



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:08 PM EDT

PDB ID : 4Q4A / pdb_00004q4a
Title : Improved model of AMP-PNP bound TM287/288
Authors : Hohl, M.; Gruetter, M.G.; Seeger, M.A.
Deposited on : 2014-04-14
Resolution : 2.60 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

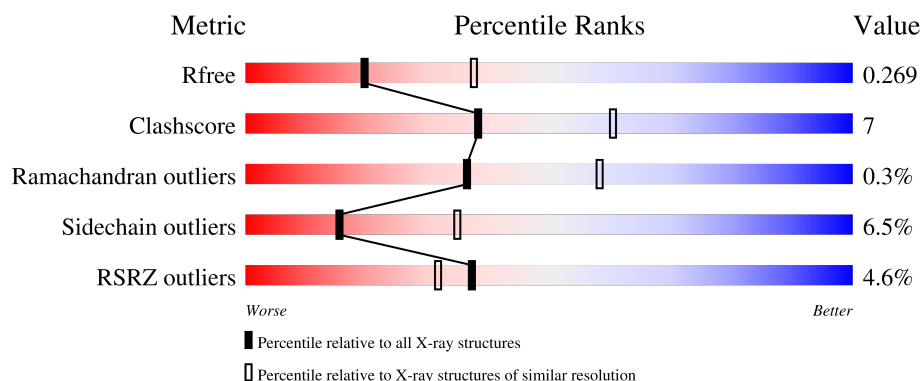
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

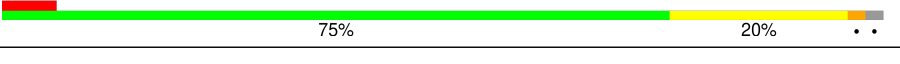
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	587	 3% 76% 19% . .
2	B	598	 6% 75% 20% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9166 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 ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4485	2889	772	805	19			

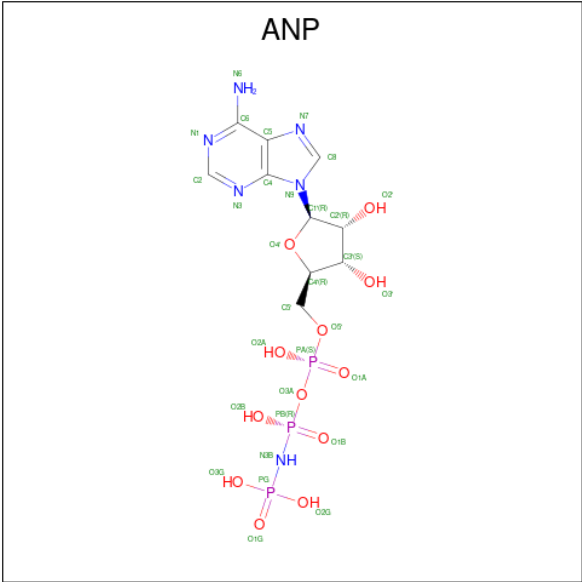
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	584	Total	C	N	O	S	0	0	0
			4649	3006	783	846	14			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

