



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:29 AM UTC

PDB ID : 2QPT / pdb_00002qpt
Title : Crystal structure of an EHD ATPase involved in membrane remodelling
Authors : Daumke, O.
Deposited on : 2007-07-25
Resolution : 3.10 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

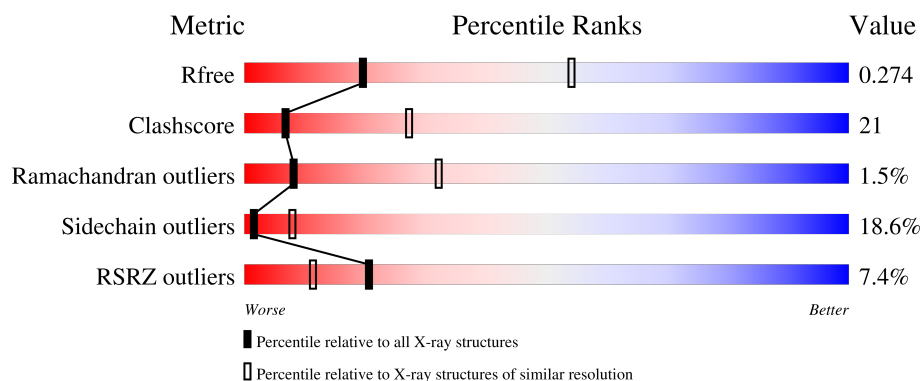
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	550	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3834 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 EH DOMAIN-CONTAINING PROTEIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	6	0	0
			3795	2437	652	689	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q8BH64
A	-5	PRO	-	expression tag	UNP Q8BH64
A	-4	HIS	-	expression tag	UNP Q8BH64
A	-3	MET	-	expression tag	UNP Q8BH64
A	-2	GLY	-	expression tag	UNP Q8BH64
A	-1	GLY	-	expression tag	UNP Q8BH64
A	0	SER	-	expression tag	UNP Q8BH64
A	410	ALA	GLN	engineered mutation	UNP Q8BH64

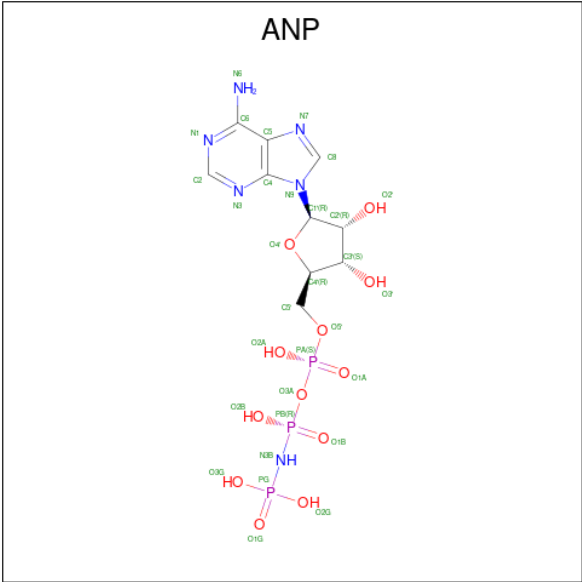
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

