



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:34 AM UTC

PDB ID : 2OZO / pdb_00002ozo
Title : Autoinhibited intact human ZAP-70
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Deposited on : 2007-02-26
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

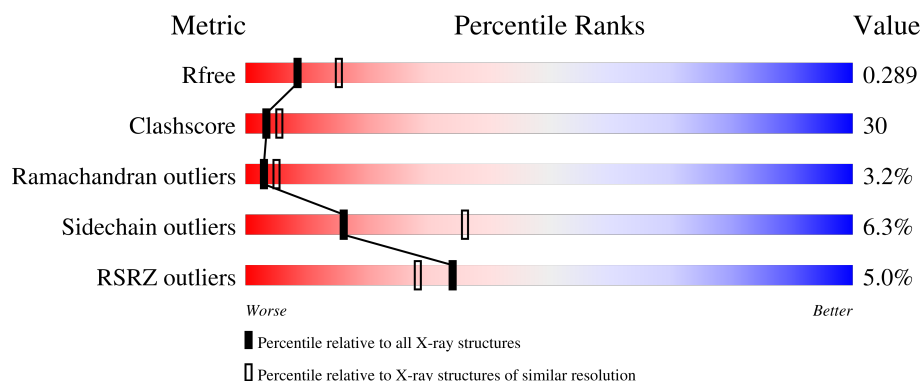
1 Overall quality at a glance

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	613	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4326 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 Tyrosine-protein kinase ZAP-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4225	2705	727	759	34	0	0	0

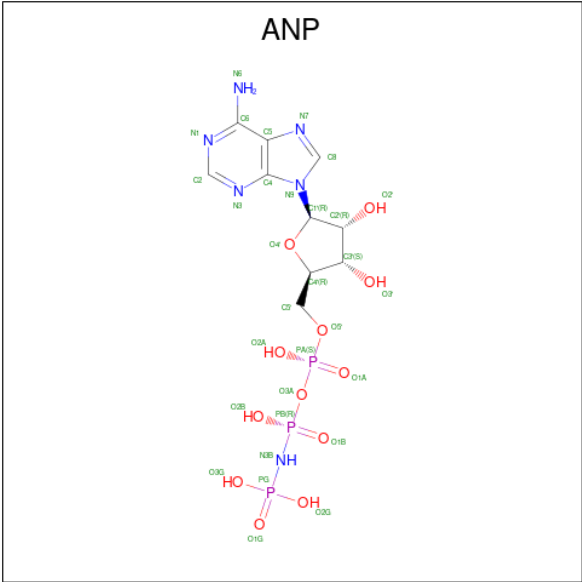
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	PHE	TYR	engineered mutation	UNP P43403
A	319	PHE	TYR	engineered mutation	UNP P43403
A	461	ASN	ASP	engineered mutation	UNP P43403
A	607	GLY	-	cloning artifact	UNP P43403
A	608	SER	-	cloning artifact	UNP P43403
A	609	ALA	-	cloning artifact	UNP P43403
A	610	LEU	-	cloning artifact	UNP P43403
A	611	GLU	-	cloning artifact	UNP P43403
A	612	VAL	-	cloning artifact	UNP P43403
A	613	ALA	-	cloning artifact	UNP P43403

- 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 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total	0	0
			69 O 69 69		

- Molecule 1: Tyrosine-protein kinase ZAP-70



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.30Å 52.93Å 69.33Å 105.91° 92.94° 103.72°	Depositor
Resolution (Å)	500.00 – 2.60 66.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (500.00-2.60) 88.3 (66.16-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.290 0.219 , 0.289	Depositor DCC
R_{free} test set	1911 reflections (9.31%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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: ANP, MG

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	0.51	0/4328	1.04	18/5855 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	GLU	N-CA-C	-12.33	99.12	112.93
1	A	326	LYS	N-CA-C	10.31	124.54	109.69
1	A	319	PHE	N-CA-C	-10.23	100.93	113.41
1	A	372	LYS	N-CA-C	-8.70	100.99	111.69
1	A	470	VAL	N-CA-C	-8.10	103.00	111.58
1	A	380	THR	N-CA-C	-7.42	104.20	113.18
1	A	166	SER	N-CA-C	7.09	121.38	112.87
1	A	344	LEU	N-CA-C	-6.75	103.63	112.41
1	A	179	SER	N-CA-C	6.20	119.29	110.68
1	A	565	PRO	CA-C-N	5.68	124.87	118.97
1	A	565	PRO	C-N-CA	5.68	124.87	118.97
1	A	343	GLU	N-CA-C	5.48	117.76	110.53
1	A	327	ASP	N-CA-C	-5.36	99.38	110.80
1	A	433	ILE	N-CA-C	5.36	112.44	107.56
1	A	100	LYS	CA-C-N	5.24	126.05	120.13
1	A	100	LYS	C-N-CA	5.24	126.05	120.13
1	A	324	GLU	N-CA-C	-5.07	104.36	110.44
1	A	603	LYS	N-CA-C	5.01	121.48	110.80

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	4225	0	4104	251	0
2	A	1	0	0	0	0
3	A	31	0	13	1	0
4	A	69	0	0	9	0
All	All	4326	0	4117	252	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 30.

