,54,58,60	0
1	TPO	A	403	11/12	0.93	0.10	31,33,35,35	0
1	TPO	B	555	11/12	0.95	0.09	19,32,36,36	0
1	TPO	A	555	11/12	0.97	0.06	18,25,32,33	0

6.3 Carbohydrates [i](#)

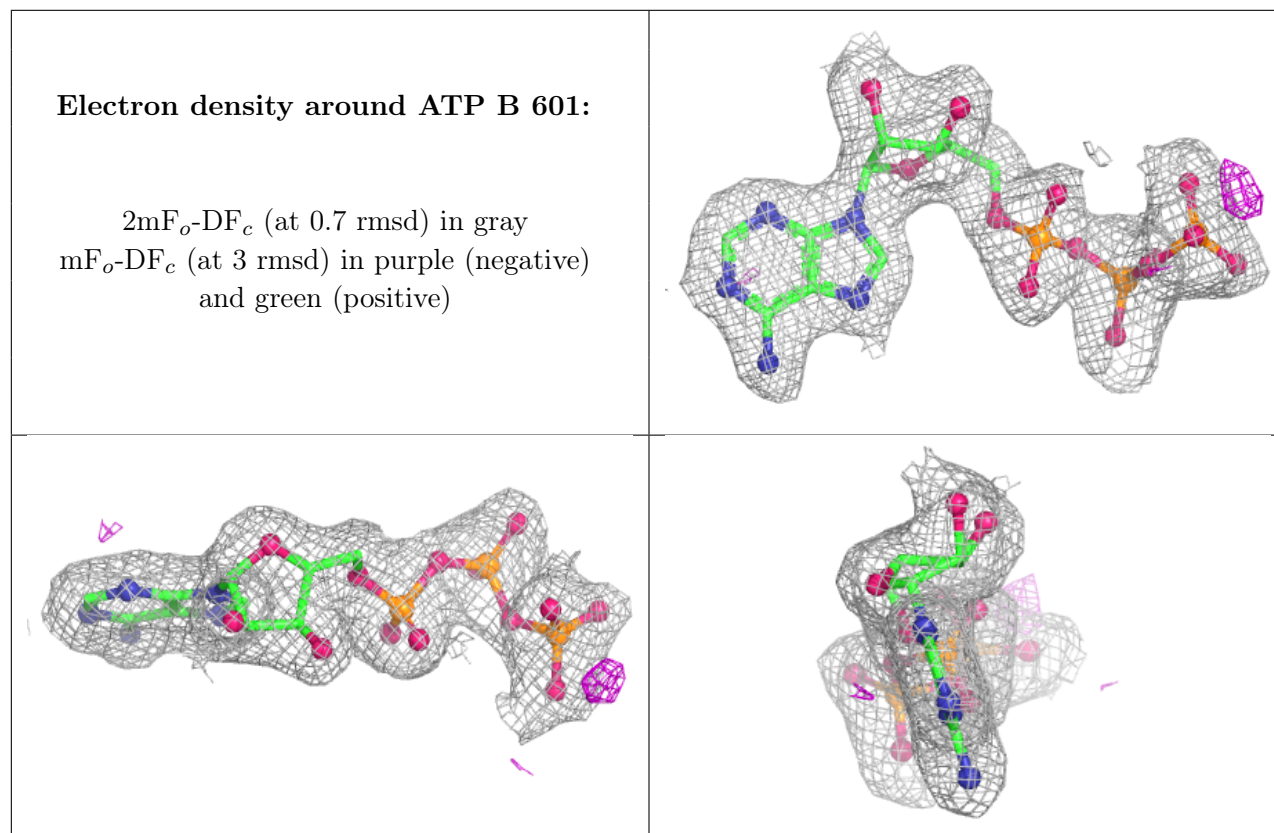
There are no monosaccharides in this entry.