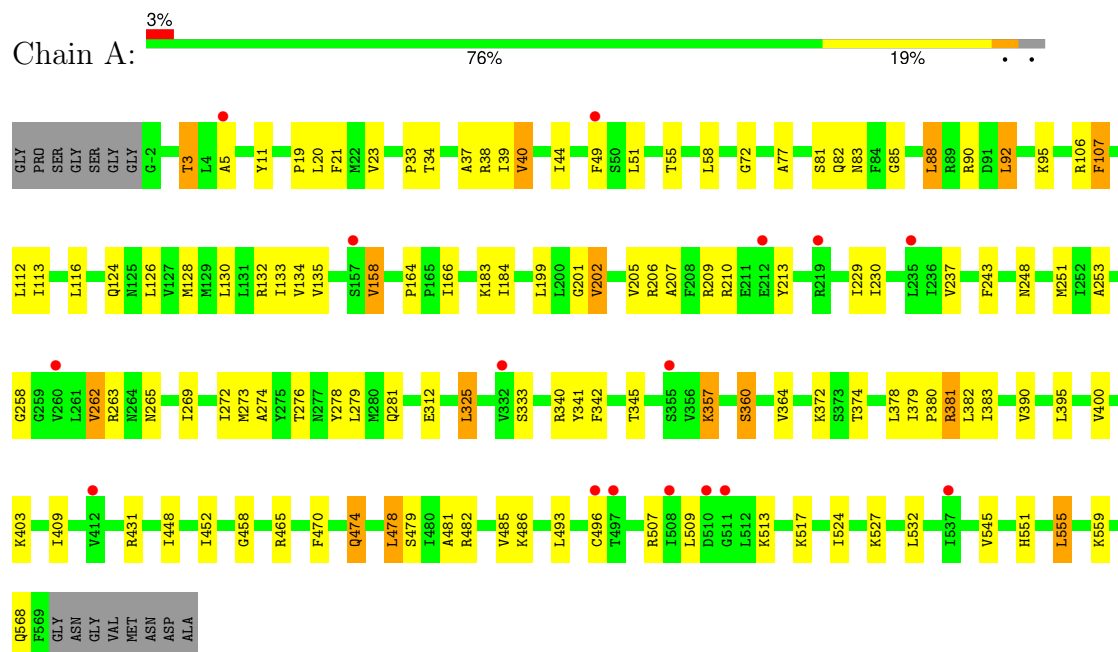
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

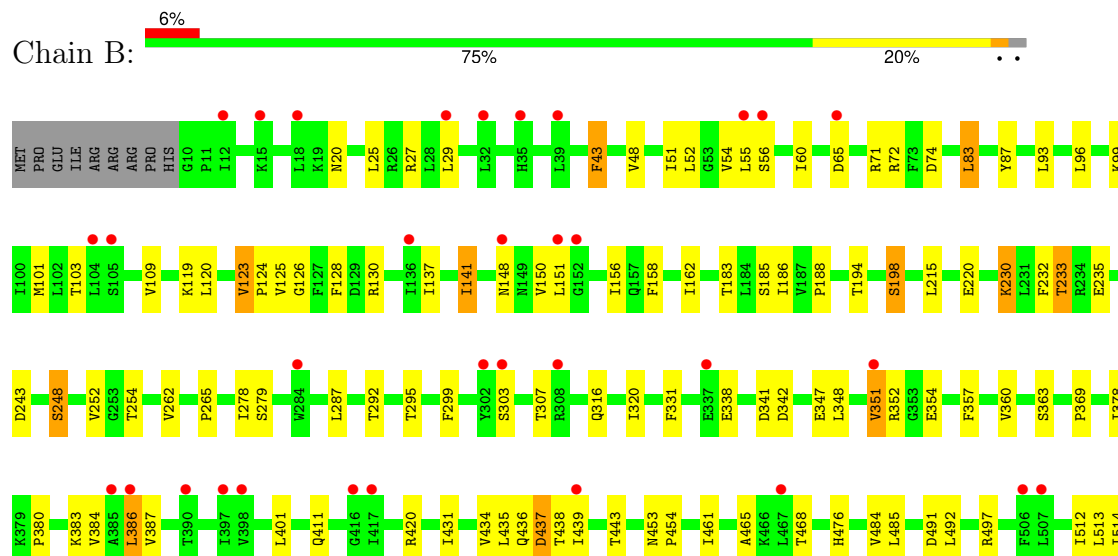
3 Residue-property plots [i](#)

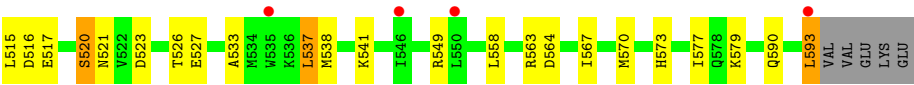
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ABC transporter



• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.33Å 84.31Å 115.78Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	24.93 – 2.60 24.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (24.93-2.60) 99.2 (24.93-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.226 , 0.268 0.228 , 0.269	Depositor DCC
R_{free} test set	3193 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: MG, ANP

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	0.38	0/4560	0.78	3/6166 (0.0%)
2	B	0.33	0/4730	0.76	0/6396
All	All	0.36	0/9290	0.77	3/12562 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	PRO	N-CA-C	5.63	117.57	110.70
1	A	325	LEU	CA-C-N	5.00	124.49	119.19
1	A	325	LEU	C-N-CA	5.00	124.49	119.19

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	4485	0	4682	71	0
2	B	4649	0	4840	75	0
3	A	31	0	13	2	0
4	A	1	0	0	0	0
All	All	9166	0	9535	129	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 7.