All (252) 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:430:ARG:HH12	1:A:562:PRO:HB2	1.17	1.08
1:A:604:VAL:HG23	1:A:605:GLU:H	1.19	1.05
1:A:27:ALA:HB3	1:A:33:LEU:HD21	1.48	0.96
1:A:605:GLU:HB2	1:A:610:LEU:HD22	1.48	0.96
1:A:41:ARG:HH22	1:A:226:GLY:HA3	1.35	0.92
1:A:559:GLU:CD	1:A:559:GLU:H	1.76	0.91
1:A:471:ASN:C	1:A:471:ASN:HD22	1.79	0.89
1:A:398:ILE:HD12	1:A:477:ILE:HB	1.56	0.87
1:A:230:ASP:HB2	1:A:234:GLN:HE22	1.38	0.86
1:A:170:ARG:CZ	1:A:190:ARG:HH22	1.91	0.84
1:A:485:ALA:HA	4:A:664:HOH:O	1.79	0.81
1:A:502:PRO:C	1:A:503:LEU:HD22	2.07	0.80
1:A:502:PRO:HD3	4:A:657:HOH:O	1.82	0.79
1:A:604:VAL:HG23	1:A:605:GLU:N	1.96	0.78
1:A:181:ALA:O	1:A:186:LYS:HE2	1.82	0.78
1:A:63:ARG:HH11	1:A:63:ARG:HB3	1.49	0.77
1:A:321:ASP:OD1	1:A:323:GLU:HG2	1.85	0.77
1:A:430:ARG:NH1	1:A:562:PRO:HB2	1.97	0.76
1:A:97:ASN:HD21	1:A:99:ARG:HE	1.33	0.74
1:A:517:SER:H	1:A:520:SER:HB3	1.51	0.74
1:A:343:GLU:OE1	1:A:351:SER:HB2	1.87	0.73
1:A:450:LYS:O	1:A:454:GLU:HG2	1.87	0.73
1:A:611:GLU:C	1:A:613:ALA:H	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HB3	1:A:41:ARG:NH1	2.06	0.71
1:A:398:ILE:CD1	1:A:477:ILE:HB	2.21	0.71
1:A:231:THR:OG1	1:A:234:GLN:HG3	1.91	0.70
1:A:314:VAL:HG12	1:A:319:PHE:CD1	2.26	0.70
1:A:610:LEU:C	1:A:612:VAL:H	1.98	0.69
1:A:354:GLN:HG3	1:A:416:MET:CE	2.23	0.68
1:A:479:ASP:HB3	1:A:482:LEU:HD11	1.74	0.68
1:A:611:GLU:C	1:A:613:ALA:N	2.49	0.68
1:A:318:PRO:HB3	4:A:632:HOH:O	1.92	0.68
1:A:450:LYS:HE3	1:A:587:LEU:HD12	1.77	0.67
1:A:552:ILE:HG23	1:A:557:ARG:HH12	1.58	0.67
1:A:314:VAL:HG13	1:A:474:TYR:CG	2.29	0.66
1:A:375:THR:CB	1:A:380:THR:HG22	2.25	0.66
1:A:40:LEU:H	1:A:40:LEU:HD22	1.61	0.65
1:A:354:GLN:HG2	1:A:355:GLY:N	2.11	0.65
1:A:471:ASN:C	1:A:471:ASN:ND2	2.52	0.65
1:A:220:LYS:HE3	1:A:230:ASP:OD2	1.95	0.65
1:A:170:ARG:HB2	1:A:170:ARG:HH11	1.62	0.65
1:A:342:ILE:N	1:A:342:ILE:HD12	2.11	0.64
1:A:577:ILE:HB	1:A:583:ARG:HG2	1.79	0.64
1:A:2:PRO:HB3	1:A:119:ARG:NH2	2.12	0.64
1:A:314:VAL:HG12	1:A:319:PHE:HD1	1.61	0.64
1:A:216:ASP:OD2	1:A:228:LYS:HE3	1.98	0.64
1:A:316:GLU:HB2	4:A:627:HOH:O	1.97	0.64
1:A:330:LEU:HD22	1:A:404:VAL:HG12	1.79	0.64
1:A:316:GLU:O	1:A:317:SER:HB2	1.97	0.63
1:A:198:TYR:HE1	1:A:221:TYR:HE2	1.47	0.63
1:A:552:ILE:HG23	1:A:557:ARG:NH1	2.13	0.63
1:A:603:LYS:O	1:A:604:VAL:HG22	1.99	0.62
1:A:119:ARG:HD2	1:A:150:GLU:OE1	1.99	0.62
1:A:230:ASP:HB2	1:A:234:GLN:NE2	2.14	0.61
1:A:169:THR:OG1	1:A:172:GLU:HG3	2.01	0.61
1:A:471:ASN:ND2	1:A:473:HIS:H	1.98	0.60
1:A:333:LYS:HB2	1:A:336:ASN:HD22	1.67	0.60
1:A:559:GLU:CD	1:A:559:GLU:N	2.56	0.60
1:A:529:MET:HB3	1:A:572:MET:HE2	1.83	0.60
1:A:349:PHE:CE1	1:A:482:LEU:HD13	2.37	0.59
1:A:441:LEU:O	1:A:445:VAL:HG23	2.03	0.59
1:A:390:MET:HE3	1:A:480:PHE:O	2.03	0.59
1:A:97:ASN:ND2	1:A:99:ARG:HE	2.00	0.58
