



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:43 AM UTC

PDB ID : 1ROR / pdb_00001ror
Title : CRYSTAL STRUCTURES OF THE CATALYTIC DOMAIN OF PHOSPHO-DIESTERASE 4B2B COMPLEXED WITH AMP
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Deposited on : 2003-12-02
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

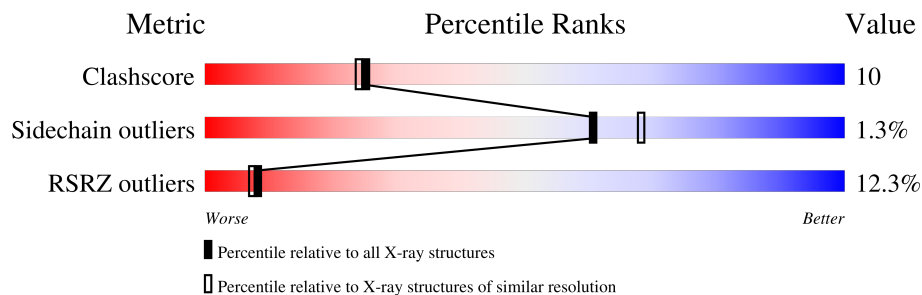
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	378	
1	B	378	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5892 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2724	1718	462	525	19	0	0	0
1	B	337	2719	1715	461	524	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	initiating methionine	UNP Q07343
A	487	ALA	SER	engineered mutation	UNP Q07343
A	489	ALA	SER	engineered mutation	UNP Q07343
B	151	MET	-	initiating methionine	UNP Q07343
B	487	ALA	SER	engineered mutation	UNP Q07343
B	489	ALA	SER	engineered mutation	UNP Q07343

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 4 is water.

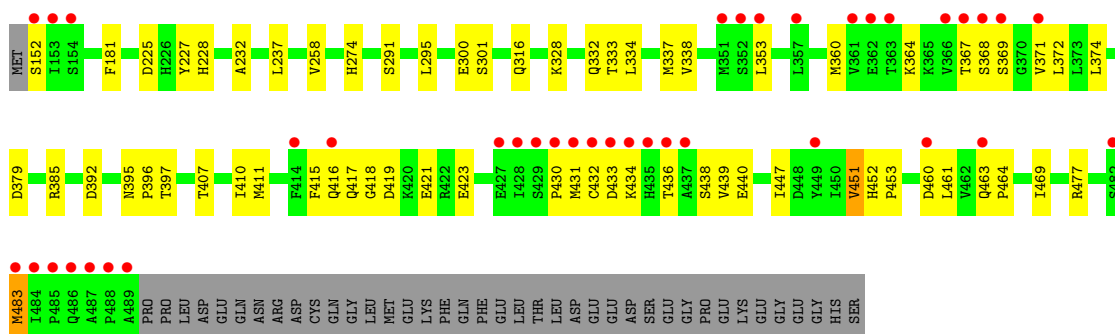
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		
4	B	151	Total	O	0	0
			151	151		

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.