All (129) 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:85:GLY:HA3	1:A:124:GLN:HE21	1.53	0.72
1:A:527:LYS:HA	1:A:568:GLN:HE22	1.54	0.71
1:A:380:PRO:O	1:A:382:LEU:N	2.25	0.70
2:B:401:LEU:HD22	2:B:514:ILE:HD11	1.72	0.70
2:B:378:ILE:HD12	2:B:384:VAL:HG21	1.75	0.69
1:A:207:ALA:O	1:A:209:ARG:NH1	2.27	0.68
1:A:206:ARG:NH2	2:B:123:VAL:O	2.27	0.66
1:A:448:ILE:HG12	1:A:478:LEU:HD13	1.76	0.66
2:B:517:GLU:HB3	2:B:549:ARG:HH21	1.61	0.65
2:B:109:VAL:HG11	2:B:148:ASN:HB2	1.81	0.62
2:B:527:GLU:OE2	2:B:549:ARG:NH1	2.32	0.62
1:A:88:LEU:HD22	1:A:92:LEU:HD22	1.82	0.61
1:A:482:ARG:HD3	2:B:232:PHE:CZ	2.36	0.60
1:A:95:LYS:NZ	1:A:312:GLU:O	2.30	0.59
2:B:60:ILE:HD11	2:B:83:LEU:HD21	1.84	0.59
2:B:72:ARG:NH1	2:B:74:ASP:OD1	2.37	0.57
1:A:465:ARG:NH1	2:B:220:GLU:OE1	2.38	0.56
1:A:403:LYS:HG3	2:B:233:THR:HG21	1.89	0.55
1:A:19:PRO:HB3	1:A:135:VAL:HG21	1.87	0.55
1:A:210:ARG:HG3	1:A:213:TYR:HB3	1.88	0.54
1:A:132:ARG:HG3	1:A:133:ILE:H	1.72	0.54
1:A:372:LYS:HD2	1:A:524:ILE:HG23	1.88	0.54
1:A:107:PHE:HB2	1:A:112:LEU:HD13	1.90	0.53
1:A:49:PHE:HE1	2:B:287:LEU:HB3	1.73	0.53
1:A:11:TYR:CZ	1:A:83:ASN:HB3	2.44	0.53
1:A:40:VAL:HG11	1:A:273:MET:HE2	1.91	0.52
2:B:363:SER:HB3	2:B:369:PRO:HA	1.91	0.52
1:A:342:PHE:CE2	3:A:601:ANP:H2	2.45	0.52
2:B:316:GLN:O	2:B:320:ILE:HG12	2.09	0.52
1:A:3:THR:HG23	1:A:5:ALA:H	1.76	0.51
2:B:119:LYS:NZ	2:B:338:GLU:OE2	2.44	0.51
1:A:379:ILE:HG22	1:A:409:ILE:HD13	1.91	0.51
1:A:44:ILE:HA	2:B:287:LEU:HD21	1.93	0.51
2:B:573:HIS:CE1	2:B:577:ILE:HD11	2.47	0.50
2:B:183:THR:O	2:B:186:ILE:HG12	2.11	0.50
2:B:436:GLN:HA	2:B:516:ASP:O	2.12	0.50
2:B:56:SER:O	2:B:60:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:LEU:O	2:B:497:ARG:NH1	2.45	0.49
1:A:452:ILE:O	1:A:458:GLY:HA2	2.14	0.48
2:B:101:MET:HG3	2:B:156:ILE:HD13	1.96	0.48
2:B:563:ARG:HD3	2:B:564:ASP:HB2	1.95	0.48
2:B:435:LEU:H	2:B:435:LEU:HD12	1.79	0.48
1:A:357:LYS:O	1:A:360:SER:OG	2.31	0.48
2:B:515:LEU:HD22	2:B:538:MET:HE2	1.96	0.47
1:A:106:ARG:NH2	1:A:312:GLU:OE2	2.46	0.47
1:A:184:ILE:HD13	1:A:229:ILE:HG12	1.96	0.47
1:A:479:SER:HA	1:A:482:ARG:HB3	1.97	0.47
1:A:263:ARG:O	2:B:71:ARG:NH1	2.48	0.47
2:B:52:LEU:HA	2:B:55:LEU:HD12	1.97	0.47
2:B:278:ILE:HD12	2:B:303:SER:HB3	1.97	0.47
1:A:341:TYR:OH	1:A:374:THR:HG22	2.14	0.47
1:A:92:LEU:HB3	1:A:116:LEU:HG	1.96	0.47
1:A:470:PHE:HB3	1:A:474:GLN:HG3	1.97	0.46
1:A:364:VAL:HB	1:A:524:ILE:HG13	1.97	0.46
1:A:251:MET:HE1	1:A:276:THR:HB	1.97	0.46
1:A:199:LEU:HD21	2:B:120:LEU:HD11	1.98	0.45
2:B:25:LEU:O	2:B:29:LEU:HG	2.16	0.45
2:B:533:ALA:O	2:B:537:LEU:HB2	2.16	0.45
2:B:262:VAL:C	2:B:265:PRO:HD2	2.40	0.45
2:B:411:GLN:HB2	2:B:420:ARG:HH22	1.81	0.45
2:B:437:ASP:OD1	2:B:437:ASP:N	2.48	0.45
1:A:166:ILE:HD13	1:A:243:PHE:HE1	1.82	0.45
1:A:357:LYS:H	1:A:357:LYS:HG2	1.46	0.45
2:B:123:VAL:HG22	2:B:124:PRO:HD2	1.98	0.45
1:A:90:ARG:NH2	2:B:243:ASP:OD2	2.48	0.45
2:B:51:ILE:O	2:B:54:VAL:HG22	2.17	0.45
2:B:194:THR:O	2:B:198:SER:HB2	2.17	0.45
2:B:520:SER:OG	2:B:521:ASN:N	2.50	0.45