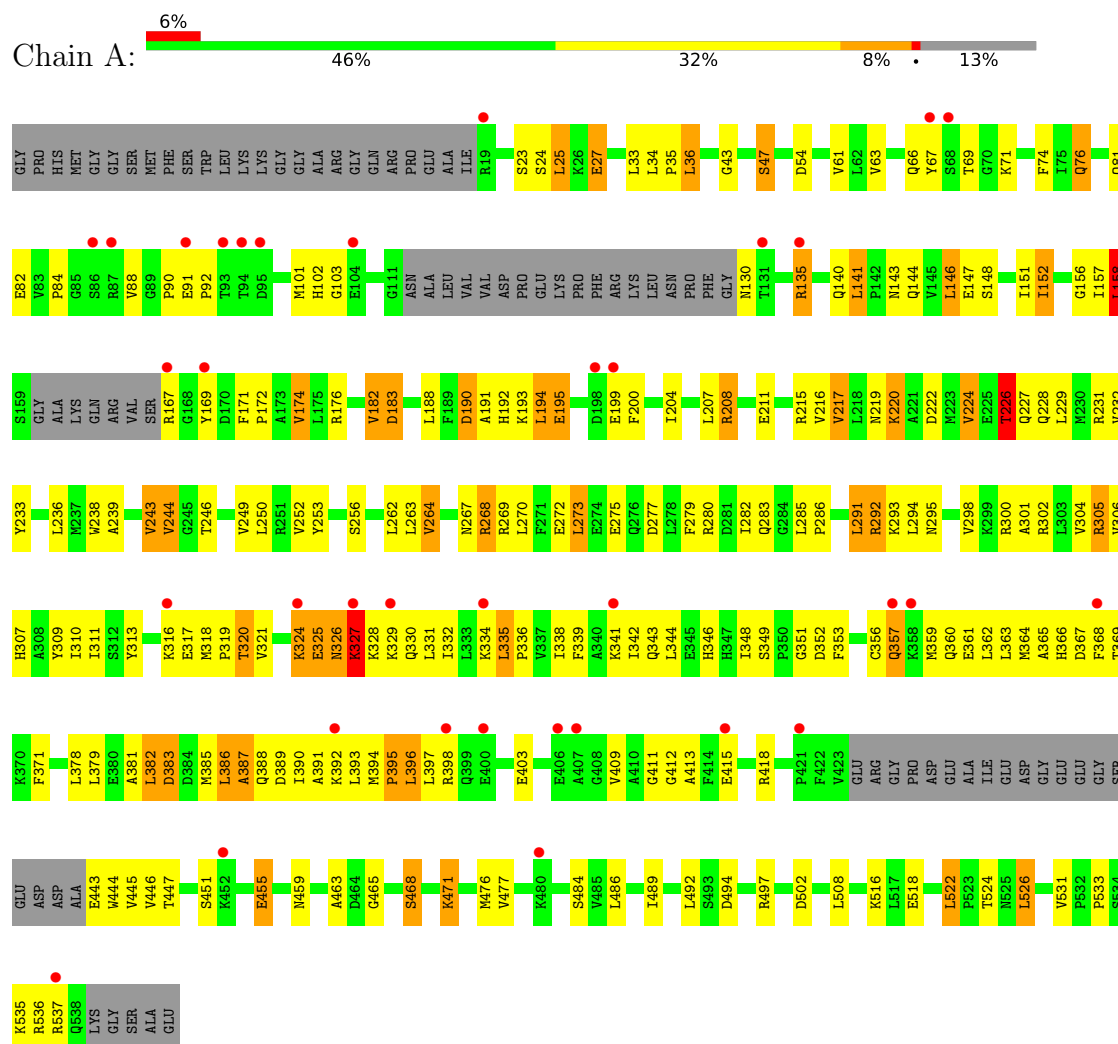
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		

3 Residue-property plots

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: EH DOMAIN-CONTAINING PROTEIN-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.85Å 134.65Å 56.07Å 90.00° 106.05° 90.00°	Depositor
Resolution (Å)	19.96 – 3.10 19.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.96-3.10) 98.3 (19.96-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.40 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.234 , 0.276 0.231 , 0.274	Depositor DCC
R_{free} test set	623 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3834	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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: MG, CA, 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	0.61	5/3877 (0.1%)	0.90	13/5236 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CG-CD	15.53	1.90	1.52
1	A	395	PRO	C-O	12.46	1.40	1.24
1	A	395	PRO	C-N	10.20	1.47	1.33
1	A	158	LEU	CB-CG	-9.01	1.35	1.53
1	A	392	LYS	C-O	8.14	1.34	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	GLU	CB-CG-CD	-15.09	86.94	112.60
1	A	395	PRO	CA-C-N	-9.85	106.31	120.29
1	A	395	PRO	C-N-CA	-9.85	106.31	120.29
1	A	395	PRO	O-C-N	7.51	131.25	122.17
1	A	396	LEU	N-CA-C	-5.99	104.83	111.36
1	A	327	LYS	N-CA-C	-5.76	105.00	111.28
1	A	455	GLU	CG-CD-OE1	-5.75	105.17	118.40
1	A	366	HIS	N-CA-C	5.47	118.53	110.59
1	A	243	VAL	N-CA-C	5.25	115.36	110.42
1	A	135	ARG	N-CA-C	-5.23	106.75	112.72
1	A	226	THR	N-CA-C	5.20	116.64	110.97
1	A	413	ALA	N-CA-C	-5.06	106.35	112.88
1	A	182	VAL	N-CA-C	5.04	115.55	110.05

There are no chirality outliers.

There are no planarity outliers.

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	3795	0	3849	164	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	13	3	0
5	A	6	0	0	0	0
All	All	3834	0	3862	164	1

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 21.

