



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 3A8W / pdb_00003a8w
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	:	4-5-2 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

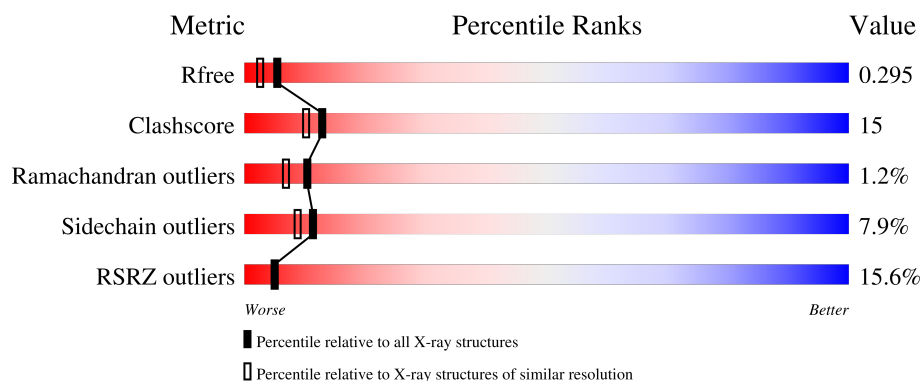
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	6% 77% 15% • 5%
1	B	345	24% 57% 33% 5% • 5%

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

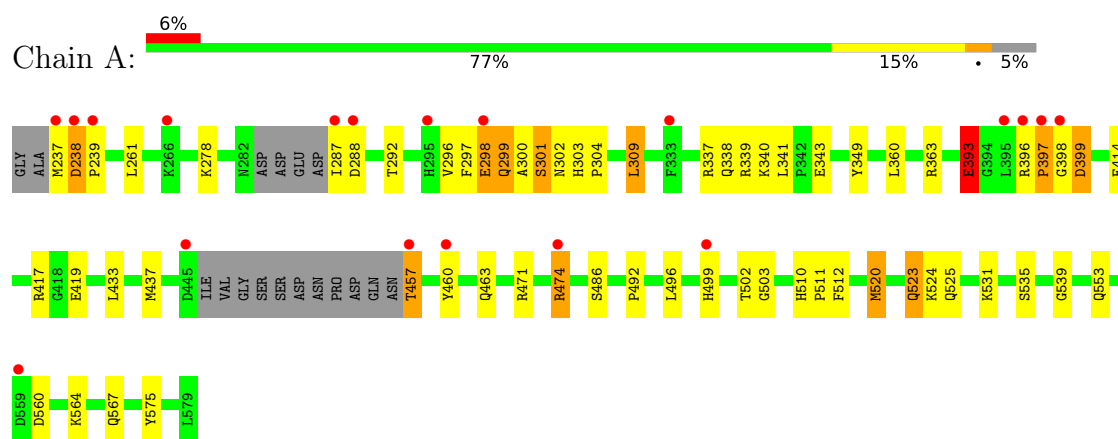
- Molecule 4 is water.

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

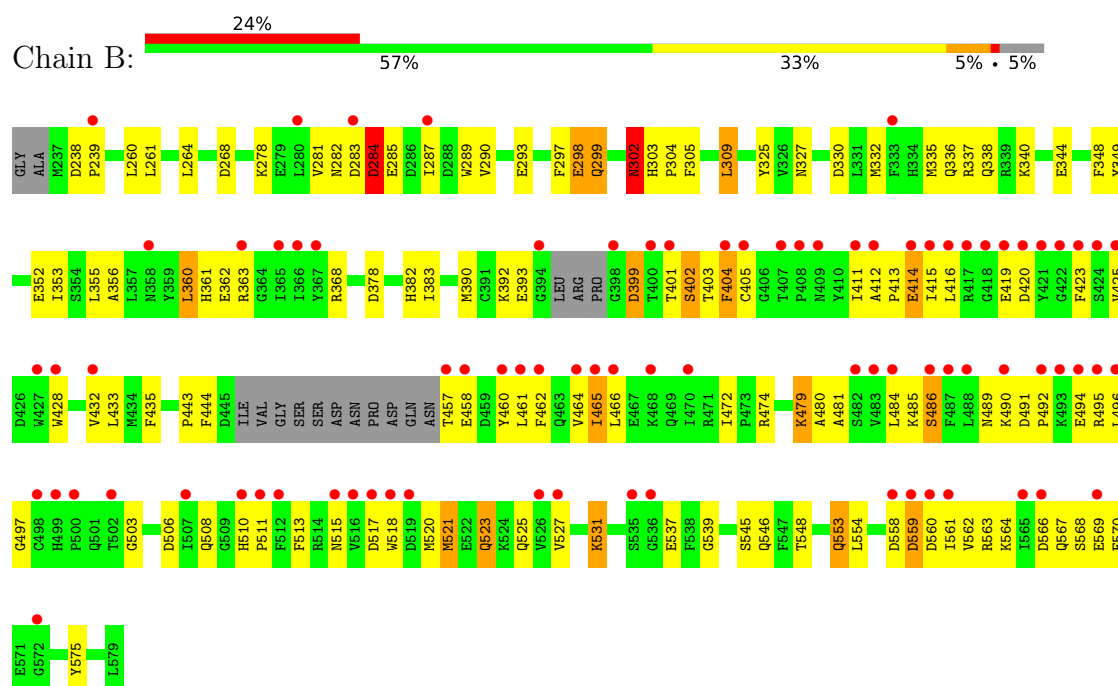
3 Residue-property plots [i](#)