1:A:258:GLY:O	1:A:262:VAL:HG12	2.17	0.45
1:A:39:ILE:HD12	2:B:279:SER:HB3	1.99	0.45
1:A:37:ALA:HB2	1:A:274:ALA:HB2	1.99	0.44
2:B:48:VAL:HG23	2:B:93:LEU:HD13	1.99	0.44
2:B:523:ASP:OD1	2:B:526:THR:OG1	2.27	0.44
1:A:166:ILE:HD13	1:A:243:PHE:CE1	2.52	0.44
1:A:493:LEU:HB3	1:A:496:CYS:SG	2.57	0.44
1:A:532:LEU:CD1	2:B:593:LEU:HB2	2.48	0.44
1:A:33:PRO:HG2	1:A:278:TYR:CE1	2.52	0.44
1:A:113:ILE:HD13	2:B:220:GLU:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HA	1:A:134:VAL:HB	1.99	0.44
2:B:431:ILE:HG12	2:B:512:ILE:HB	1.99	0.44
1:A:378:LEU:HB3	1:A:390:VAL:HG21	1.99	0.44
1:A:481:ALA:O	1:A:485:VAL:HG23	2.18	0.44
1:A:378:LEU:HD23	1:A:383:ILE:HG13	2.00	0.44
1:A:20:LEU:O	1:A:23:VAL:HG22	2.17	0.43
1:A:82:GLN:HG3	2:B:254:THR:HA	2.00	0.43
1:A:248:ASN:HB3	2:B:87:TYR:CD2	2.53	0.43
1:A:551:HIS:O	1:A:555:LEU:HB2	2.18	0.43
1:A:21:PHE:CD2	1:A:72:GLY:HA3	2.53	0.43
1:A:158:VAL:HG21	1:A:253:ALA:HB1	2.01	0.43
2:B:434:VAL:HB	2:B:515:LEU:HD12	2.01	0.43
2:B:386:LEU:HD12	2:B:386:LEU:H	1.83	0.43
2:B:341:ASP:HB3	2:B:342:ASP:H	1.73	0.42
1:A:340:ARG:HD3	1:A:345:THR:O	2.19	0.42
2:B:461:ILE:O	2:B:465:ALA:N	2.50	0.42
2:B:248:SER:O	2:B:252:VAL:HG23	2.19	0.42
2:B:579:LYS:HB3	2:B:579:LYS:HE2	1.84	0.42
1:A:77:ALA:O	1:A:81:SER:HB2	2.20	0.42
2:B:357:PHE:HD2	2:B:360:VAL:HG21	1.84	0.42
1:A:38:ARG:HE	1:A:55:THR:HG21	1.85	0.42
1:A:201:GLY:HA2	2:B:439:ILE:HD13	2.01	0.42
1:A:202:VAL:HG21	2:B:128:PHE:CE2	2.55	0.42
2:B:158:PHE:CE2	2:B:162:ILE:HD11	2.55	0.41
1:A:509:LEU:O	1:A:513:LYS:HE3	2.20	0.41
1:A:409:ILE:O	1:A:486:LYS:NZ	2.45	0.41
2:B:183:THR:HG21	2:B:299:PHE:HD1	1.85	0.41
2:B:230:LYS:NZ	2:B:235:GLU:OE1	2.53	0.41
1:A:265:ASN:O	1:A:265:ASN:ND2	2.54	0.41
1:A:431:ARG:HD3	1:A:485:VAL:O	2.20	0.41
2:B:52:LEU:HD23	2:B:55:LEU:HD12	2.03	0.41
2:B:537:LEU:O	2:B:541:LYS:HE2	2.21	0.41
1:A:128:MET:HE3	1:A:132:ARG:CZ	2.51	0.41
2:B:573:HIS:O	2:B:577:ILE:HG13	2.20	0.41
1:A:199:LEU:HD12	2:B:137:ILE:HD11	2.02	0.41
2:B:351:VAL:HG12	2:B:352:ARG:H	1.85	0.41
1:A:374:THR:HG23	3:A:601:ANP:O1A	2.21	0.41
2:B:453:ASN:HA	2:B:454:PRO:HD2	1.89	0.41
2:B:60:ILE:CD1	2:B:83:LEU:HD21	2.51	0.41
2:B:96:LEU:HD23	2:B:96:LEU:HA	1.92	0.41
1:A:555:LEU:HD22	1:A:555:LEU:HA	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ARG:HD3	2:B:331:PHE:CD2	2.57	0.40
1:A:325:LEU:HD11	1:A:400:VAL:HG11	2.04	0.40
2:B:185:SER:O	2:B:188:PRO:HD2	2.22	0.40
2:B:354:GLU:HG2	2:B:380:PRO:HD3	2.03	0.40
2:B:141:ILE:HD12	2:B:141:ILE:HA	1.92	0.40
1:A:474:GLN:H	1:A:474:GLN:HG2	1.71	0.40
2:B:43:PHE:HD1	2:B:43:PHE:HA	1.70	0.40
2:B:65:ASP:OD2	2:B:292:THR:OG1	2.32	0.40
2:B:126:GLY:O	2:B:130:ARG:HG3	2.22	0.40
2:B:558:LEU:HD21	2:B:570:MET:HE3	2.03	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	570/587 (97%)	551 (97%)	18 (3%)	1 (0%)	43	66
2	B	582/598 (97%)	548 (94%)	31 (5%)	3 (0%)	24	46
All	All	1152/1185 (97%)	1099 (95%)	49 (4%)	4 (0%)	36	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ARG
2	B	520	SER
2	B	590	GLN
2	B	20	ASN