All (164) 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:305:ARG:HH21	1:A:305:ARG:HG2	1.17	1.08
1:A:357:GLN:HA	1:A:360:GLN:HE21	1.16	1.06
1:A:188:LEU:HD22	1:A:217:VAL:HG22	1.47	0.96
1:A:66:GLN:NE2	1:A:195:GLU:O	2.00	0.94
1:A:208:ARG:HH11	1:A:208:ARG:HG2	1.32	0.93
1:A:334:LYS:O	1:A:334:LYS:HG2	1.73	0.87
1:A:357:GLN:HA	1:A:360:GLN:NE2	1.91	0.85
1:A:277:ASP:HA	1:A:280:ARG:HH12	1.41	0.85
1:A:403:GLU:HA	1:A:403:GLU:OE1	1.80	0.82
1:A:277:ASP:HA	1:A:280:ARG:NH1	1.96	0.81
1:A:91:GLU:HG3	1:A:92:PRO:HD2	1.65	0.79
1:A:208:ARG:HG2	1:A:208:ARG:NH1	1.94	0.79
1:A:244:VAL:HG23	1:A:246:THR:HG22	1.65	0.77
1:A:382:LEU:HD13	1:A:386:LEU:HD21	1.67	0.76
1:A:171:PHE:HB3	1:A:172:PRO:HD3	1.67	0.76
1:A:533:PRO:HA	1:A:535:LYS:HE3	1.69	0.75
1:A:194:LEU:HG	1:A:232:VAL:HG13	1.70	0.73
1:A:415:GLU:HG3	1:A:418:ARG:HG3	1.70	0.73
1:A:305:ARG:HG2	1:A:305:ARG:NH2	1.97	0.72
1:A:394:MET:HB2	1:A:395:PRO:HD3	1.72	0.70
1:A:305:ARG:HH21	1:A:305:ARG:CG	2.02	0.69
1:A:200:PHE:HD2	1:A:204:ILE:CD1	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:O	1:A:272:GLU:HG2	1.94	0.67
1:A:302:ARG:O	1:A:306:VAL:HG23	1.95	0.67
1:A:216:VAL:O	1:A:252:VAL:HA	1.97	0.65
1:A:208:ARG:HH11	1:A:208:ARG:CG	2.07	0.65
1:A:363:LEU:HD12	1:A:368:PHE:CZ	2.32	0.65
1:A:386:LEU:O	1:A:390:ILE:HB	1.98	0.63
1:A:200:PHE:CD2	1:A:204:ILE:HD11	2.33	0.63
1:A:388:GLN:O	1:A:391:ALA:HB3	1.99	0.63
1:A:200:PHE:HD2	1:A:204:ILE:HD12	1.64	0.63
1:A:76:GLN:NE2	1:A:82:GLU:HA	2.14	0.63
1:A:200:PHE:CD2	1:A:204:ILE:CD1	2.82	0.63
1:A:275:GLU:HG2	1:A:279:PHE:CE2	2.35	0.62
1:A:318:MET:HG3	1:A:368:PHE:HB3	1.81	0.61
1:A:361:GLU:O	1:A:364:MET:HB3	2.00	0.61
1:A:494:ASP:CG	1:A:497:ARG:HA	2.26	0.60
1:A:233:TYR:CE2	1:A:252:VAL:HG21	2.37	0.60
1:A:190:ASP:OD2	1:A:220:LYS:HE2	2.02	0.59
1:A:27:GLU:HA	1:A:27:GLU:OE1	2.01	0.59
1:A:220:LYS:HB3	4:A:600:ANP:N1	2.19	0.58
1:A:219:ASN:C	1:A:220:LYS:HG2	2.28	0.58
1:A:341:LYS:O	1:A:344:LEU:HB2	2.04	0.57
1:A:71:LYS:HE3	4:A:600:ANP:O1B	2.03	0.57
1:A:152:ILE:O	1:A:152:ILE:HG13	2.04	0.57
1:A:220:LYS:HA	1:A:256:SER:HB3	1.87	0.57
1:A:47:SER:HB3	1:A:300:ARG:NH1	2.20	0.56
1:A:394:MET:O	1:A:397:LEU:HB3	2.04	0.56
1:A:171:PHE:O	1:A:174:VAL:HG13	2.06	0.56
1:A:216:VAL:CG1	1:A:252:VAL:HG12	2.35	0.56
1:A:395:PRO:HA	1:A:398:ARG:HD3	1.87	0.56
1:A:102:HIS:CG	1:A:103:GLY:H	2.23	0.56
1:A:327:LYS:O	1:A:331:LEU:HB2	2.06	0.56
1:A:148:SER:HB2	1:A:409:VAL:HG13	1.88	0.55
1:A:307:HIS:CE1	1:A:311:ILE:HD13	2.41	0.55