1:A:459:HIS:O	1:A:460:ARG:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:C	1:A:35:LEU:HD12	2.28	0.58
1:A:231:THR:N	1:A:234:GLN:HE21	2.02	0.58
1:A:331:PHE:HZ	1:A:384:MET:HE2	1.68	0.58
1:A:460:ARG:HG2	1:A:516:PHE:CD2	2.39	0.58
1:A:27:ALA:CB	1:A:33:LEU:HD21	2.29	0.57
1:A:97:ASN:HD22	1:A:97:ASN:H	1.50	0.57
1:A:128:ARG:O	1:A:132:LYS:HA	2.03	0.57
1:A:328:LYS:HG3	1:A:328:LYS:O	2.03	0.57
1:A:33:LEU:HA	1:A:100:LYS:O	2.03	0.57
1:A:223:ILE:CG2	1:A:235:LEU:HD21	2.34	0.57
1:A:369:LYS:HZ1	1:A:479:ASP:CG	2.11	0.57
1:A:369:LYS:NZ	1:A:479:ASP:OD1	2.37	0.57
1:A:518:SER:O	1:A:522:VAL:HG23	2.05	0.56
1:A:604:VAL:CG2	1:A:605:GLU:H	2.04	0.56
1:A:83:LEU:C	1:A:83:LEU:HD23	2.30	0.56
1:A:97:ASN:HD21	1:A:99:ARG:NE	2.02	0.56
1:A:517:SER:O	1:A:520:SER:HB3	2.04	0.56
1:A:48:LEU:HB2	1:A:61:ILE:HD11	1.87	0.55
1:A:362:LYS:HD2	1:A:364:ILE:HG22	1.89	0.55
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.71	0.55
1:A:350:GLY:HA2	1:A:371:LEU:HD23	1.88	0.55
1:A:198:TYR:CE1	1:A:221:TYR:HE2	2.25	0.55
1:A:161:MET:HG3	1:A:163:TRP:CZ2	2.42	0.55
1:A:481:GLY:N	4:A:672:HOH:O	2.39	0.55
1:A:568:LEU:HD22	1:A:593:MET:CE	2.37	0.55
1:A:46:TYR:CE2	1:A:80:PRO:HG3	2.42	0.54
1:A:509:GLU:OE2	1:A:580:TRP:HB3	2.07	0.54
1:A:577:ILE:HG21	1:A:582:ASP:HB2	1.88	0.54
1:A:559:GLU:N	1:A:559:GLU:OE2	2.40	0.54
1:A:145:GLN:HG3	1:A:315:PHE:CZ	2.42	0.54
1:A:188:LEU:HD12	1:A:188:LEU:C	2.33	0.53
1:A:337:LEU:HD23	1:A:339:ILE:HD11	1.90	0.53
1:A:202:LEU:CD2	1:A:209:TYR:HB2	2.39	0.53
1:A:540:TYR:HB3	1:A:543:MET:HE3	1.89	0.53
1:A:502:PRO:O	1:A:503:LEU:HD22	2.07	0.53
1:A:336:ASN:ND2	4:A:681:HOH:O	2.40	0.53
1:A:574:ASP:O	1:A:577:ILE:HG12	2.07	0.53
1:A:460:ARG:O	1:A:506:TYR:HE1	1.91	0.52
1:A:239:LEU:HB2	1:A:250:LEU:HD12	1.92	0.52
1:A:568:LEU:HD22	1:A:593:MET:HE1	1.91	0.52
1:A:607:GLY:O	1:A:608:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:CD1	1:A:208:VAL:HG22	2.39	0.52
1:A:136:GLU:O	1:A:140:GLN:N	2.38	0.52
1:A:173:ALA:O	1:A:177:LEU:HG	2.10	0.51
1:A:314:VAL:HG13	1:A:474:TYR:CD1	2.45	0.51
1:A:334:ARG:HD3	1:A:407:ALA:CB	2.40	0.51
1:A:482:LEU:HD12	1:A:483:SER:N	2.26	0.51
1:A:322:PRO:HG2	1:A:402:ILE:CD1	2.40	0.51
1:A:549:MET:HE3	1:A:549:MET:HA	1.91	0.51
1:A:97:ASN:HD22	1:A:97:ASN:N	2.08	0.51
1:A:440:GLU:HG3	1:A:597:TYR:CZ	2.45	0.51
1:A:188:LEU:O	1:A:189:LEU:HD12	2.09	0.51
1:A:188:LEU:C	1:A:189:LEU:HD12	2.36	0.51
1:A:41:ARG:HH12	1:A:227:THR:N	2.08	0.51
1:A:161:MET:HE2	1:A:233:TRP:CD1	2.47	0.51
1:A:502:PRO:O	1:A:503:LEU:HD13	2.10	0.50
1:A:544:LYS:HG3	1:A:545:GLY:N	2.26	0.50
1:A:551:PHE:CE1	1:A:556:LYS:HB3	2.46	0.50
1:A:333:LYS:HB2	1:A:336:ASN:ND2	2.25	0.50
1:A:437:ASN:ND2	1:A:472:ARG:HH21	2.09	0.50
1:A:178:TYR:CZ	1:A:208:VAL:HG23	2.45	0.50
1:A:170:ARG:HB2	1:A:170:ARG:NH1	2.26	0.50
1:A:423:HIS:O	1:A:427:VAL:HG23	2.11	0.50
1:A:155:THR:HG22	1:A:155:THR:O	2.12	0.49