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	496/504 (98%)	464 (94%)	32 (6%)	15	35
2	B	519/533 (97%)	485 (93%)	34 (7%)	15	34
All	All	1015/1037 (98%)	949 (94%)	66 (6%)	15	35

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	34	THR
1	A	40	VAL
1	A	51	LEU
1	A	58	LEU
1	A	88	LEU
1	A	92	LEU
1	A	107	PHE
1	A	126	LEU
1	A	158	VAL
1	A	183	LYS
1	A	202	VAL
1	A	205	VAL
1	A	230	ILE
1	A	237	VAL
1	A	262	VAL
1	A	269	ILE
1	A	272	ILE
1	A	279	LEU
1	A	281	GLN
1	A	333	SER
1	A	357	LYS
1	A	360	SER
1	A	381	ARG
1	A	395	LEU
1	A	474	GLN
1	A	478	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	507	ARG
1	A	517	LYS
1	A	545	VAL
1	A	555	LEU
1	A	559	LYS
2	B	43	PHE
2	B	83	LEU
2	B	99	LYS
2	B	103	THR
2	B	123	VAL
2	B	125	VAL
2	B	141	ILE
2	B	150	VAL
2	B	151	LEU
2	B	198	SER
2	B	215	LEU
2	B	230	LYS
2	B	233	THR
2	B	248	SER
2	B	295	THR
2	B	307	THR
2	B	347	GLU
2	B	348	LEU
2	B	351	VAL
2	B	383	LYS
2	B	386	LEU
2	B	387	VAL
2	B	437	ASP
2	B	438	THR
2	B	443	THR
2	B	468	THR
2	B	476	HIS
2	B	484	VAL
2	B	485	LEU
2	B	491	ASP
2	B	513	LEU
2	B	537	LEU
2	B	567	ILE
2	B	593	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	265	ASN
1	A	266	GLN
1	A	327	ASN
1	A	447	GLN
1	A	474	GLN
1	A	541	HIS
2	B	106	GLN
2	B	121	GLN
2	B	148	ASN
2	B	359	ASN
2	B	382	GLN
2	B	531	GLN
2	B	573	HIS