1:A:188:LEU:CD2	1:A:217:VAL:HG22	2.29	0.55
1:A:91:GLU:CG	1:A:92:PRO:HD2	2.37	0.54
1:A:215:ARG:HD2	1:A:253:TYR:HE1	1.73	0.53
1:A:135:ARG:NH2	1:A:169:TYR:HB3	2.23	0.53
1:A:334:LYS:O	1:A:334:LYS:CG	2.49	0.53
1:A:291:LEU:HG	1:A:397:LEU:HD21	1.91	0.53
1:A:334:LYS:O	1:A:338:ILE:HG12	2.07	0.53
1:A:465:GLY:O	1:A:502:ASP:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ALA:O	1:A:243:VAL:HG23	2.09	0.53
1:A:102:HIS:CG	1:A:103:GLY:N	2.77	0.52
1:A:313:TYR:O	1:A:316:LYS:HG2	2.10	0.52
1:A:25:LEU:HD11	1:A:294:LEU:HD13	1.92	0.51
1:A:335:LEU:HD12	1:A:360:GLN:HG3	1.92	0.51
1:A:362:LEU:O	1:A:365:ALA:N	2.43	0.51
1:A:382:LEU:HD13	1:A:386:LEU:CD2	2.40	0.51
1:A:69:THR:HG21	1:A:188:LEU:C	2.36	0.51
1:A:190:ASP:OD2	1:A:192:HIS:HB3	2.10	0.51
1:A:329:LYS:HE2	1:A:364:MET:HE1	1.92	0.51
1:A:144:GLN:O	1:A:147:GLU:HB2	2.11	0.51
1:A:403:GLU:OE1	1:A:403:GLU:CA	2.54	0.51
1:A:335:LEU:N	1:A:336:PRO:HD2	2.26	0.50
1:A:103:GLY:HA3	1:A:140:GLN:HB3	1.92	0.50
1:A:342:ILE:O	1:A:346:HIS:HB2	2.11	0.50
1:A:102:HIS:HB2	1:A:146:LEU:O	2.12	0.50
1:A:224:VAL:HG22	1:A:228:GLN:HG2	1.94	0.50
1:A:171:PHE:HB3	1:A:172:PRO:CD	2.41	0.50
1:A:226:THR:HB	1:A:267:ASN:HD21	1.77	0.50
1:A:306:VAL:HG21	1:A:352:ASP:HB3	1.93	0.49
1:A:148:SER:OG	1:A:409:VAL:HA	2.12	0.49
1:A:386:LEU:HA	1:A:390:ILE:HD12	1.92	0.49
1:A:244:VAL:CG2	1:A:246:THR:HG22	2.37	0.49
1:A:101:MET:O	1:A:140:GLN:HA	2.12	0.49
1:A:200:PHE:CE2	1:A:204:ILE:HD11	2.47	0.48
1:A:489:ILE:CG1	1:A:522:LEU:HD21	2.43	0.48
1:A:63:VAL:HG12	1:A:71:LYS:HG2	1.95	0.48
1:A:84:PRO:HD3	1:A:141:LEU:HD13	1.96	0.48
1:A:298:VAL:HG22	1:A:390:ILE:HD13	1.96	0.48
1:A:357:GLN:O	1:A:360:GLN:HB2	2.13	0.48
1:A:190:ASP:C	1:A:192:HIS:H	2.20	0.48
1:A:378:LEU:O	1:A:381:ALA:HB3	2.14	0.47
1:A:157:ILE:HG12	1:A:171:PHE:CE2	2.49	0.47
1:A:305:ARG:HD2	1:A:309:TYR:HE1	1.80	0.47
1:A:359:MET:O	1:A:363:LEU:HB2	2.15	0.47
1:A:349:SER:C	1:A:351:GLY:N	2.72	0.47
1:A:25:LEU:HD13	1:A:393:LEU:HD13	1.96	0.47
1:A:343:GLN:HG3	1:A:353:PHE:CE2	2.50	0.47
1:A:359:MET:HG3	1:A:363:LEU:HD23	1.96	0.46
1:A:285:LEU:HB2	1:A:286:PRO:HD3	1.97	0.46
1:A:497:ARG:O	1:A:497:ARG:CG	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:O	1:A:386:LEU:HD23	2.16	0.46
1:A:204:ILE:HG21	1:A:244:VAL:HG12	1.97	0.46
1:A:385:MET:O	1:A:389:ASP:HB2	2.15	0.46
1:A:135:ARG:CZ	1:A:169:TYR:HB3	2.46	0.45
1:A:367:ASP:C	1:A:367:ASP:OD2	2.58	0.45
1:A:320:THR:OG1	1:A:321:VAL:N	2.50	0.45
