



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:22 am BST

PDB ID : 4LQS
Title : Crystal structure of the Cbk1-Mob2 kinase-coactivator complex
Authors : Gogl, G.; Remenyi, A.
Deposited on : 2013-07-19
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

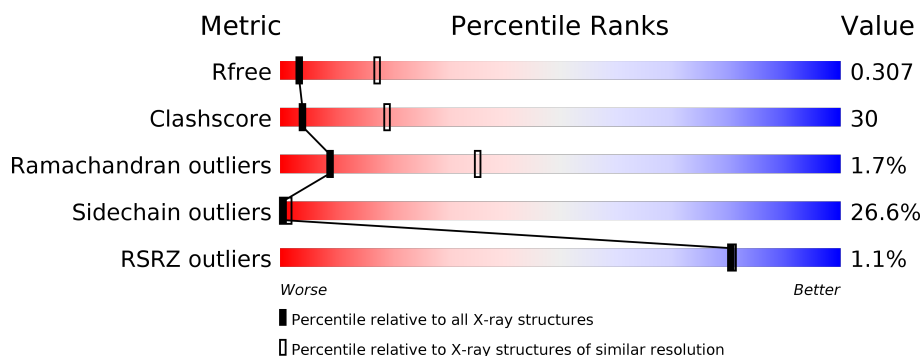
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	508	
2	B	244	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4061 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 Serine/threonine-protein kinase CBK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2911	1864	505	530	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	EXPRESSION TAG	UNP P53894
A	250	SER	-	EXPRESSION TAG	UNP P53894
A	475	ALA	ASP	ENGINEERED MUTATION	UNP P53894

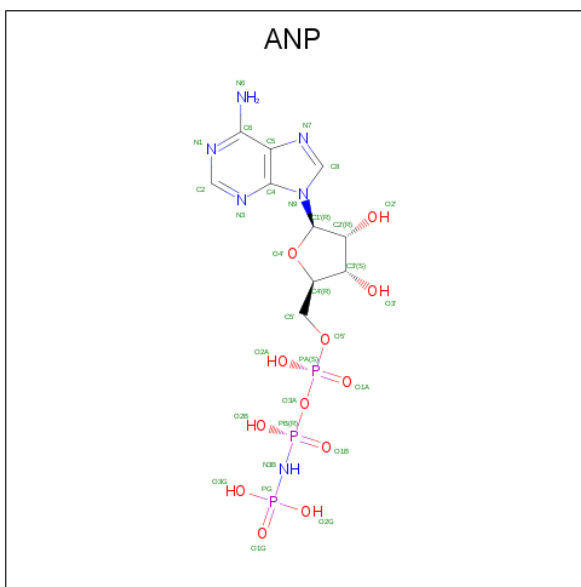
- Molecule 2 is a protein called CBK1 kinase activator protein MOB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	156	Total	C	N	O	S	0	0	0
			1119	733	187	198	1			

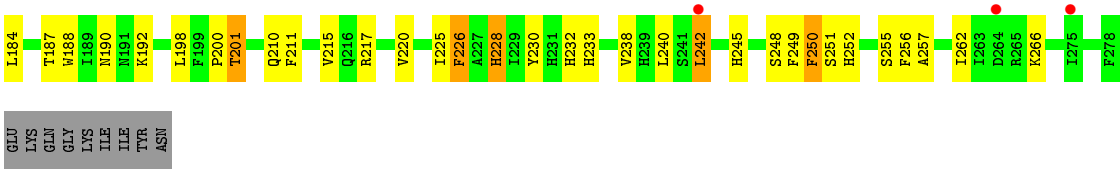
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	GLY	-	EXPRESSION TAG	UNP P43563
B	45	SER	-	EXPRESSION TAG	UNP P43563