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ANP	A	601	4	33,33,33	2.07	10 (30%)	45,52,52	1.97	12 (26%)

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	ANP	A	601	4	-	0/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ANP	PB-N3B	4.77	1.75	1.63
3	A	601	ANP	C5-C4	4.75	1.47	1.39
3	A	601	ANP	PG-N3B	4.57	1.75	1.63
3	A	601	ANP	PB-O1B	3.47	1.51	1.46
3	A	601	ANP	PG-O1G	3.35	1.51	1.46
3	A	601	ANP	C5-C6	2.73	1.48	1.41
3	A	601	ANP	PB-O3A	2.55	1.62	1.59
3	A	601	ANP	C8-N7	2.42	1.36	1.31
3	A	601	ANP	C5-N7	-2.25	1.35	1.39
3	A	601	ANP	PA-O3A	2.12	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ANP	C5-C4-N3	-5.69	118.89	126.72
3	A	601	ANP	O1G-PG-N3B	-4.65	104.92	111.77
3	A	601	ANP	N3-C4-N9	4.41	134.68	127.17
3	A	601	ANP	O2B-PB-O1B	3.93	118.30	109.87
3	A	601	ANP	C2-N3-C4	3.54	120.48	111.83
3	A	601	ANP	C4-C5-N7	-3.51	106.57	110.58
3	A	601	ANP	N3-C2-N1	-3.01	124.03	128.58
3	A	601	ANP	O2G-PG-O3G	2.52	114.37	107.59
3	A	601	ANP	C4-N9-C8	2.52	108.39	105.74
3	A	601	ANP	C5-N7-C8	2.49	107.36	103.45
3	A	601	ANP	O1B-PB-N3B	-2.21	108.51	111.77
3	A	601	ANP	C6-C5-N7	2.14	136.21	132.09

There are no chirality outliers.