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: TPO, SO4, 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	0.55	0/2722	0.84	3/3670 (0.1%)
1	B	0.60	0/2728	0.86	5/3678 (0.1%)
All	All	0.58	0/5450	0.85	8/7348 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	499	HIS	CA-C-N	7.19	128.83	119.84
1	A	499	HIS	C-N-CA	7.19	128.83	119.84
1	B	302	ASN	N-CA-C	6.02	123.62	110.80
1	B	491	ASP	CA-C-N	5.49	124.95	119.24
1	B	491	ASP	C-N-CA	5.49	124.95	119.24
1	B	433	LEU	N-CA-C	-5.41	105.46	111.36
1	A	393	GLU	N-CA-C	5.39	116.92	109.54
1	B	432	VAL	CB-CA-C	-5.00	105.39	112.14

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	55	0
1	B	2688	0	2600	112	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	5237	161	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 15.

All (161) 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:397:PRO:HD2	1:A:399:ASP:HB2	1.39	1.01
1:A:237:MET:HE3	1:B:298:GLU:HB2	1.44	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:237:MET:HE1	1:B:298:GLU:HB2	1.75	0.67
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:A:237:MET:HE2	1:B:575:TYR:CE1	2.33	0.62
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: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:349:TYR:HB2	1:A:437:MET:HE1	1.84	0.59
1:A:349:TYR:CB	1:A:437:MET:HE1	2.33	0.58
1:B:344:GLU:H	1:B:344:GLU:CD	2.11	0.58
1:B:460:TYR:O	1:B:464:VAL:HG23	2.04	0.58
1:B:278:LYS:NZ	1:B:567:GLN:HE22	2.00	0.58
1:B:355:LEU:CD1	1:B:521:MET:HG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:348:PHE:CE1	1:B:521:MET:HE1	2.44	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:A:237:MET:HE2	1:B:575:TYR:CD1	2.45	0.51
1:B:490:LYS:O	1:B:492:PRO:HD3	2.10	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: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:278:LYS:HZ3	1:B:567:GLN:HE22	1.59	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:330:ASP:OD2	1:B:330:ASP:C	2.55	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:335:MET:HE1	1:B:340:LYS:HA	1.96	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:282:ASN:ND2	1:B:282:ASN:C	2.72	0.48
1:B:444:PHE:CZ	1:B:465:ILE:HG23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLN:O	1:A:524:LYS:HB2	2.13	0.47
1:B:558:ASP:OD1	1:B:558:ASP:C	2.57	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:489:ASN:C	1:B:489:ASN:OD1	2.59	0.46
1:B:461:LEU:O	1:B:465:ILE:CG1	2.63	0.46
1:B:403:TPO:O1P	1:B:403:TPO:N	2.43	0.46
1:A:338:GLN:C	1:A:340:LYS:H	2.24	0.46
1:A:297:PHE:HB3	1:A:309:LEU:HB2	1.97	0.45
1:A:349:TYR:CD2	1:A:437:MET:HE1	2.51	0.45
1:A:297:PHE:O	1:A:301:SER:OG	2.28	0.45
1:A:341:LEU:HD12	1:A:437:MET:HE2	1.99	0.45
1:A:343:GLU:CG	1:A:512:PHE:HE1	2.29	0.45
1:A:523:GLN:HE21	1:A:523:GLN:HA	1.82	0.45
1:B:517:ASP:CG	1:B:520:MET:HG3	2.41	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:531:LYS:C	1:B:531:LYS:HD2	2.43	0.43
1:B:523:GLN:HB2	1:B:525:GLN:CD	2.40	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:A:502:THR:O	1:A:503:GLY:C	2.61	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:414:GLU:CD	1:B:492:PRO:HG3	2.45	0.42
1:A:396:ARG:CB	1:A:397:PRO:CD	2.83	0.42
1:B:378:ASP:OD2	1:B:378:ASP:C	2.63	0.42
1:B:413:PRO:HD2	1:B:414:GLU:OE2	2.19	0.42
1:B:562:VAL:C	1:B:564:LYS:N	2.76	0.42
1:A:510:HIS:HA	1:A:511:PRO:HD3	1.95	0.42
1:B:537:GLU:C	1:B:539:GLY:H	2.28	0.42
1:B:283:ASP:O	1:B:284:ASP:C	2.62	0.41
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:562:VAL:O	1:B:563:ARG:C	2.63	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:B:332:MET:HE2	1:B:336:GLN:HG3	2.02	0.41
1:B:553:GLN:HE21	1:B:553:GLN:HB3	1.68	0.41
1:B:435:PHE:CD1	1:B:443:PRO:HB3	2.57	0.40
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	10
1	B	321/345 (93%)	293 (91%)	23 (7%)	5 (2%)	7	4
All	All	641/690 (93%)	586 (91%)	47 (7%)	8 (1%)	10	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%)	276 (94%)	16 (6%)	19	18
1	B	293/306 (96%)	263 (90%)	30 (10%)	7	4
All	All	585/612 (96%)	539 (92%)	46 (8%)	11	9