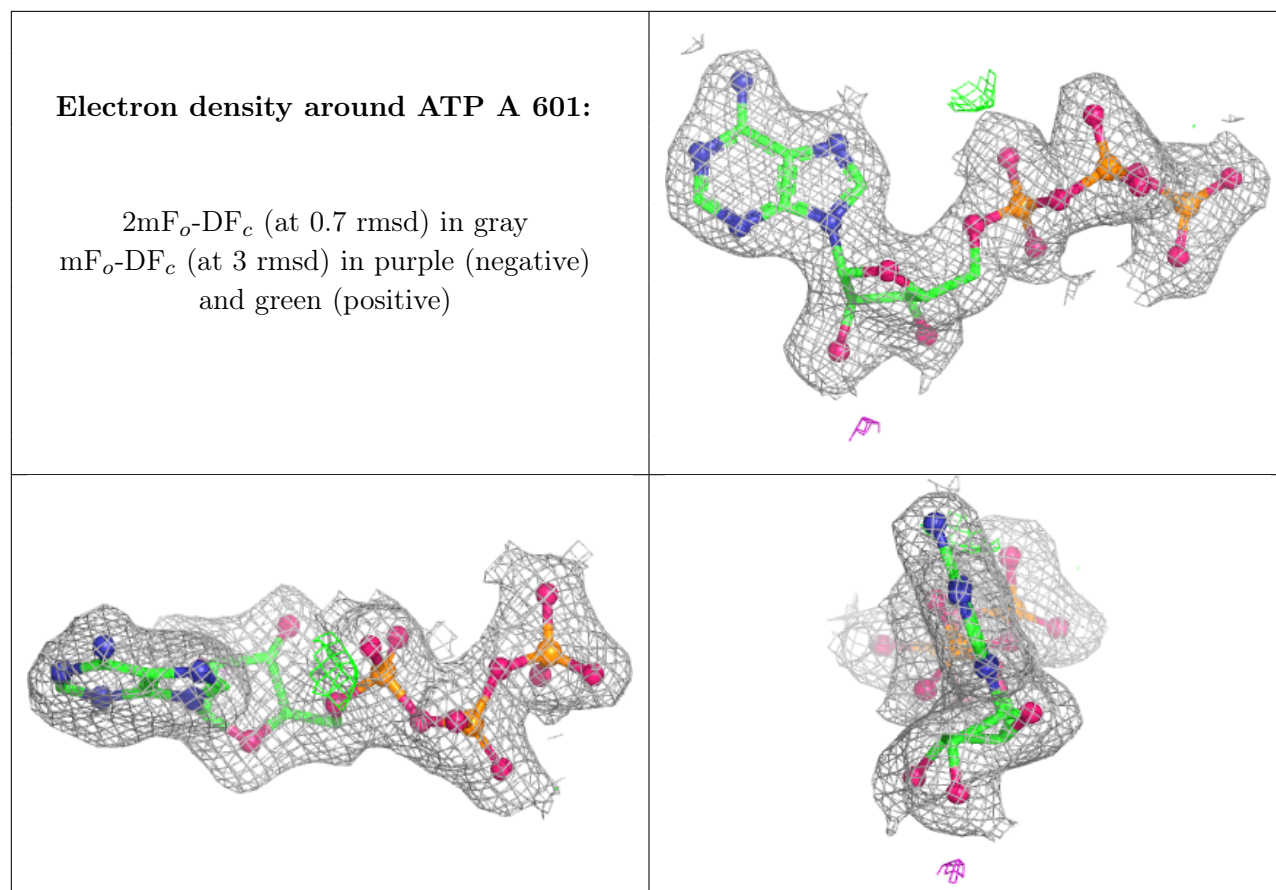
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
2	ATP	B	601	31/31	0.97	0.06	8,15,28,33	0
3	SO4	B	611	5/5	0.97	0.06	31,33,36,37	0
2	ATP	A	601	31/31	0.98	0.05	14,20,24,27	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 ⓘ

There are no such residues in this entry.