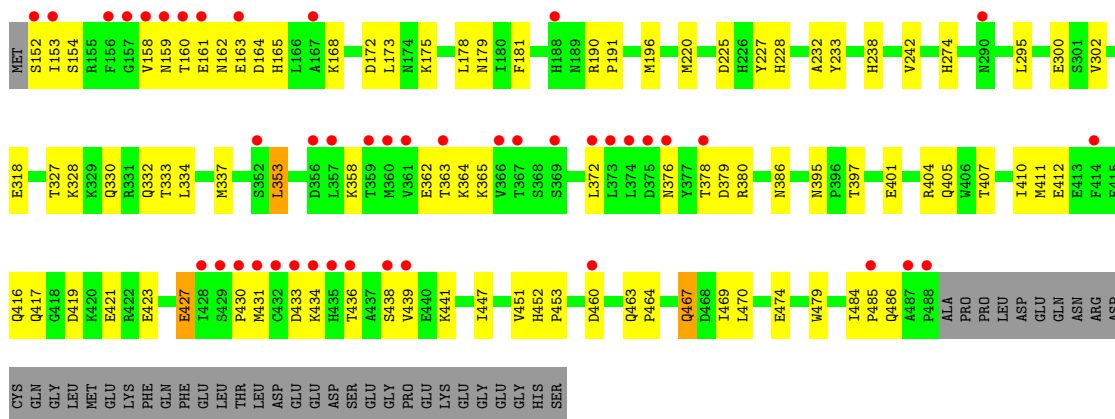
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain A: 



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.11Å 159.86Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.00) 93.9 (20.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.228 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5892	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.45	0/2781	0.90	4/3773 (0.1%)
1	B	0.42	0/2776	0.91	6/3766 (0.2%)
All	All	0.44	0/5557	0.91	10/7539 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ALA	N-CA-C	7.21	120.05	111.33
1	A	274	HIS	N-CA-C	6.93	121.35	112.34
1	A	232	ALA	N-CA-C	6.26	118.11	111.28
1	A	227	TYR	N-CA-C	-6.20	99.55	109.96
1	B	274	HIS	N-CA-C	5.94	119.63	112.38
1	B	484	ILE	CA-C-N	5.71	126.98	119.84
1	B	484	ILE	C-N-CA	5.71	126.98	119.84
1	B	227	TYR	N-CA-C	-5.23	101.19	109.76
1	A	451	VAL	N-CA-C	5.20	115.42	110.42
1	B	302	VAL	N-CA-C	5.02	115.45	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2724	0	2649	49	0
1	B	2719	0	2644	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	23	0	12	2	0
3	B	23	0	12	2	0
4	A	248	0	0	5	0
4	B	151	0	0	8	0
All	All	5892	0	5317	105	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 10.

All (105) 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:152:SER:HA	4:A:626:HOH:O	1.67	0.92
1:A:483:MET:HE3	1:A:483:MET:HA	1.60	0.83
1:A:438:SER:HB2	4:A:815:HOH:O	1.87	0.73
1:B:295:LEU:HG	4:B:821:HOH:O	1.87	0.73
1:A:291:SER:O	1:A:295:LEU:HD13	1.94	0.68
1:A:333:THR:HG22	1:A:337:MET:HE2	1.76	0.67
1:A:395:ASN:HB2	1:A:396:PRO:HD3	1.75	0.67