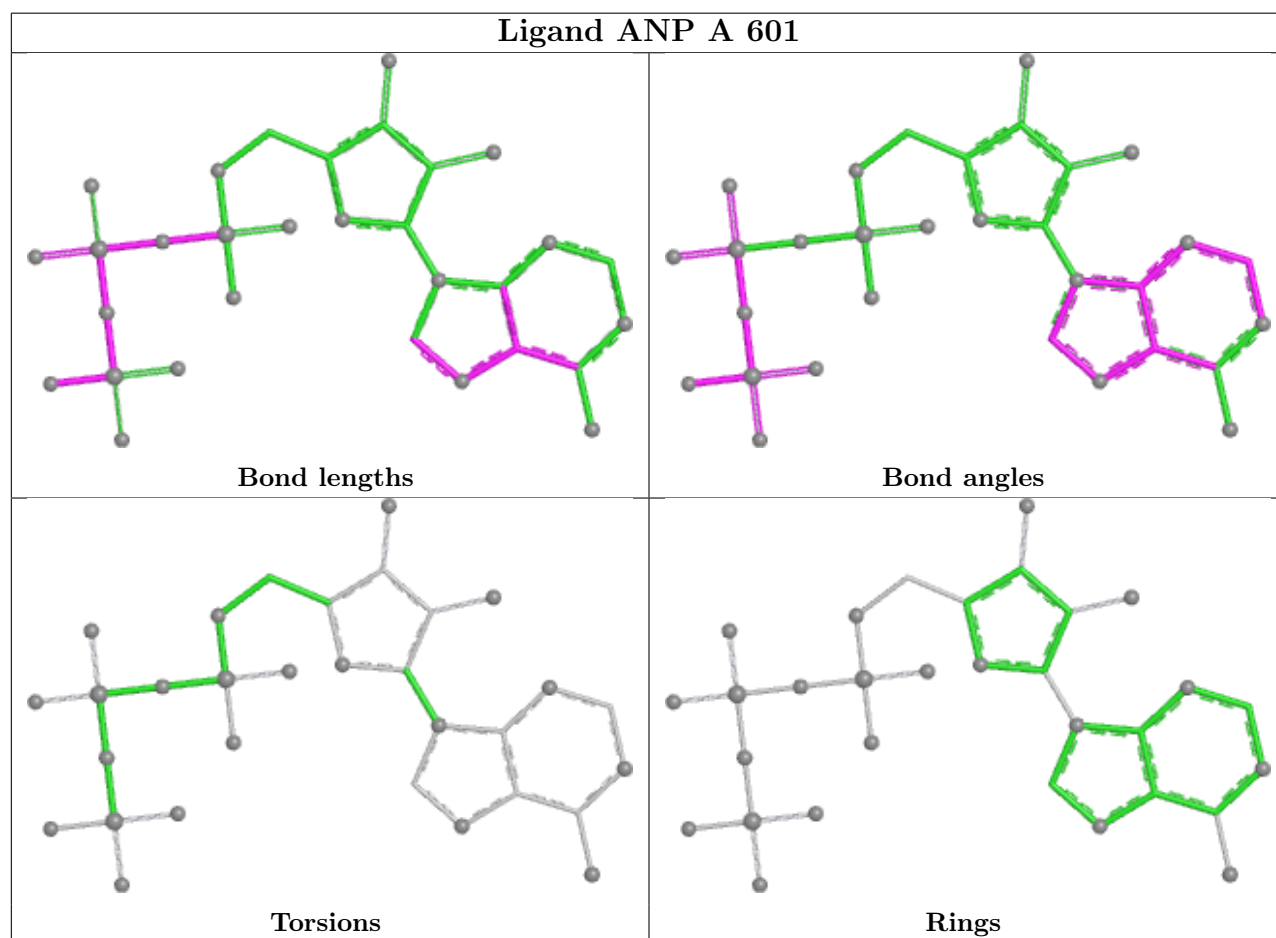
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ANP	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 ⓘ

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	572/587 (97%)	0.19	16 (2%)	55 49	72, 109, 152, 183	0
2	B	584/598 (97%)	0.37	37 (6%)	26 20	80, 137, 179, 234	0
All	All	1156/1185 (97%)	0.28	53 (4%)	37 32	72, 121, 173, 234	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	105	SER	6.3
1	A	260	VAL	6.1
2	B	151	LEU	5.6
2	B	416	GLY	5.3
2	B	32	LEU	5.3
2	B	152	GLY	5.1
2	B	467	LEU	4.7
1	A	412	VAL	4.0
2	B	507	LEU	3.9
1	A	496	CYS	3.5
2	B	337	GLU	3.4
1	A	355	SER	3.4
2	B	546	ILE	3.2
1	A	235	LEU	3.1
2	B	39	LEU	3.1
1	A	508	ILE	3.1
2	B	386	LEU	3.0
1	A	511	GLY	3.0
2	B	104	LEU	2.9
1	A	332	VAL	2.8
2	B	398	VAL	2.8
2	B	29	LEU	2.8
2	B	284	TRP	2.7
2	B	15	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	212	GLU	2.6
2	B	12	ILE	2.6
2	B	308	ARG	2.5
2	B	55	LEU	2.4
2	B	56	SER	2.4
2	B	148	ASN	2.4
2	B	397	ILE	2.4
1	A	5	ALA	2.4
2	B	385	ALA	2.4
2	B	18	LEU	2.3
2	B	417	ILE	2.3
2	B	136	ILE	2.3
2	B	65	ASP	2.3
2	B	593	LEU	2.3
1	A	49	PHE	2.3
1	A	537	ILE	2.2
2	B	302	TYR	2.2
2	B	303	SER	2.2
2	B	351	VAL	2.2
2	B	535	TRP	2.2
2	B	390	THR	2.2
1	A	510	ASP	2.1
1	A	157	SER	2.1
1	A	497	THR	2.1
2	B	35	HIS	2.1
2	B	439	ILE	2.1
2	B	506	PHE	2.1
1	A	219	ARG	2.0
2	B	550	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