All (46) 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

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Mol	Chain	Res	Type
1	A	531	LYS
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	299	GLN
1	B	302	ASN
1	B	309	LEU
1	B	337	ARG
1	B	360	LEU
1	B	362	GLU
1	B	402	SER
1	B	411	ILE
1	B	414	GLU
1	B	419	GLU
1	B	425	VAL
1	B	458	GLU
1	B	465	ILE
1	B	474	ARG
1	B	479	LYS
1	B	485	LYS
1	B	486	SER
1	B	515	ASN
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	336	GLN
1	A	523	GLN
1	A	567	GLN
1	B	291	GLN
1	B	302	ASN
1	B	358	ASN

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Mol	Chain	Res	Type
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	A	555	1	8,10,11	0.84	0	10,14,16	1.03	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	B	555	1	8,10,11	0.99	0	10,14,16	1.20	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	A	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	B	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ATP	A	601	-	32,33,33	1.38	6 (18%)	48,52,52	1.84	13 (27%)
2	ATP	B	601	-	32,33,33	1.62	6 (18%)	48,52,52	1.90	14 (29%)
3	SO4	B	611	-	4,4,4	0.22	0	6,6,6	0.25	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
2	ATP	A	601	-	-	2/22/38/38	0/3/3/3
2	ATP	B	601	-	-	2/22/38/38	0/3/3/3