1:B:419:ASP:O	1:B:423:GLU:HG3	1.96	0.65
1:A:416:GLN:NE2	1:A:416:GLN:HA	2.12	0.64
1:B:353:LEU:HD22	1:B:386:ASN:OD1	1.97	0.64
1:A:416:GLN:HA	1:A:416:GLN:HE21	1.62	0.64
1:A:328:LYS:O	1:A:332:GLN:HG3	1.99	0.63
1:B:164:ASP:HB3	4:B:837:HOH:O	1.99	0.63
1:B:460:ASP:O	1:B:463:GLN:HG3	1.98	0.62
1:B:467:GLN:HG2	4:B:774:HOH:O	1.99	0.61
1:A:415:PHE:CE1	1:A:434:LYS:HA	2.36	0.61
1:B:404:ARG:HD3	1:B:479:TRP:CH2	2.35	0.61
1:A:440:GLU:H	1:A:440:GLU:CD	2.09	0.61
1:B:412:GLU:O	1:B:416:GLN:HG3	2.00	0.61
1:B:397:THR:HB	1:B:469:ILE:HG23	1.83	0.60
1:A:397:THR:HB	1:A:469:ILE:HG23	1.83	0.59
1:B:196:MET:HG3	1:B:220:MET:HE2	1.82	0.59
1:A:360:MET:HE1	1:A:379:ASP:HA	1.84	0.59
1:A:316:GLN:HG2	4:A:732:HOH:O	2.01	0.58
1:A:460:ASP:O	1:A:463:GLN:HG3	2.02	0.58
1:A:430:PRO:O	1:A:431:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASN:HB3	1:B:379:ASP:OD2	2.04	0.57
1:B:404:ARG:HD3	1:B:479:TRP:CZ3	2.41	0.55
1:B:153:ILE:O	1:B:153:ILE:HG13	2.07	0.55
1:B:159:ASN:OD1	1:B:161:GLU:HB3	2.06	0.54
1:A:483:MET:CE	1:B:485:PRO:HG3	2.38	0.54
1:A:483:MET:HA	1:A:483:MET:CE	2.36	0.54
1:A:483:MET:HE2	1:B:485:PRO:HG3	1.89	0.54
1:B:411:MET:HE2	1:B:439:VAL:HG22	1.88	0.54
1:A:417:GLN:O	1:A:421:GLU:HG3	2.08	0.53
1:B:152:SER:C	1:B:154:SER:H	2.16	0.53
1:B:404:ARG:HD2	4:B:846:HOH:O	2.09	0.53
1:A:416:GLN:HE21	1:A:416:GLN:CA	2.23	0.52
1:B:158:VAL:HG13	1:B:162:ASN:HB2	1.92	0.51
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.93	0.51
1:B:334:LEU:C	1:B:334:LEU:HD23	2.36	0.51
1:B:470:LEU:O	1:B:474:GLU:HG3	2.11	0.51
1:A:368:SER:O	1:A:369:SER:HB3	2.10	0.51