1:A:63:ARG:HB3	1:A:63:ARG:NH1	2.23	0.49
1:A:505:TRP:HZ2	1:A:531:GLU:CD	2.20	0.49
1:A:125:ASP:O	1:A:129:GLN:HB2	2.12	0.49
1:A:134:GLU:HG3	1:A:135:GLY:N	2.27	0.49
1:A:146:ALA:HB3	1:A:147:PRO:HD3	1.95	0.49
1:A:434:PRO:HG2	1:A:437:ASN:HB2	1.94	0.49
1:A:471:ASN:ND2	1:A:473:HIS:N	2.60	0.49
1:A:128:ARG:NH1	1:A:134:GLU:OE1	2.46	0.49
3:A:615:ANP:H5'1	4:A:655:HOH:O	2.12	0.49
1:A:41:ARG:HH12	1:A:226:GLY:C	2.21	0.48
1:A:334:ARG:O	1:A:334:ARG:HG3	2.11	0.48
1:A:28:GLY:O	1:A:30:ALA:N	2.46	0.48
1:A:359:MET:HE2	1:A:364:ILE:HG23	1.95	0.48
1:A:215:GLN:HG3	1:A:219:GLY:O	2.14	0.48
1:A:127:VAL:HB	1:A:138:LEU:HD11	1.95	0.48
1:A:134:GLU:HG3	1:A:135:GLY:H	1.77	0.48
1:A:602:SER:O	1:A:604:VAL:N	2.41	0.48
1:A:331:PHE:CZ	1:A:384:MET:HE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD22	1:A:475:ALA:HB2	1.95	0.48
1:A:332:LEU:HD21	1:A:403:GLY:HA3	1.96	0.48
1:A:505:TRP:CZ2	1:A:539:PRO:HG2	2.49	0.48
1:A:572:MET:O	1:A:575:CYS:HB2	2.14	0.47
1:A:425:PHE:CD2	1:A:469:LEU:HD11	2.50	0.47
1:A:368:ILE:HD12	1:A:368:ILE:N	2.30	0.47
1:A:544:LYS:O	1:A:545:GLY:O	2.32	0.47
1:A:194:GLU:HB3	1:A:197:THR:OG1	2.15	0.47
1:A:133:LEU:HD23	1:A:138:LEU:HA	1.95	0.47
1:A:376:GLU:O	1:A:377:LYS:CB	2.63	0.47
1:A:544:LYS:HG3	1:A:545:GLY:H	1.79	0.47
1:A:529:MET:CB	1:A:572:MET:HE2	2.45	0.47
1:A:544:LYS:NZ	4:A:657:HOH:O	2.48	0.47
1:A:239:LEU:HD13	1:A:246:LEU:HD11	1.97	0.47
1:A:440:GLU:OE2	1:A:473:HIS:HD2	1.98	0.47
1:A:460:ARG:HG3	1:A:460:ARG:HH11	1.79	0.47
1:A:146:ALA:N	1:A:147:PRO:CD	2.79	0.46
1:A:544:LYS:CG	1:A:545:GLY:N	2.77	0.46
1:A:108:LEU:HD12	1:A:109:GLU:H	1.81	0.46
1:A:604:VAL:CG2	1:A:605:GLU:N	2.69	0.46
1:A:577:ILE:O	1:A:583:ARG:HD3	2.16	0.46
1:A:64:GLN:HB2	1:A:66:ASN:OD1	2.16	0.46
1:A:187:PHE:CD1	1:A:187:PHE:C	2.94	0.46
1:A:223:ILE:HG22	1:A:235:LEU:HD21	1.97	0.45
1:A:525:TYR:OH	1:A:593:MET:HG3	2.15	0.45
1:A:354:GLN:HE21	1:A:416:MET:HE3	1.82	0.45
1:A:429:LYS:HD3	1:A:432:GLU:OE1	2.16	0.45
1:A:460:ARG:HG2	1:A:516:PHE:HD2	1.81	0.45
1:A:229:PHE:CD1	1:A:235:LEU:HG	2.52	0.44
1:A:50:LEU:HD23	1:A:57:HIS:HB2	1.98	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.85	0.44
1:A:203:ILE:HD11	1:A:208:VAL:HG22	1.98	0.44
1:A:462:LEU:HD23	1:A:525:TYR:N	2.33	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.75	0.44
1:A:341:ASP:C	1:A:342:ILE:HD12	2.42	0.44
1:A:480:PHE:O	1:A:480:PHE:CD1	2.71	0.44
1:A:223:ILE:O	1:A:224:PRO:C	2.59	0.44
1:A:337:LEU:CD2	1:A:339:ILE:HD11	2.48	0.44
1:A:440:GLU:HG3	1:A:597:TYR:OH	2.18	0.44
1:A:70:ALA:HB2	1:A:76:ALA:HA	1.99	0.43
1:A:175:ARG:O	1:A:175:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HD3	4:A:662:HOH:O	2.18	0.43
1:A:450:LYS:HE3	1:A:587:LEU:CD1	2.47	0.43
1:A:231:THR:N	1:A:234:GLN:NE2	2.67	0.43
1:A:322:PRO:HG2	1:A:402:ILE:HD12	2.00	0.43
1:A:40:LEU:H	1:A:40:LEU:CD2	2.30	0.43
1:A:146:ALA:O	1:A:150:GLU:HG3	2.18	0.43