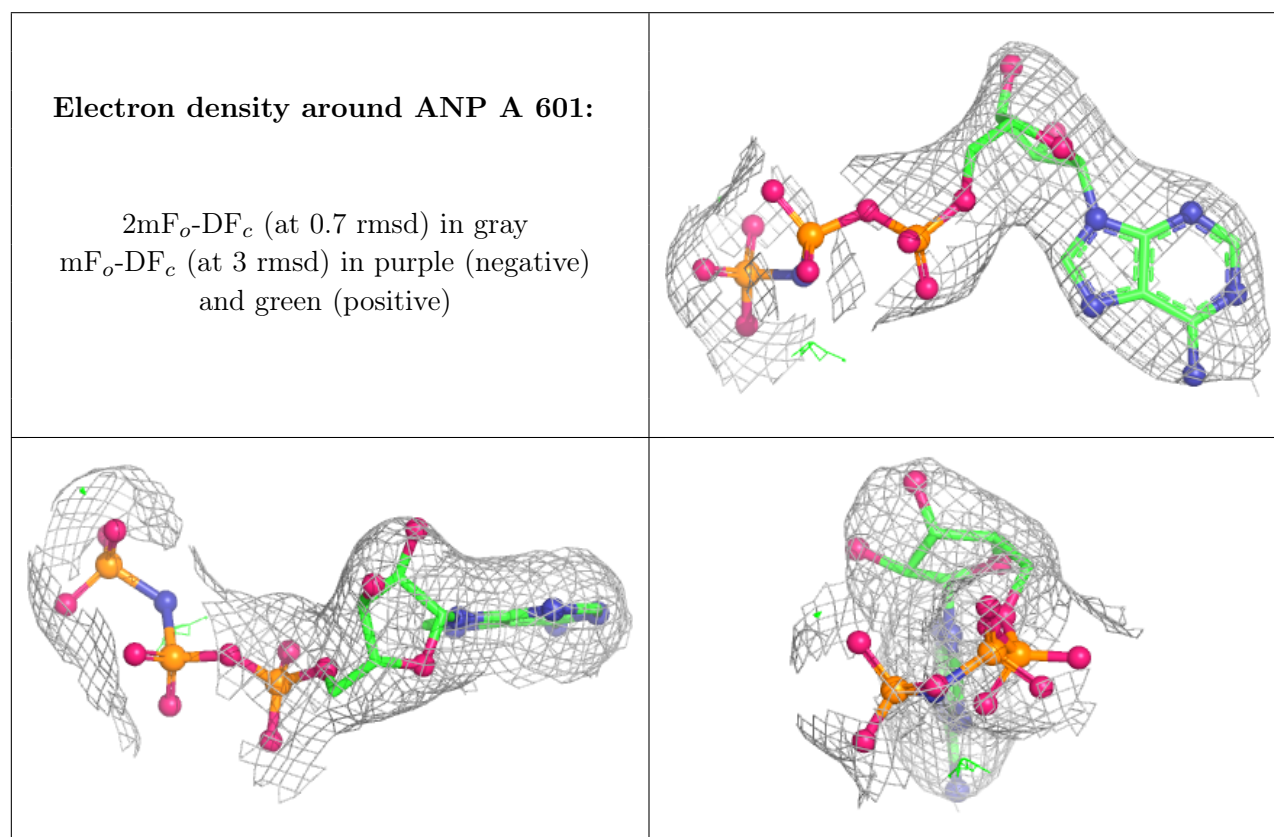
There are no oligosaccharides in this entry.

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	ANP	A	601	31/31	0.95	0.07	85,116,121,124	0
4	MG	A	602	1/1	0.95	0.11	109,109,109,109	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.