1:B:438:SER:HB3	1:B:441:LYS:HB2	1.91	0.51
1:A:300:GLU:HB2	4:A:835:HOH:O	2.11	0.50
1:A:334:LEU:O	1:A:338:VAL:HG23	2.10	0.50
1:A:353:LEU:HD21	1:A:385:ARG:HD3	1.91	0.50
1:B:395:ASN:ND2	4:B:736:HOH:O	2.43	0.50
1:B:401:GLU:O	1:B:405:GLN:HG3	2.12	0.50
1:B:411:MET:HG3	1:B:439:VAL:HG22	1.93	0.50
1:B:358:LYS:O	1:B:362:GLU:HG3	2.12	0.49
1:B:238:HIS:O	1:B:242:VAL:HG23	2.12	0.49
1:B:434:LYS:O	1:B:434:LYS:HG2	2.12	0.49
1:A:300:GLU:O	1:A:301:SER:C	2.56	0.49
1:B:417:GLN:O	1:B:421:GLU:HG3	2.13	0.49
1:B:196:MET:HG3	1:B:220:MET:CE	2.43	0.48
1:B:233:TYR:CD1	1:B:410:ILE:HG13	2.48	0.48
1:A:364:LYS:HE3	1:A:372:LEU:HD21	1.95	0.48
1:B:410:ILE:HD13	3:B:703:AMP:C6	2.49	0.48
1:A:477:ARG:HD3	1:A:477:ARG:C	2.39	0.47
1:A:419:ASP:O	1:A:423:GLU:HG3	2.15	0.47
1:A:410:ILE:HD11	3:A:603:AMP:H2'	1.96	0.47
1:B:327:THR:OG1	1:B:330:GLN:HG3	2.14	0.47
1:B:228:HIS:N	1:B:228:HIS:CD2	2.81	0.47
1:B:380:ARG:HG3	1:B:380:ARG:HH11	1.80	0.47
1:A:152:SER:CB	4:A:828:HOH:O	2.63	0.47
1:B:376:ASN:OD1	1:B:378:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:THR:HA	1:B:410:ILE:HD12	1.97	0.47
1:B:363:THR:O	1:B:365:LYS:HG3	2.16	0.46
1:B:364:LYS:HE3	1:B:372:LEU:HD21	1.97	0.45
1:B:410:ILE:HD13	3:B:703:AMP:N6	2.31	0.45
1:A:228:HIS:N	1:A:228:HIS:CD2	2.84	0.45
1:A:411:MET:HE2	1:A:439:VAL:HG22	1.98	0.45
1:B:430:PRO:O	1:B:431:MET:HB2	2.17	0.45
1:A:258:VAL:HG11	1:A:374:LEU:HD12	1.99	0.45
1:A:418:GLY:HA3	1:A:432:CYS:O	2.17	0.44
1:B:295:LEU:HB3	4:B:768:HOH:O	2.17	0.44
1:B:172:ASP:OD1	1:B:175:LYS:HD2	2.18	0.43
1:B:427:GLU:H	1:B:427:GLU:HG3	1.52	0.43