1:A:325:GLU:O	1:A:328:LYS:HB3	2.17	0.45
1:A:182:VAL:CG1	1:A:183:ASP:N	2.78	0.45
1:A:326:ASN:O	1:A:330:GLN:HB3	2.17	0.45
1:A:494:ASP:OD2	1:A:497:ARG:HA	2.16	0.45
1:A:157:ILE:HG23	1:A:199:GLU:HG2	1.99	0.45
1:A:292:ARG:HG3	1:A:293:LYS:N	2.32	0.44
1:A:43:GLY:HA2	1:A:47:SER:O	2.17	0.44
1:A:368:PHE:HA	1:A:371:PHE:CD1	2.53	0.44
1:A:273:LEU:HD13	1:A:273:LEU:HA	1.73	0.43
1:A:324:LYS:HE3	1:A:369:THR:HG21	2.00	0.43
1:A:394:MET:CB	1:A:395:PRO:HD3	2.47	0.43
1:A:193:LYS:HE2	1:A:193:LYS:HB3	1.68	0.43
1:A:385:MET:HA	1:A:389:ASP:OD2	2.18	0.43
1:A:222:ASP:O	1:A:264:VAL:HG12	2.19	0.43
1:A:531:VAL:O	1:A:535:LYS:HE2	2.18	0.43
1:A:383:ASP:OD1	1:A:383:ASP:N	2.51	0.43
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.86	0.43
1:A:141:LEU:HD23	1:A:141:LEU:N	2.34	0.43
1:A:282:ILE:O	1:A:285:LEU:HG	2.18	0.43
1:A:526:LEU:HD12	1:A:531:VAL:HG22	2.01	0.42
1:A:226:THR:HB	1:A:267:ASN:ND2	2.33	0.42
1:A:300:ARG:O	1:A:301:ALA:C	2.62	0.42
1:A:468:SER:HB3	1:A:471:LYS:HG3	2.02	0.42
1:A:283:GLN:HA	1:A:409:VAL:CG2	2.50	0.42
1:A:386:LEU:O	1:A:387:ALA:C	2.63	0.42
1:A:33:LEU:HD21	1:A:301:ALA:HA	2.02	0.42
1:A:102:HIS:CA	1:A:146:LEU:HB3	2.50	0.42
1:A:191:ALA:HA	1:A:232:VAL:HG11	2.01	0.42
1:A:476:MET:HB3	1:A:486:LEU:HD22	2.01	0.42
1:A:293:LYS:O	1:A:294:LEU:C	2.62	0.42
1:A:215:ARG:HD2	1:A:253:TYR:CE1	2.54	0.41
1:A:305:ARG:NH2	1:A:305:ARG:CG	2.69	0.41
1:A:317:GLU:HB3	1:A:331:LEU:HD11	2.02	0.41
1:A:385:MET:O	1:A:386:LEU:C	2.62	0.41
1:A:47:SER:HB3	1:A:300:ARG:HH12	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLU:HG3	1:A:444:TRP:N	2.34	0.41
1:A:71:LYS:NZ	1:A:156:GLY:HA2	2.35	0.41
1:A:394:MET:HB2	1:A:395:PRO:CD	2.47	0.41
1:A:61:VAL:CG2	1:A:151:ILE:HG23	2.50	0.41
1:A:81:GLN:HE21	1:A:143:ASN:HD22	1.69	0.41
1:A:200:PHE:O	1:A:204:ILE:HD12	2.21	0.41
1:A:61:VAL:HG23	1:A:151:ILE:HG23	2.02	0.41
1:A:319:PRO:HD3	1:A:327:LYS:HG3	2.01	0.41
1:A:356:CYS:O	1:A:360:GLN:HG3	2.21	0.41
1:A:67:TYR:CE1	1:A:158:LEU:HA	2.56	0.41
1:A:71:LYS:O	1:A:74:PHE:HB3	2.21	0.41
1:A:256:SER:HB2	4:A:600:ANP:HN62	1.86	0.41
1:A:34:LEU:N	1:A:35:PRO:CD	2.84	0.41
1:A:36:LEU:HD22	1:A:304:VAL:HG12	2.02	0.40
1:A:190:ASP:HB2	1:A:220:LYS:HG3	2.04	0.40
1:A:310:ILE:HD13	1:A:339:PHE:CE1	2.57	0.40
1:A:226:THR:O	1:A:227:GLN:C	2.63	0.40
1:A:302:ARG:HB3	1:A:352:ASP:OD1	2.21	0.40
1:A:157:ILE:HG12	1:A:171:PHE:HE2	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLU:OE1	1:A:443:GLU:OE1[2_553]	1.56	0.64