1:A:354:GLN:HG2	1:A:355:GLY:H	1.80	0.43
1:A:95:PRO:O	1:A:96:CYS:HB3	2.19	0.43
1:A:399:VAL:HG21	1:A:478:SER:HB3	2.00	0.43
1:A:519:ARG:NH1	1:A:581:GLU:HA	2.34	0.43
1:A:523:TRP:O	1:A:527:VAL:HG23	2.19	0.43
1:A:519:ARG:HH12	1:A:581:GLU:HA	1.81	0.43
1:A:202:LEU:HD23	1:A:209:TYR:HB2	1.99	0.43
1:A:459:HIS:C	1:A:459:HIS:ND1	2.77	0.43
1:A:324:GLU:O	1:A:325:LEU:CB	2.67	0.42
1:A:341:ASP:N	1:A:342:ILE:HD12	2.33	0.42
1:A:612:VAL:O	1:A:613:ALA:C	2.62	0.42
1:A:34:PHE:HA	1:A:49:SER:O	2.19	0.42
1:A:41:ARG:HH22	1:A:226:GLY:CA	2.19	0.42
1:A:453:GLU:HG3	1:A:518:SER:CB	2.48	0.42
1:A:607:GLY:N	1:A:610:LEU:HD21	2.34	0.42
1:A:321:ASP:OD1	1:A:322:PRO:N	2.53	0.42
1:A:540:TYR:CE2	1:A:558:MET:HG3	2.55	0.42
1:A:177:LEU:HB3	1:A:203:ILE:HD11	2.01	0.42
1:A:551:PHE:CZ	1:A:556:LYS:HB3	2.55	0.42
1:A:40:LEU:HD22	1:A:40:LEU:N	2.31	0.42
1:A:370:VAL:O	1:A:371:LEU:O	2.38	0.42
1:A:612:VAL:O	1:A:612:VAL:HG12	2.19	0.42
1:A:391:HIS:HE1	1:A:402:ILE:O	2.03	0.42
1:A:445:VAL:O	1:A:449:MET:HG2	2.19	0.42
1:A:31:ASP:HA	1:A:51:VAL:O	2.20	0.42
1:A:198:TYR:CE1	1:A:221:TYR:CE2	3.07	0.42
1:A:539:PRO:O	1:A:540:TYR:C	2.63	0.42
1:A:579:LYS:HB2	1:A:582:ASP:OD1	2.20	0.42
1:A:314:VAL:HG12	1:A:314:VAL:O	2.19	0.41
1:A:548:VAL:O	1:A:549:MET:C	2.62	0.41
1:A:202:LEU:HD21	1:A:209:TYR:HB2	2.01	0.41
1:A:28:GLY:C	1:A:30:ALA:N	2.79	0.41
1:A:369:LYS:NZ	1:A:479:ASP:CG	2.78	0.41
1:A:437:ASN:HD22	1:A:472:ARG:HH21	1.69	0.41
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:HG13	1:A:474:TYR:CD2	2.56	0.41
1:A:77:HIS:HE1	1:A:86:PHE:CG	2.38	0.41
1:A:203:ILE:HD13	1:A:208:VAL:HG22	2.03	0.41
1:A:212:LEU:HD12	1:A:213:ILE:N	2.36	0.41
1:A:561:PRO:HA	1:A:562:PRO:HD3	1.98	0.41
1:A:127:VAL:O	1:A:128:ARG:C	2.63	0.41
1:A:550:ALA:O	1:A:551:PHE:C	2.64	0.41
1:A:610:LEU:C	1:A:612:VAL:N	2.66	0.41
1:A:141:ALA:HB1	1:A:315:PHE:CE2	2.56	0.41
1:A:344:LEU:HD11	1:A:354:GLN:HB2	2.02	0.41
1:A:529:MET:HB3	1:A:529:MET:HE2	1.98	0.41
1:A:145:GLN:O	1:A:149:VAL:HG23	2.21	0.41
1:A:192:ARG:NH1	1:A:192:ARG:HB3	2.35	0.41
1:A:354:GLN:HG3	1:A:416:MET:HE2	2.01	0.41
1:A:567:GLU:CD	1:A:567:GLU:H	2.28	0.41
1:A:586:PHE:HA	1:A:589:VAL:HB	2.03	0.41
1:A:347:GLY:O	1:A:348:ASN:C	2.63	0.40
1:A:606:GLY:C	1:A:610:LEU:HD21	2.46	0.40
1:A:239:LEU:HB2	1:A:250:LEU:CD1	2.51	0.40
1:A:565:PRO:HB2	1:A:567:GLU:OE2	2.21	0.40
1:A:11:PHE:CZ	1:A:13:GLY:HA2	2.55	0.40
1:A:239:LEU:HA	1:A:242:LYS:O	2.21	0.40
1:A:342:ILE:N	1:A:342:ILE:CD1	2.79	0.40
1:A:449:MET:SD	1:A:477:ILE:HD13	2.61	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	539/613 (88%)	469 (87%)	53 (10%)	17 (3%)	3 5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	325	LEU
1	A	327	ASP
1	A	373	GLN
1	A	377	LYS
1	A	603	LYS
1	A	92	ASP
1	A	349	PHE
1	A	350	GLY
1	A	371	LEU
1	A	545	GLY
1	A	604	VAL
1	A	318	PRO
1	A	544	LYS
1	A	612	VAL
1	A	106	SER
1	A	580	TRP