All (12) 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	A	601	ATP	C5-C4	4.54	1.47	1.39
2	B	601	ATP	C5-C4	4.45	1.47	1.39
2	B	601	ATP	PB-O3A	2.71	1.62	1.59
2	A	601	ATP	C8-N7	2.68	1.36	1.31
2	A	601	ATP	C5-N7	-2.60	1.34	1.39
2	B	601	ATP	C8-N7	2.59	1.36	1.31
2	B	601	ATP	PB-O3B	2.37	1.62	1.59
2	A	601	ATP	C5-C6	2.29	1.47	1.41
2	B	601	ATP	C5-C6	2.14	1.46	1.41
2	A	601	ATP	C4-N9	-2.07	1.33	1.37
2	A	601	ATP	PA-O3A	2.02	1.61	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	C5-C4-N3	-5.52	119.12	126.72
2	A	601	ATP	C5-C4-N3	-5.27	119.46	126.72
2	B	601	ATP	N3-C4-N9	4.67	135.12	127.17
2	B	601	ATP	N3-C2-N1	-4.20	122.22	128.58
2	B	601	ATP	C2-N3-C4	3.96	121.51	111.83
2	A	601	ATP	N3-C4-N9	3.93	133.85	127.17
2	A	601	ATP	N3-C2-N1	-3.80	122.83	128.58
2	A	601	ATP	C4-C5-N7	-3.74	106.30	110.58
2	A	601	ATP	C2-N3-C4	3.61	120.64	111.83
2	A	601	ATP	C2'-C1'-N9	-3.34	105.00	113.30
2	B	601	ATP	C4-N9-C8	3.33	109.23	105.74
2	A	601	ATP	O3B-PB-O1B	-3.12	101.32	110.70
2	B	601	ATP	C2'-C1'-N9	-3.07	105.67	113.30
2	A	601	ATP	C5-N7-C8	2.78	107.82	103.45
2	A	601	ATP	C4-N9-C8	2.76	108.64	105.74
2	B	601	ATP	C4-C5-N7	-2.70	107.49	110.58
2	A	601	ATP	C6-C5-N7	2.46	136.82	132.09
2	A	601	ATP	N9-C8-N7	-2.39	110.55	113.94
2	B	601	ATP	O3G-PG-O2G	2.36	116.64	107.80
2	B	601	ATP	C2-N1-C6	2.31	122.52	118.73
2	B	601	ATP	N9-C8-N7	-2.31	110.67	113.94
2	A	601	ATP	C2-N1-C6	2.28	122.48	118.73
2	B	601	ATP	O3B-PB-O1B	-2.28	103.86	110.70
2	B	601	ATP	C5-N7-C8	2.20	106.91	103.45
2	B	601	ATP	N6-C6-N1	2.19	123.26	118.38
2	B	601	ATP	C6-C5-N7	2.02	135.97	132.09
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:

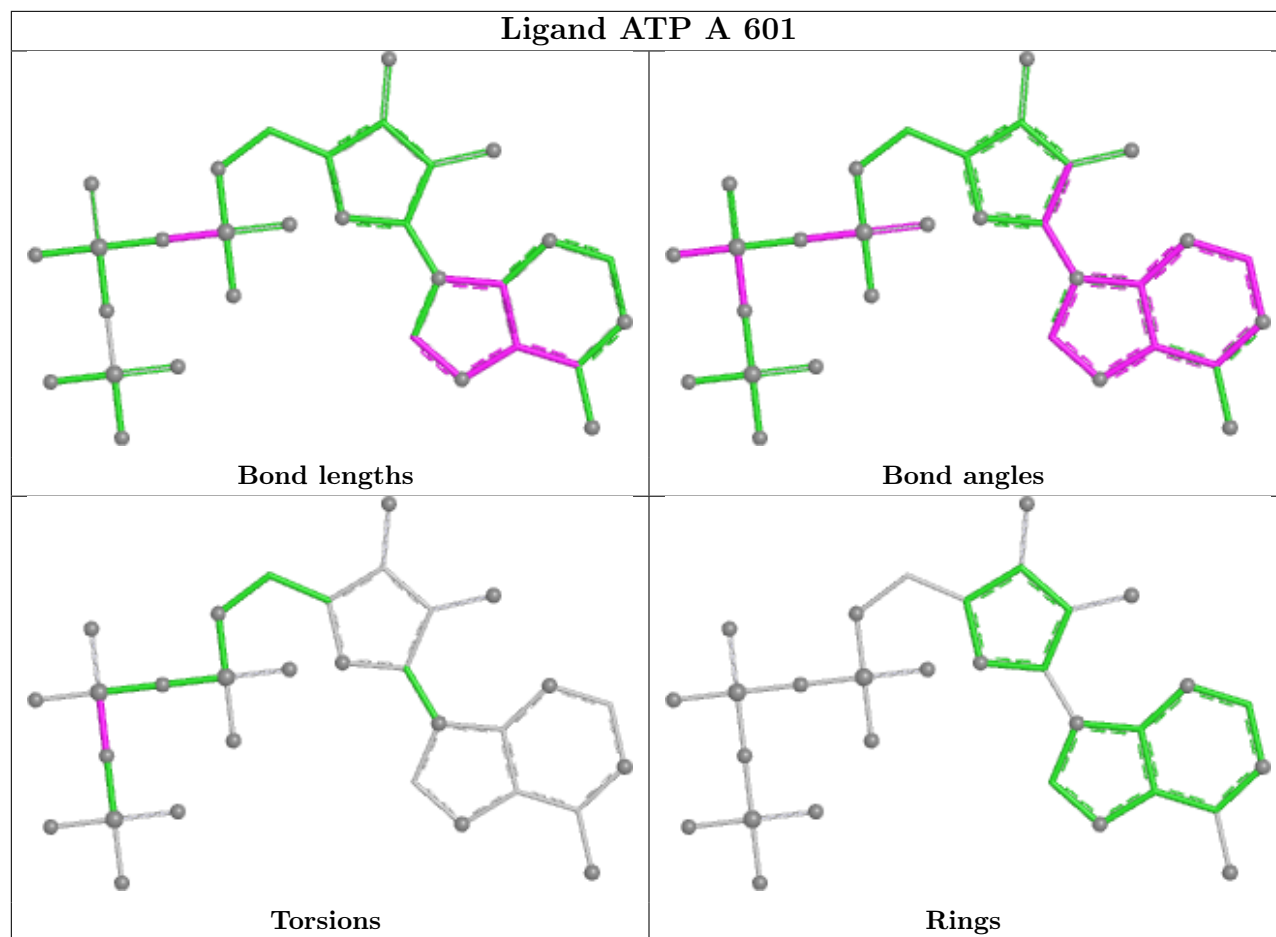
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	PG-O3B-PB-O1B
2	B	601	ATP	PG-O3B-PB-O2B
2	A	601	ATP	PG-O3B-PB-O2B
2	B	601	ATP	PG-O3B-PB-O1B