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	468/550 (85%)	404 (86%)	57 (12%)	7 (2%)	8	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ALA
1	A	90	PRO
1	A	411	GLY
1	A	463	ALA
1	A	325	GLU
1	A	412	GLY
1	A	320	THR

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	413/468 (88%)	336 (81%)	77 (19%)	1 8

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	24	SER
1	A	25	LEU
1	A	27	GLU
1	A	36	LEU
1	A	47	SER
1	A	54	ASP
1	A	76	GLN
1	A	88	VAL
1	A	130	ASN
1	A	141	LEU
1	A	146	LEU
1	A	152	ILE
1	A	158	LEU
1	A	167	ARG
1	A	174	VAL
1	A	176	ARG
1	A	183	ASP

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Mol	Chain	Res	Type
1	A	190	ASP
1	A	194	LEU
1	A	195	GLU
1	A	207	LEU
1	A	208	ARG
1	A	211	GLU
1	A	217	VAL
1	A	220	LYS
1	A	224	VAL
1	A	226	THR
1	A	229	LEU
1	A	231	ARG
1	A	236	LEU
1	A	238	TRP
1	A	244	VAL
1	A	249	VAL
1	A	250	LEU
1	A	262	LEU
1	A	263	LEU
1	A	264	VAL
1	A	268	ARG
1	A	269	ARG
1	A	270	LEU
1	A	273	LEU
1	A	291	LEU
1	A	292	ARG
1	A	295	ASN
1	A	305	ARG
1	A	324	LYS
1	A	326	ASN
1	A	327	LYS
1	A	332	ILE
1	A	335	LEU
1	A	348	ILE
1	A	357	GLN
1	A	379	LEU
1	A	382	LEU
1	A	383	ASP
1	A	386	LEU
1	A	396	LEU
1	A	445	VAL
1	A	446	VAL

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Mol	Chain	Res	Type
1	A	447	THR
1	A	451	SER
1	A	455	GLU
1	A	459	ASN
1	A	468	SER
1	A	471	LYS
1	A	477	VAL
1	A	484	SER
1	A	492	LEU
1	A	508	LEU
1	A	516	LYS
1	A	518	GLU
1	A	522	LEU
1	A	524	THR
1	A	526	LEU
1	A	536	ARG
1	A	537	ARG

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	76	GLN
1	A	81	GLN
1	A	134	ASN
1	A	192	HIS
1	A	267	ASN
1	A	276	GLN
1	A	283	GLN
1	A	288	HIS
1	A	295	ASN
1	A	326	ASN
1	A	343	GLN
1	A	357	GLN
1	A	360	GLN
1	A	399	GLN

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 2 are 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	$\# Z > 2$
4	ANP	A	600	2	33,33,33	1.93	10 (30%)	45,52,52	2.00	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
4	ANP	A	600	2	-	9/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ANP	PB-N3B	4.31	1.74	1.63
4	A	600	ANP	C5-C4	4.29	1.46	1.39
4	A	600	ANP	PG-N3B	4.22	1.74	1.63
4	A	600	ANP	PG-O1G	3.54	1.51	1.46
4	A	600	ANP	PB-O1B	3.36	1.51	1.46
4	A	600	ANP	C5-C6	2.51	1.48	1.41
4	A	600	ANP	C8-N7	2.36	1.36	1.31
4	A	600	ANP	C5-N7	-2.24	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ANP	PB-O2B	-2.02	1.51	1.56
4	A	600	ANP	PG-O3G	-2.01	1.51	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ANP	C5-C4-N3	-5.61	118.99	126.72
4	A	600	ANP	O1G-PG-N3B	-4.77	104.75	111.77
4	A	600	ANP	N3-C4-N9	4.49	134.80	127.17
4	A	600	ANP	O2B-PB-O1B	4.00	118.45	109.87
4	A	600	ANP	C2-N3-C4	3.66	120.77	111.83
4	A	600	ANP	C4-C5-N7	-3.41	106.68	110.58
4	A	600	ANP	N3-C2-N1	-3.28	123.61	128.58
4	A	600	ANP	C4-N9-C8	3.11	109.00	105.74
4	A	600	ANP	C5-N7-C8	2.64	107.59	103.45
4	A	600	ANP	N9-C8-N7	-2.41	110.52	113.94
4	A	600	ANP	O2G-PG-O3G	2.24	113.61	107.59
4	A	600	ANP	C6-C5-N7	2.09	136.12	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ANP	PG-N3B-PB-O1B
4	A	600	ANP	PG-N3B-PB-O3A
4	A	600	ANP	C5'-O5'-PA-O2A
4	A	600	ANP	C5'-O5'-PA-O3A
4	A	600	ANP	O4'-C4'-C5'-O5'
4	A	600	ANP	C3'-C4'-C5'-O5'
4	A	600	ANP	C5'-O5'-PA-O1A
4	A	600	ANP	C2'-C1'-N9-C8
4	A	600	ANP	PB-N3B-PG-O1G