1:A:181:PHE:CD1	1:A:237:LEU:HD21	2.54	0.43
1:A:360:MET:HE2	1:A:379:ASP:CG	2.43	0.43
1:B:165:HIS:O	1:B:168:LYS:HB3	2.20	0.42
1:B:485:PRO:O	1:B:486:GLN:C	2.63	0.42
1:A:353:LEU:HD21	1:A:385:ARG:CD	2.50	0.42
1:A:367:THR:HG23	1:A:371:VAL:O	2.19	0.42
1:A:372:LEU:HD11	1:A:461:LEU:O	2.20	0.42
1:B:433:ASP:HB3	1:B:436:THR:OG1	2.20	0.42
1:B:179:ASN:OD1	1:B:181:PHE:HB2	2.20	0.41
1:B:328:LYS:O	1:B:332:GLN:HG3	2.20	0.41
1:B:447:ILE:HA	1:B:451:VAL:HB	2.01	0.41
1:B:452:HIS:HB3	1:B:453:PRO:HD3	2.01	0.41
1:A:433:ASP:HB3	1:A:436:THR:OG1	2.20	0.41
1:A:463:GLN:HA	1:A:464:PRO:HA	1.82	0.41
1:B:173:LEU:HA	1:B:178:LEU:CD1	2.50	0.41
1:A:368:SER:O	1:A:369:SER:CB	2.68	0.41
1:B:160:THR:HA	1:B:163:GLU:HB3	2.03	0.41
1:B:190:ARG:N	1:B:191:PRO:CD	2.84	0.41
1:B:333:THR:O	1:B:337:MET:HG3	2.19	0.41
1:B:318:GLU:HB3	4:B:716:HOH:O	2.20	0.41
1:B:159:ASN:N	4:B:839:HOH:O	2.50	0.40
1:A:328:LYS:HE2	1:A:328:LYS:HB2	1.83	0.40
1:A:460:ASP:HA	1:A:463:GLN:HG3	2.03	0.40
1:A:392:ASP:OD2	3:A:603:AMP:O1P	2.40	0.40
1:A:407:THR:O	1:A:410:ILE:HG22	2.20	0.40
1:A:447:ILE:HA	1:A:451:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	305/341 (89%)	303 (99%)	2 (1%)	76	82
1	B	305/341 (89%)	299 (98%)	6 (2%)	48	54
All	All	610/682 (89%)	602 (99%)	8 (1%)	61	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ASP
1	A	483	MET
1	B	225	ASP
1	B	300	GLU
1	B	353	LEU
1	B	427	GLU
1	B	464	PRO
1	B	467	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	A	332	GLN
1	A	395	ASN
1	A	416	GLN
1	B	201	GLN
1	B	284	GLN
1	B	463	GLN
1	B	467	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	AMP	B	703	2	25,25,25	1.70	6 (24%)	37,38,38	1.35	4 (10%)