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	430/519 (83%)	403 (94%)	27 (6%)	16	36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	40	LEU
1	A	63	ARG
1	A	65	LEU
1	A	97	ASN
1	A	109	GLU
1	A	175	ARG
1	A	200	LEU

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Mol	Chain	Res	Type
1	A	202	LEU
1	A	235	LEU
1	A	249	CYS
1	A	313	SER
1	A	315	PHE
1	A	318	PRO
1	A	320	SER
1	A	330	LEU
1	A	342	ILE
1	A	356	VAL
1	A	381	GLU
1	A	452	LEU
1	A	471	ASN
1	A	514	ARG
1	A	537	GLN
1	A	559	GLU
1	A	567	GLU
1	A	593	MET
1	A	605	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	38	GLN
1	A	64	GLN
1	A	77	HIS
1	A	97	ASN
1	A	103	ASN
1	A	129	GLN
1	A	140	GLN
1	A	234	GLN
1	A	336	ASN
1	A	354	GLN
1	A	391	HIS
1	A	395	ASN
1	A	406	GLN
1	A	423	HIS
1	A	437	ASN
1	A	471	ASN
1	A	473	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	615	2	33,33,33	1.48	7 (21%)	45,52,52	1.44	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	615	2	-	4/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	ANP	PB-O3A	-3.41	1.54	1.59
3	A	615	ANP	PG-O1G	3.32	1.51	1.46
3	A	615	ANP	PB-O2B	-2.89	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	ANP	C4-N3	2.85	1.39	1.34
3	A	615	ANP	PG-O3G	-2.75	1.49	1.56
3	A	615	ANP	PG-O2G	-2.28	1.50	1.56
3	A	615	ANP	C1'-N9	2.03	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	615	ANP	O1G-PG-N3B	-4.38	105.32	111.77
3	A	615	ANP	C3'-C2'-C1'	3.81	108.67	101.46
3	A	615	ANP	O2B-PB-O1B	3.77	117.96	109.87
3	A	615	ANP	O1B-PB-N3B	-2.39	108.24	111.77
3	A	615	ANP	O3A-PB-N3B	-2.21	100.47	106.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