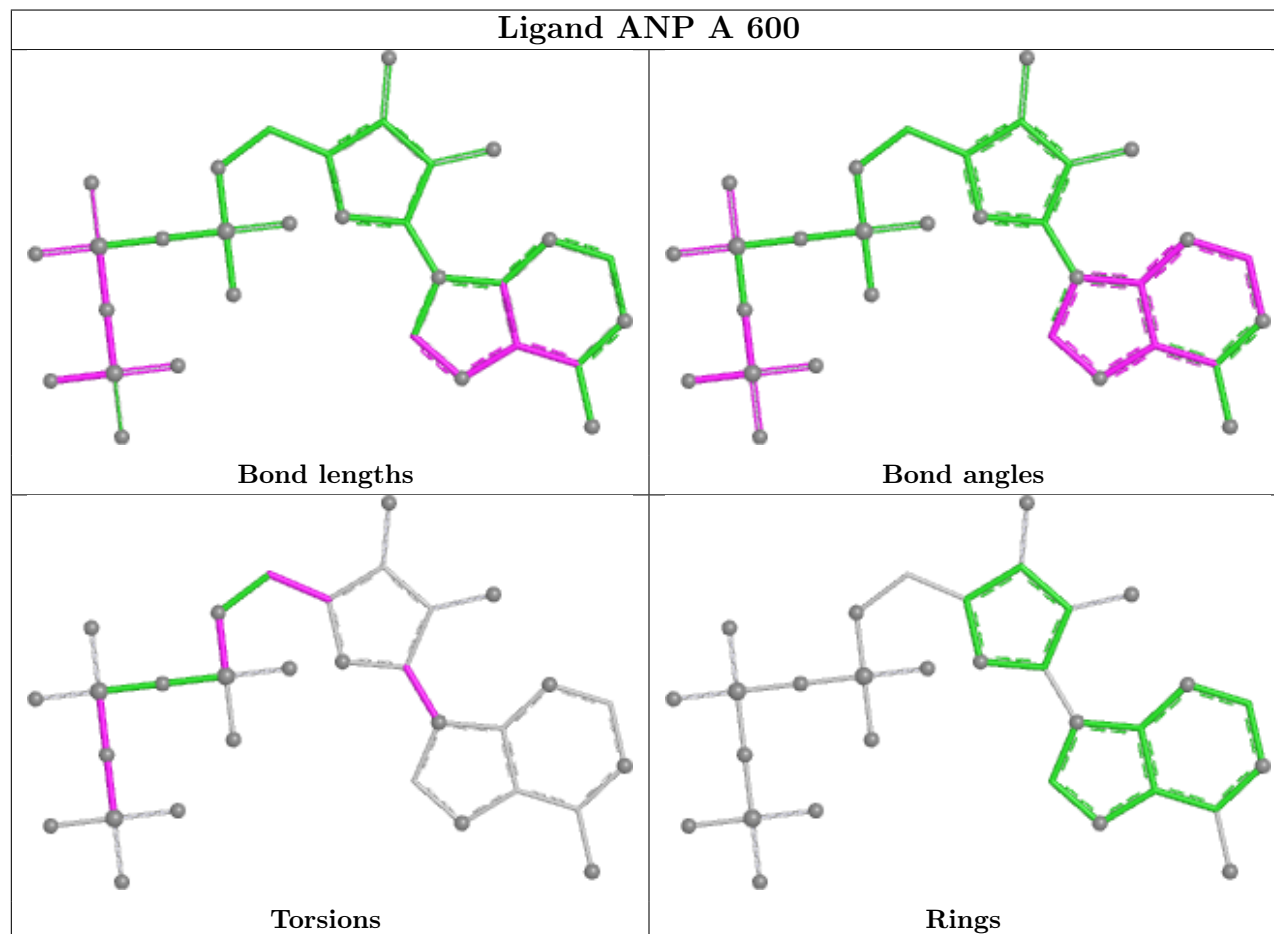
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	ANP	3	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	476/550 (86%)	0.51	35 (7%) 20 11	28, 59, 66, 70	31 (6%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ARG	6.0
1	A	94	THR	4.7
1	A	324	LYS	4.6
1	A	91	GLU	4.5
1	A	537	ARG	4.4
1	A	93	THR	4.2
1	A	67	TYR	4.1
1	A	400	GLU	4.1
1	A	406	GLU	4.1
1	A	198	ASP	4.0
1	A	135	ARG	3.9
1	A	316	LYS	3.6
1	A	95	ASP	3.6
1	A	415	GLU	3.5
1	A	407	ALA	3.2
1	A	199	GLU	3.2
1	A	68	SER	3.2
1	A	392	LYS	3.2
1	A	357	GLN	3.1
1	A	86	SER	3.1
1	A	327	LYS	3.0
1	A	358	LYS	2.8
1	A	398	ARG	2.7
1	A	167	ARG	2.7
1	A	104	GLU	2.6
1	A	329	LYS	2.6
1	A	19	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	169	TYR	2.4
1	A	131	THR	2.3
1	A	368	PHE	2.3
1	A	452	LYS	2.2
1	A	334	LYS	2.2
1	A	421	PRO	2.1
1	A	341	LYS	2.0
1	A	480	LYS	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](#)