3	AMP	A	603	2	25,25,25	1.67	6 (24%)	37,38,38	1.33	4 (10%)

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
3	AMP	B	703	2	-	1/10/26/26	0/3/3/3
3	AMP	A	603	2	-	0/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	AMP	C4-N3	3.73	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	AMP	C5-C4	3.73	1.45	1.39
3	A	603	AMP	C4-N3	3.61	1.41	1.34
3	B	703	AMP	C5-C4	3.57	1.45	1.39
3	B	703	AMP	P-O3P	-3.37	1.42	1.54
3	A	603	AMP	C2-N1	3.25	1.39	1.33
3	B	703	AMP	C2-N1	2.94	1.39	1.33
3	A	603	AMP	P-O3P	-2.53	1.45	1.54
3	B	703	AMP	C2-N3	2.45	1.38	1.33
3	A	603	AMP	C2-N3	2.43	1.38	1.33
3	A	603	AMP	C8-N7	2.16	1.35	1.31
3	B	703	AMP	C8-N7	2.05	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	AMP	N3-C2-N1	-4.02	122.49	128.58
3	A	603	AMP	N3-C2-N1	-3.94	122.62	128.58
3	B	703	AMP	C5-C4-N3	-2.98	122.62	126.72
3	A	603	AMP	O5'-P-O1P	2.90	114.27	106.44
3	A	603	AMP	C5-C4-N3	-2.76	122.92	126.72
3	B	703	AMP	C2-N3-C4	2.36	117.60	111.83
3	B	703	AMP	O5'-P-O1P	2.28	112.59	106.44
3	A	603	AMP	C2-N3-C4	2.26	117.36	111.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	AMP	C4'-C5'-O5'-P

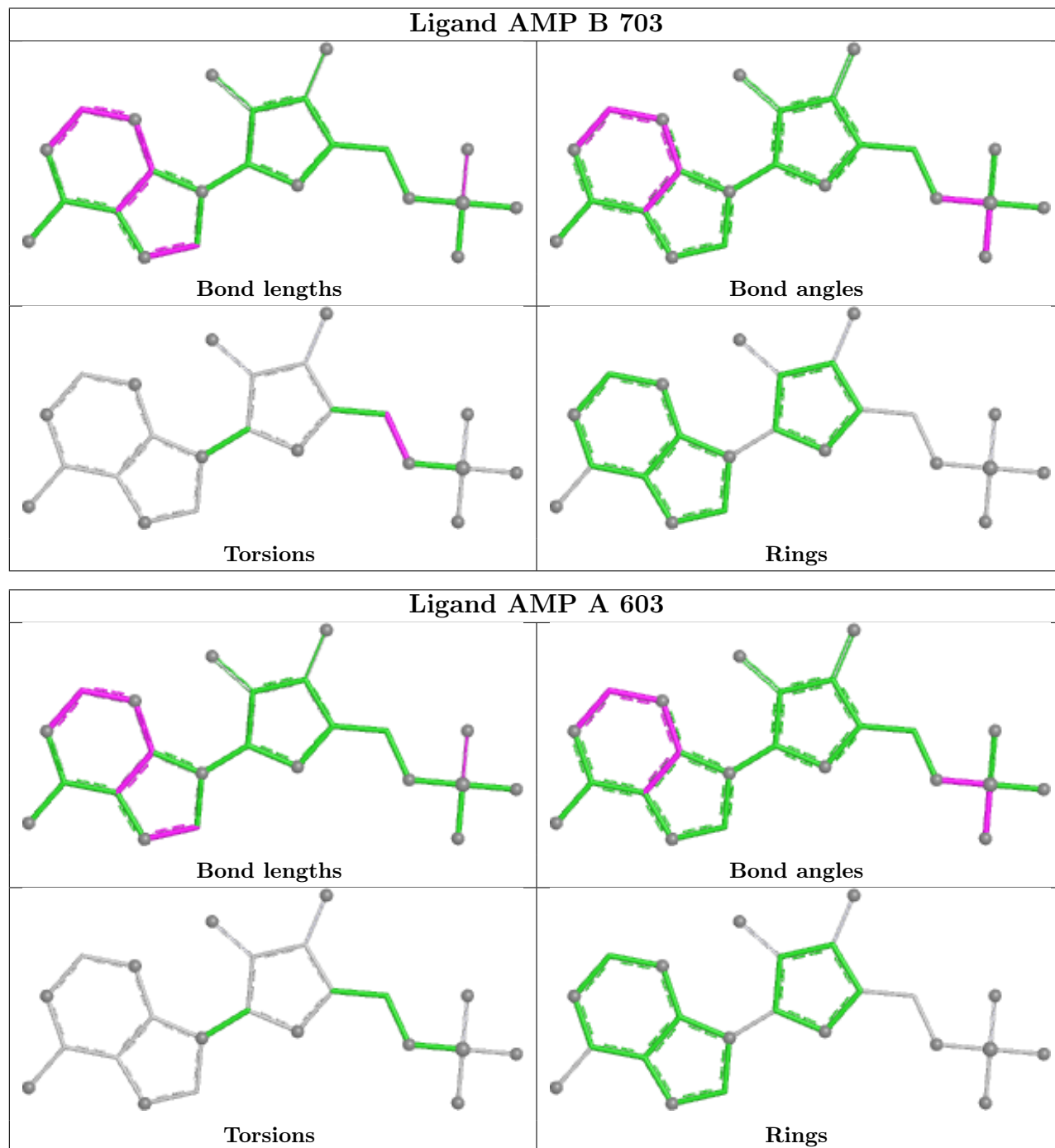
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	AMP	2	0
3	A	603	AMP	2	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	338/378 (89%)	0.42	39 (11%) 9 8	16, 28, 64, 79	0
1	B	337/378 (89%)	0.82	44 (13%) 7 6	22, 37, 68, 72	0
All	All	675/756 (89%)	0.62	83 (12%) 8 7	16, 33, 65, 79	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	PRO	7.8