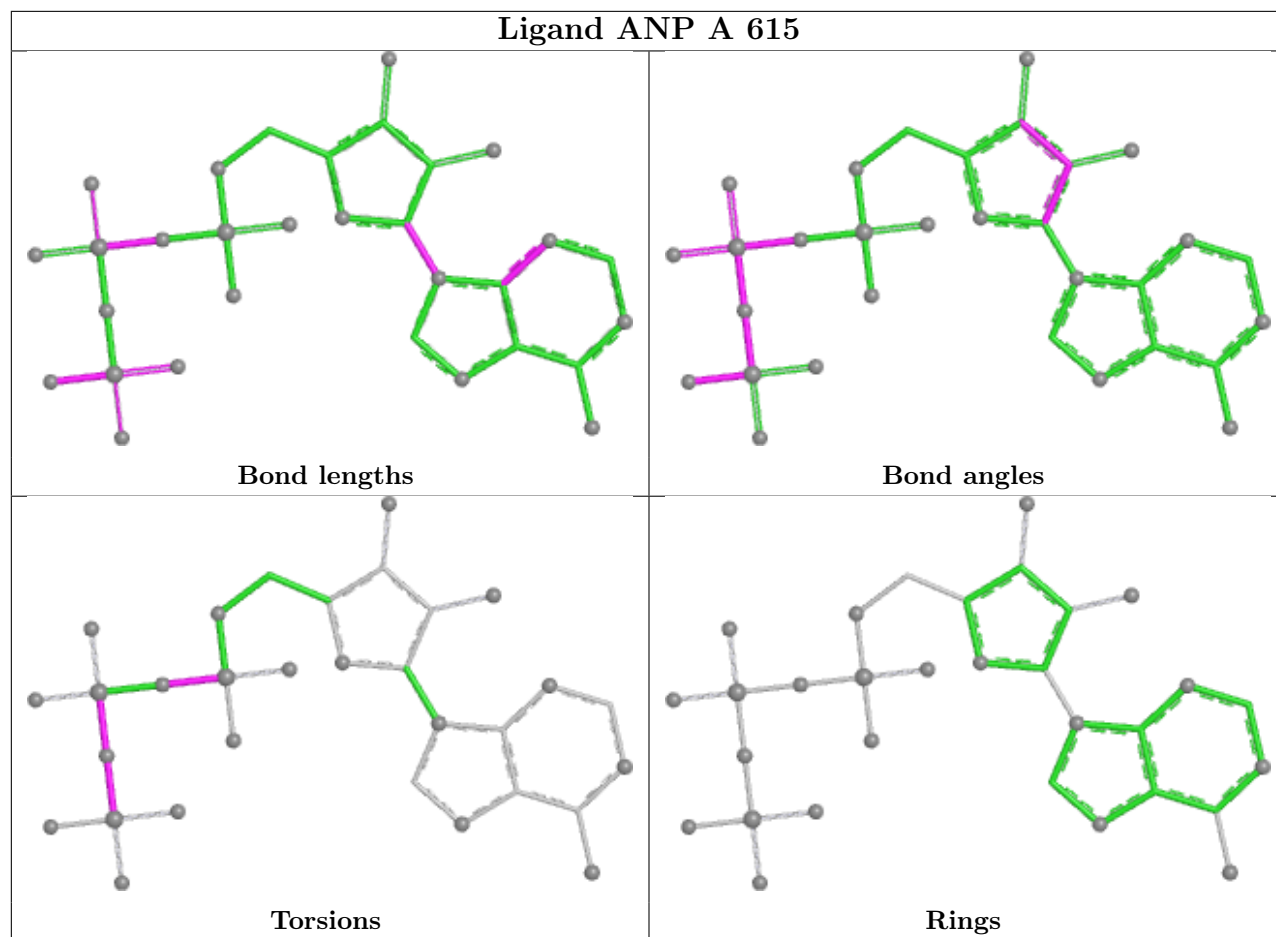
Mol	Chain	Res	Type	Atoms
3	A	615	ANP	PB-N3B-PG-O1G
3	A	615	ANP	PB-O3A-PA-O1A
3	A	615	ANP	PG-N3B-PB-O1B
3	A	615	ANP	PB-O3A-PA-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	615	ANP	1	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	545/613 (88%)	0.20	27 (4%) 34 28	18, 42, 66, 79	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	GLY	4.4
1	A	613	ALA	4.0
1	A	606	GLY	3.8
1	A	612	VAL	3.7
1	A	609	ALA	3.5
1	A	376	GLU	3.3
1	A	327	ASP	3.1
1	A	378	ALA	3.1
1	A	544	LYS	2.9
1	A	485	ALA	2.9
1	A	325	LEU	2.8
1	A	2	PRO	2.8
1	A	372	LYS	2.7
1	A	318	PRO	2.6
1	A	342	ILE	2.6
1	A	166	SER	2.5
1	A	610	LEU	2.4
1	A	483	SER	2.3
1	A	546	PRO	2.3
1	A	326	LYS	2.3
1	A	377	LYS	2.2
1	A	349	PHE	2.2
1	A	503	LEU	2.1
1	A	487	GLY	2.1
1	A	31	ASP	2.1
1	A	371	LEU	2.1
1	A	315	PHE	2.1