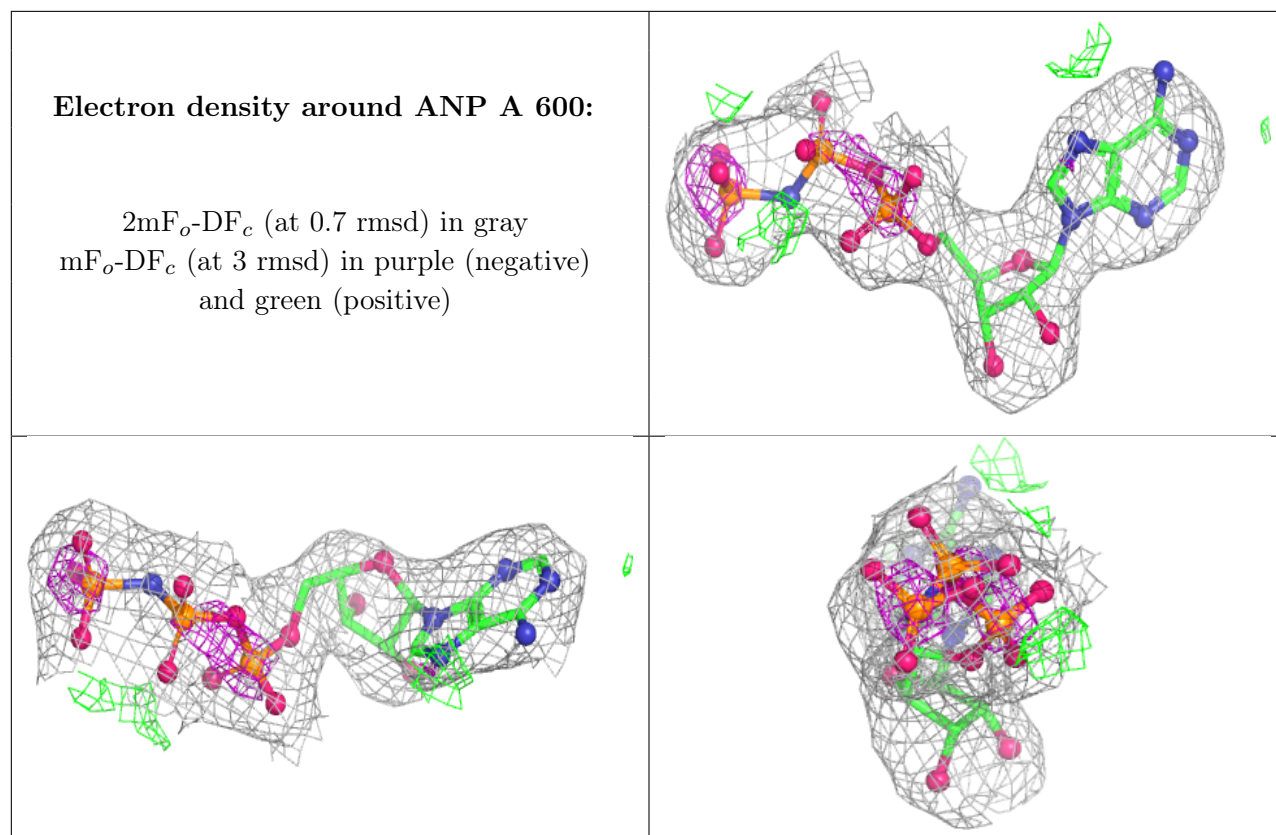
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	MG	A	700	1/1	0.86	0.10	48,48,48,48	0
4	ANP	A	600	31/31	0.95	0.10	51,52,53,53	0
3	CA	A	701	1/1	0.98	0.04	48,48,48,48	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.