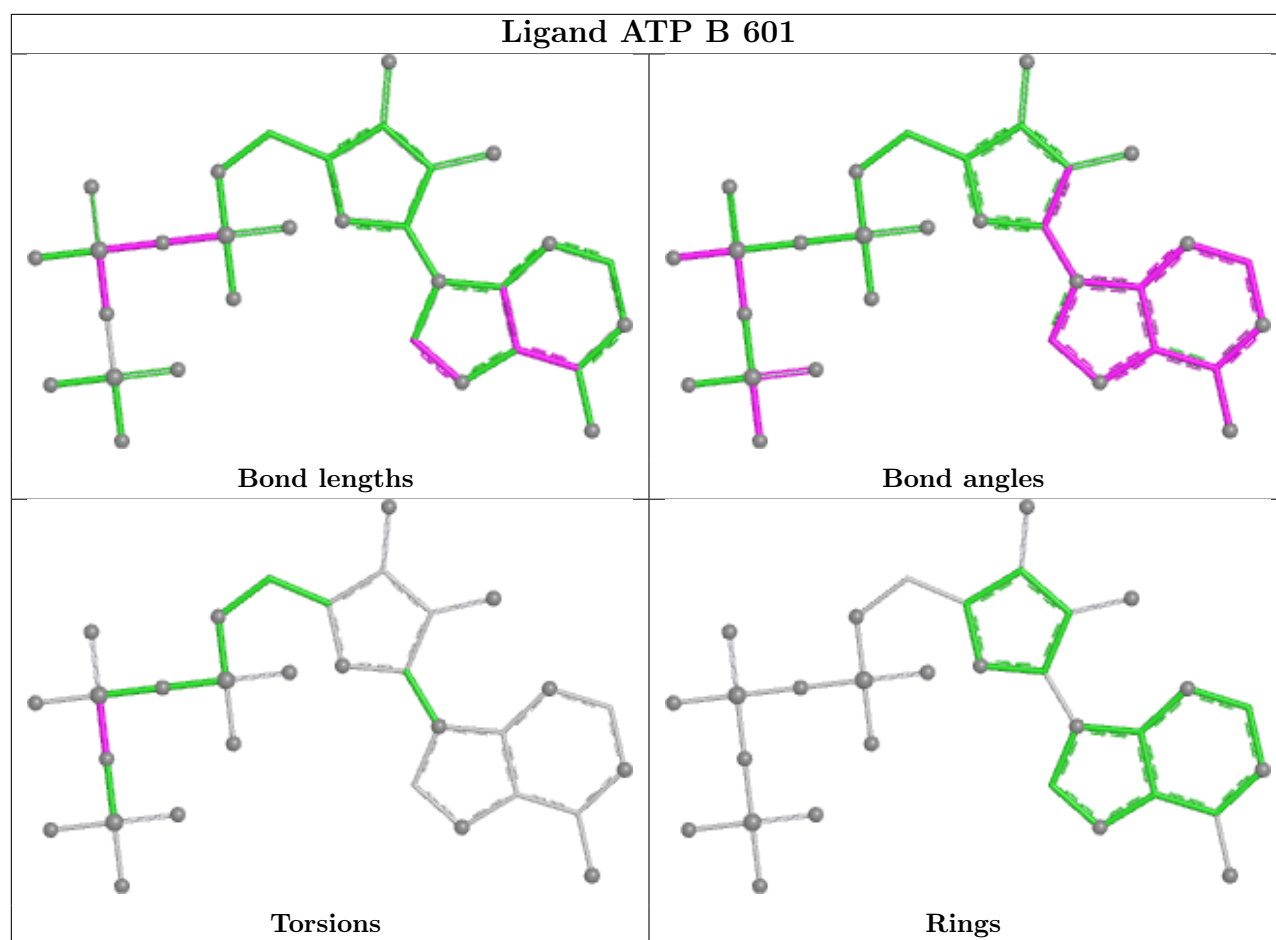
There are no ring outliers.