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](#)

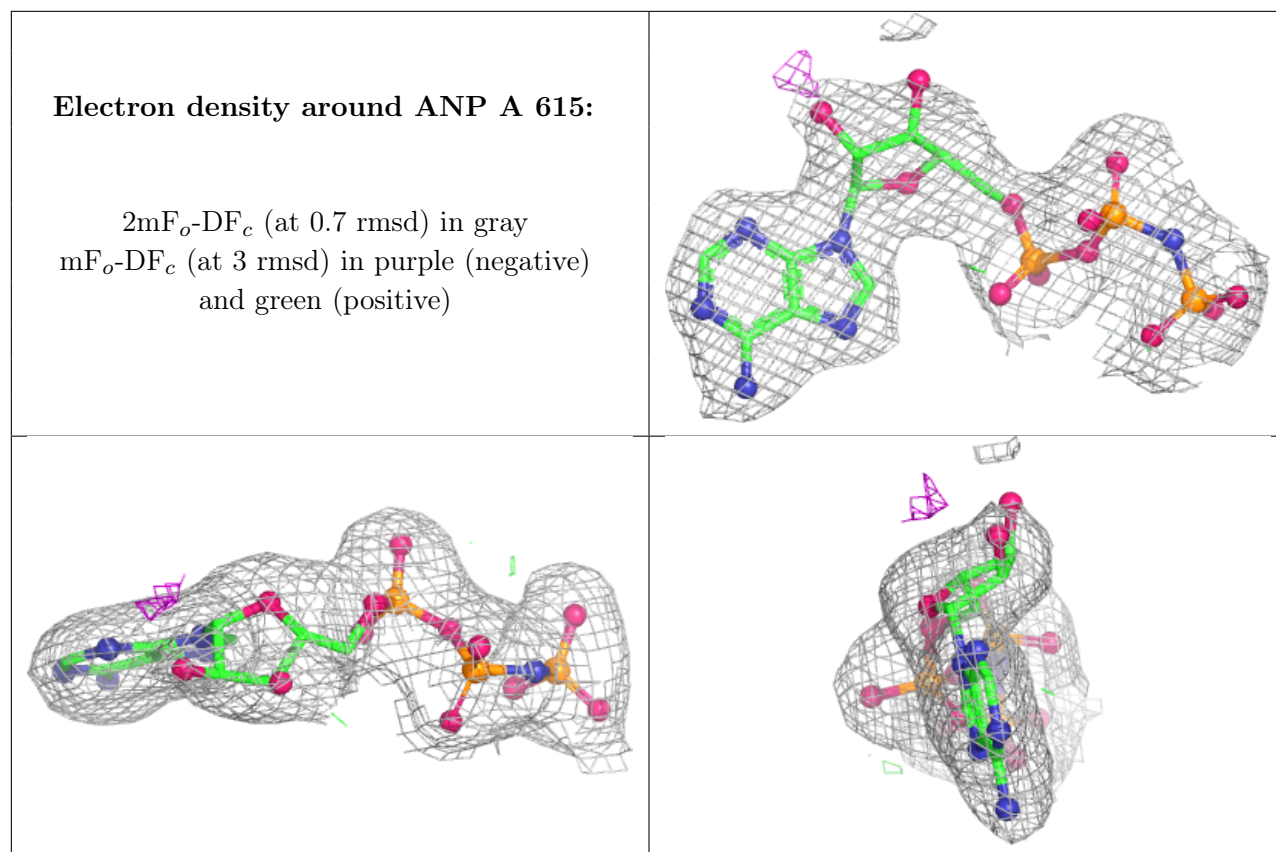
There are no oligosaccharides in this entry.

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
3	ANP	A	615	31/31	0.94	0.09	27,37,48,52	0
2	MG	A	614	1/1	0.98	0.08	28,28,28,28	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.