1	A	430	PRO	7.0
1	B	488	PRO	7.0
1	B	428	ILE	5.6
1	B	429	SER	5.5
1	B	160	THR	5.2
1	A	488	PRO	4.9
1	B	435	HIS	4.8
1	A	487	ALA	4.7
1	A	428	ILE	4.7
1	A	434	LYS	4.6
1	A	431	MET	4.5
1	A	489	ALA	4.5
1	A	485	PRO	4.1
1	A	437	ALA	4.0
1	B	188	HIS	4.0
1	B	152	SER	3.9
1	A	435	HIS	3.9
1	B	158	VAL	3.8
1	A	433	ASP	3.8
1	A	429	SER	3.6
1	B	157	GLY	3.5
1	B	431	MET	3.5
1	A	484	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	432	CYS	3.4
1	A	449	TYR	3.3
1	B	487	ALA	3.3
1	B	159	ASN	3.3
1	A	486	GLN	3.2
1	A	414	PHE	3.1
1	A	427	GLU	3.1
1	B	156	PHE	3.1
1	A	368	SER	3.0
1	B	372	LEU	3.0
1	B	375	ASP	2.9
1	B	485	PRO	2.9
1	A	482	SER	2.9
1	B	376	ASN	2.8
1	B	414	PHE	2.8
1	B	153	ILE	2.8
1	B	369	SER	2.8
1	B	374	LEU	2.8
1	A	363	THR	2.7
1	B	361	VAL	2.7
1	A	357	LEU	2.6
1	B	432	CYS	2.6
1	A	436	THR	2.6
1	A	152	SER	2.6
1	A	154	SER	2.6
1	B	360	MET	2.5
1	B	433	ASP	2.5
1	B	167	ALA	2.5
1	B	373	LEU	2.5
1	A	361	VAL	2.5
1	B	434	LYS	2.5
1	B	352	SER	2.5
1	A	366	VAL	2.5
1	A	352	SER	2.5
1	B	367	THR	2.5
1	A	483	MET	2.5
1	A	367	THR	2.4
1	A	463	GLN	2.4
1	B	161	GLU	2.4
1	A	351	MET	2.4
1	B	378	THR	2.4
1	B	439	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	153	ILE	2.3
1	A	369	SER	2.3
1	A	371	VAL	2.3
1	A	353	LEU	2.3
1	B	366	VAL	2.2
1	A	460	ASP	2.2
1	B	290	ASN	2.2
1	B	363	THR	2.2
1	B	436	THR	2.2
1	B	356	ASP	2.2
1	B	359	THR	2.2
1	B	460	ASP	2.2
1	B	357	LEU	2.1
1	A	362	GLU	2.1
1	B	163	GLU	2.1
1	B	438	SER	2.1
1	A	416	GLN	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](#)

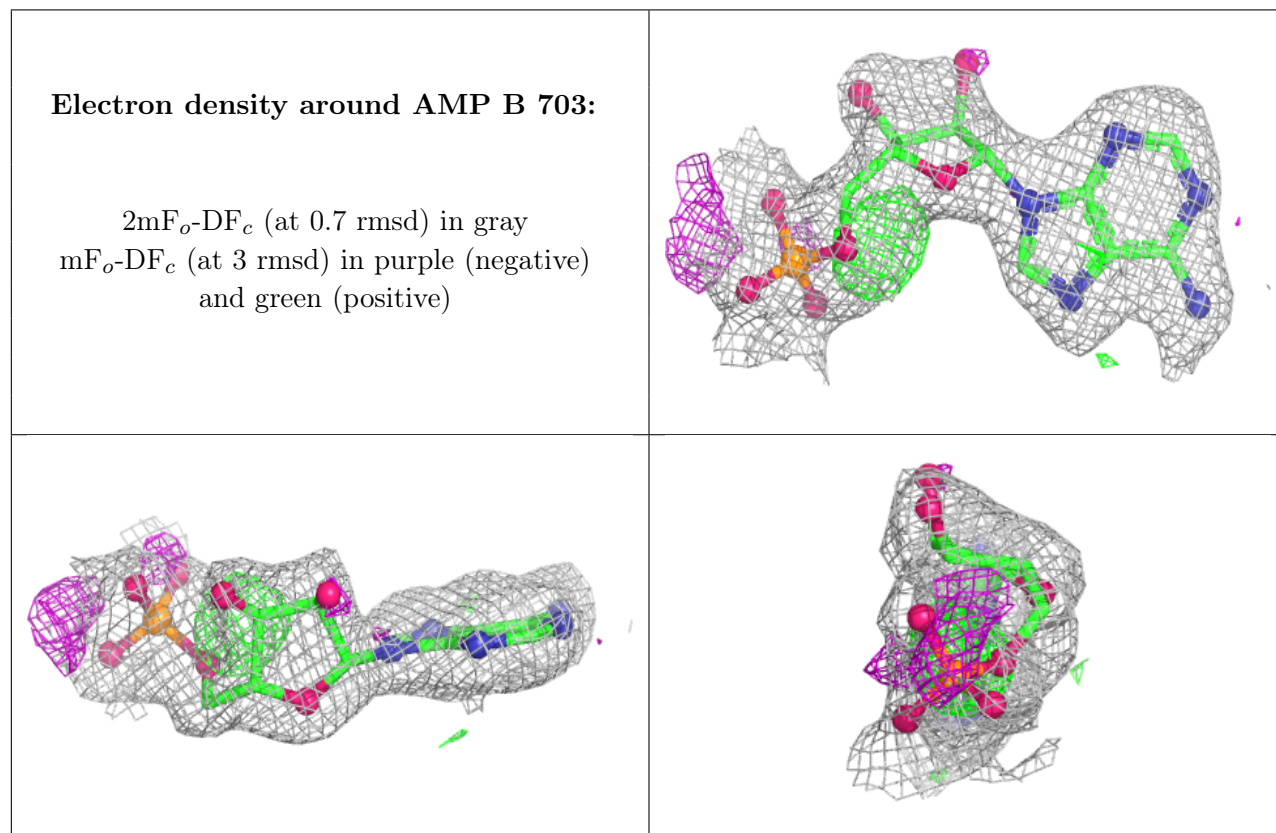
There are no oligosaccharides in this entry.