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.

Ligand ATP A 601





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%)	0.50	19 (5%) 29 30	14, 30, 49, 62	0
1	B	327/345 (94%)	1.20	83 (25%) 1 2	8, 33, 55, 70	0
All	All	653/690 (94%)	0.85	102 (15%) 5 5	8, 31, 53, 70	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	PHE	5.8
1	A	287	ILE	5.7
1	B	420	ASP	5.5
1	B	470	ILE	4.9
1	B	423	PHE	4.4
1	B	561	ILE	4.3
1	A	238	ASP	4.2
1	B	415	ILE	4.1
1	B	421	TYR	4.1
1	B	461	LEU	4.0
1	B	464	VAL	3.9
1	B	496	LEU	3.8
1	B	408	PRO	3.8
1	B	526	VAL	3.7
1	B	411	ILE	3.7
1	B	488	LEU	3.6
1	B	460	TYR	3.6
1	B	565	ILE	3.5
1	B	536	GLY	3.5
1	B	417	ARG	3.5
1	B	492	PRO	3.4
1	B	424	SER	3.4
1	B	465	ILE	3.4
1	B	466	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	366	ILE	3.3
1	B	493	LYS	3.3
1	B	560	ASP	3.3
1	B	457	THR	3.2
1	B	502	THR	3.2
1	A	397	PRO	3.2
1	B	468	LYS	3.2
1	B	394	GLY	3.1
1	B	515	ASN	3.1
1	B	412	ALA	3.1
1	B	427	TRP	3.1
1	B	458	GLU	3.1
1	B	418	GLY	3.1
1	B	462	PHE	3.1
1	B	512	PHE	3.1
1	B	518	TRP	3.1
1	B	398	GLY	3.1
1	B	416	LEU	3.1
1	A	395	LEU	3.0
1	B	425	VAL	3.0
1	B	409	ASN	3.0
1	A	333	PHE	3.0
1	A	460	TYR	2.9
1	B	484	LEU	2.9
1	B	487	PHE	2.8
1	B	566	ASP	2.8
1	B	428	TRP	2.8
1	B	495	ARG	2.8
1	B	499	HIS	2.8
1	B	363	ARG	2.8
1	B	507	ILE	2.8
1	B	432	VAL	2.7
1	B	365	ILE	2.7
1	B	511	PRO	2.7
1	B	287	ILE	2.7
1	B	535	SER	2.6
1	B	483	VAL	2.6
1	A	474	ARG	2.6
1	A	237	MET	2.6
1	B	239	PRO	2.6
1	B	401	THR	2.6
1	B	367	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	445	ASP	2.6
1	B	414	GLU	2.5
1	B	516	VAL	2.5
1	A	398	GLY	2.5
1	B	422	GLY	2.5
1	A	288	ASP	2.5
1	B	280	LEU	2.5
1	B	498	CYS	2.5
1	B	559	ASP	2.5
1	B	558	ASP	2.4
1	B	405	CYS	2.4
1	A	239	PRO	2.4
1	A	396	ARG	2.4
1	B	519	ASP	2.4
1	B	569	GLU	2.4
1	B	572	GLY	2.4
1	A	559	ASP	2.4
1	B	517	ASP	2.4
1	B	486	SER	2.3
1	B	400	THR	2.3
1	B	358	ASN	2.3
1	B	527	VAL	2.2
1	A	499	HIS	2.2
1	B	333	PHE	2.1
1	B	494	GLU	2.1
1	B	510	HIS	2.1
1	A	266	LYS	2.1
1	A	298	GLU	2.1
1	B	283	ASP	2.1
1	A	457	THR	2.1
1	B	482	SER	2.1
1	B	500	PRO	2.1
1	B	490	LYS	2.1
1	A	295	HIS	2.1
1	B	419	GLU	2.0
1	B	407	THR	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($\text{\AA}^2$)	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

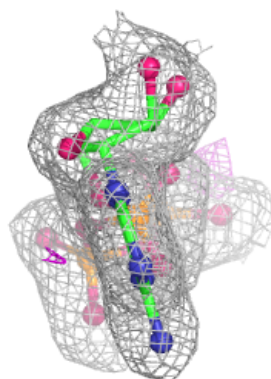
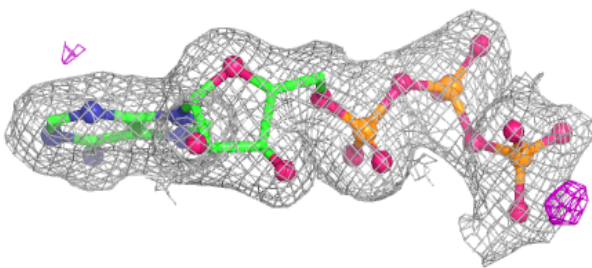
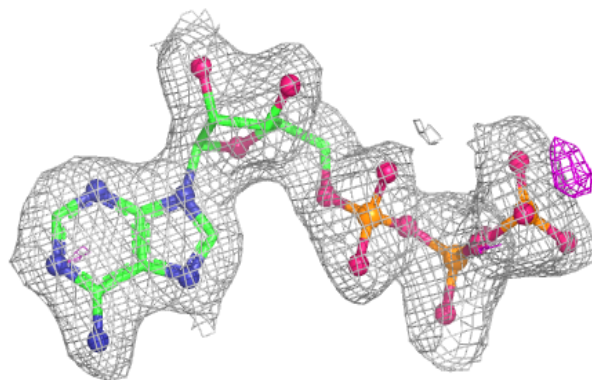
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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

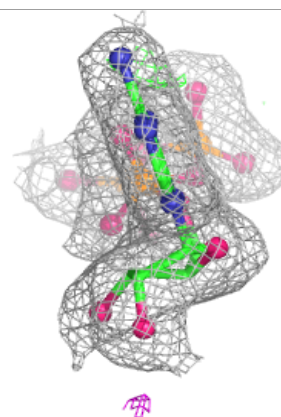
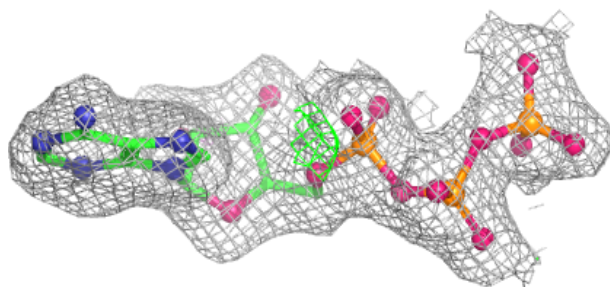
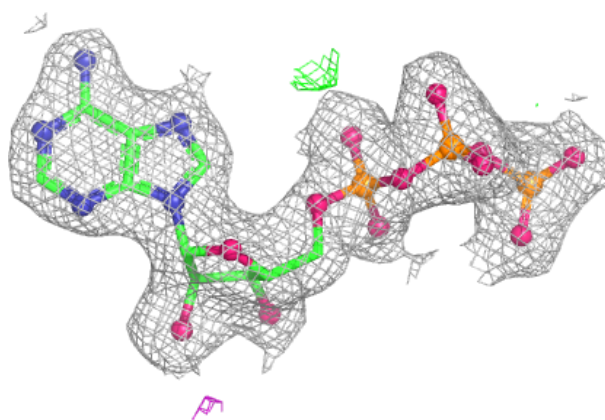
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.