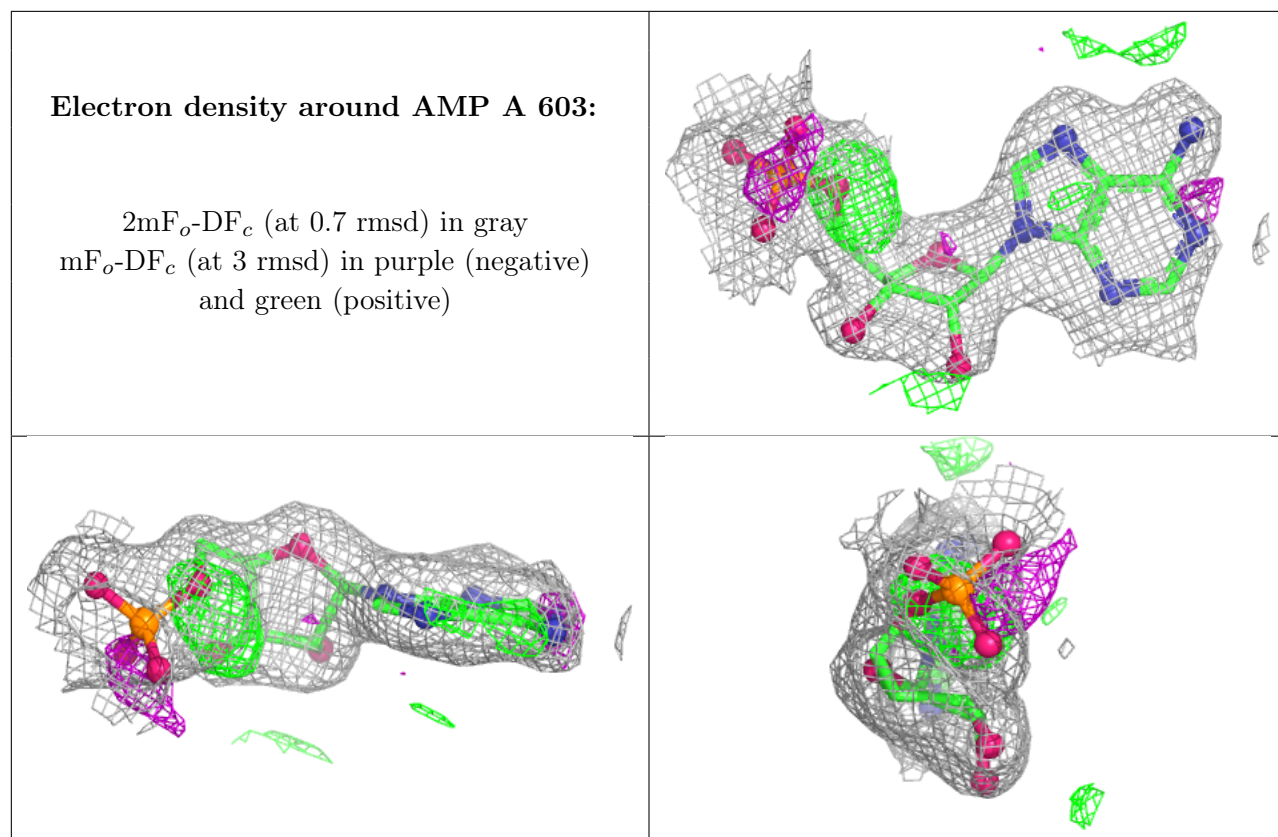
6.4 Ligands [i](#)

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	AMP	B	703	23/23	0.83	0.12	41,47,48,49	0
3	AMP	A	603	23/23	0.84	0.12	42,45,46,47	0
2	ZN	B	702	1/1	0.98	0.13	50,50,50,50	0
2	ZN	A	602	1/1	0.99	0.06	46,46,46,46	0
2	ZN	B	701	1/1	1.00	0.02	28,28,28,28	0
2	ZN	A	601	1/1	1.00	0.03	24,24,24,24	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.