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.43 Å 79.98 Å 117.58 Å 90.00° 117.60° 90.00°	Depositor
Resolution (Å)	47.34 – 3.30 47.34 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.34-3.30) 93.0 (47.34-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.33 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.270 , 0.307 0.273 , 0.307	Depositor DCC
R_{free} test set	875 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 123.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4061	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: 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	0.56	0/2982	0.92	6/4041 (0.1%)
2	B	0.34	0/1153	0.58	0/1589
All	All	0.51	0/4135	0.84	6/5630 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	1
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	341	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	495	GLY	N-CA-C	6.78	130.05	113.10
1	A	664	ASP	N-CA-C	-6.33	93.92	111.00
1	A	583	PHE	N-CA-C	-6.00	94.80	111.00
1	A	432	LEU	CA-CB-CG	-5.56	102.50	115.30
1	A	491	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	GLU	Peptide
1	A	447	PHE	Peptide
1	A	572	VAL	Peptide
1	A	582	ILE	Peptide
1	A	618	GLU	Peptide
1	A	619	THR	Peptide
1	A	635	ASP	Peptide
2	B	181	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2911	0	2711	197	0
2	B	1119	0	917	45	0
3	A	31	0	13	2	0
All	All	4061	0	3641	233	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 (233) 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:341:ARG:HH11	1:A:341:ARG:HG2	1.35	0.89
1:A:448:THR:HA	1:A:451:VAL:HB	1.59	0.84
2:B:181:TYR:O	2:B:183:ASP:N	2.11	0.84
1:A:464:GLU:OE1	1:A:468:LYS:NZ	2.13	0.82
1:A:345:THR:OG1	1:A:346:ARG:N	2.12	0.80
1:A:453:ARG:HB2	1:A:453:ARG:HH11	1.45	0.80
1:A:564:ARG:HH21	1:A:609:PRO:HD3	1.49	0.78
1:A:306:GLU:HA	1:A:309:VAL:HB	1.67	0.77
1:A:494:PHE:H	1:A:494:PHE:HD2	1.33	0.76
1:A:446:LEU:HB2	1:A:448:THR:HG23	1.65	0.76
1:A:654:ASP:HB2	1:A:656:ARG:NH1	2.01	0.76
1:A:304:ARG:HA	1:A:307:ARG:HB3	1.69	0.75
1:A:344:ARG:HA	1:A:742:TYR:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:HD13	1:A:489:ILE:HD11	1.70	0.74
1:A:304:ARG:HB3	1:A:304:ARG:HH11	1.53	0.73
2:B:240:LEU:HD23	2:B:242:LEU:HG	1.71	0.71
1:A:343:ARG:HB3	1:A:345:THR:HG22	1.72	0.70
1:A:490:LYS:HE2	1:A:681:ARG:HH22	1.56	0.70
1:A:410:PRO:HB2	1:A:681:ARG:HE	1.56	0.70
1:A:307:ARG:HH22	1:A:311:LEU:HD22	1.57	0.69
1:A:446:LEU:O	1:A:448:THR:OG1	2.11	0.69
1:A:456:MET:O	1:A:458:GLU:N	2.28	0.67
1:A:480:ASN:ND2	3:A:801:ANP:O1G	2.27	0.67
1:A:613:SER:OG	1:A:619:THR:OG1	2.09	0.67
2:B:226:PHE:HE1	2:B:250:PHE:HA	1.60	0.67
1:A:462:ALA:O	1:A:465:THR:OG1	2.13	0.66
1:A:458:GLU:HG2	1:A:489:ILE:HB	1.76	0.66
1:A:494:PHE:O	1:A:497:SER:N	2.18	0.66
2:B:132:GLU:O	2:B:135:THR:OG1	2.12	0.66
1:A:439:THR:HA	1:A:442:ILE:HD12	1.79	0.65
1:A:464:GLU:HG2	1:A:663:ALA:HB1	1.78	0.65
2:B:251:SER:O	2:B:255:SER:OG	2.14	0.65
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.62	0.64
1:A:342:LEU:O	1:A:343:ARG:NH2	2.31	0.64
1:A:626:PHE:O	1:A:629:THR:N	2.30	0.64
1:A:697:THR:H	1:A:698:ARG:NH2	1.96	0.63
1:A:681:ARG:HH11	1:A:681:ARG:HG2	1.62	0.63
1:A:708:VAL:O	1:A:710:ASP:N	2.32	0.63
1:A:342:LEU:HB2	1:A:747:PHE:CZ	2.34	0.62
2:B:211:PHE:O	2:B:215:VAL:N	2.23	0.62
1:A:340:LEU:H	1:A:340:LEU:HD23	1.64	0.62
1:A:654:ASP:HB2	1:A:656:ARG:HH12	1.64	0.61
1:A:417:TYR:HB2	1:A:744:TYR:OH	2.00	0.61
1:A:294:TYR:HE1	2:B:145:ALA:HB3	1.65	0.61
1:A:475:ALA:HA	1:A:577:TYR:CZ	2.36	0.61
1:A:304:ARG:NH1	1:A:304:ARG:HB3	2.15	0.61
1:A:630:LEU:HD11	1:A:650:LEU:HD23	1.84	0.60
2:B:187:THR:HA	2:B:190:ASN:HB2	1.83	0.60
1:A:345:THR:HG1	1:A:346:ARG:H	1.45	0.60
2:B:225:ILE:HD12	2:B:225:ILE:H	1.66	0.60
2:B:148:VAL:HG23	2:B:180:GLN:HB2	1.83	0.59
1:A:660:HIS:ND1	1:A:662:GLY:HA3	2.17	0.59
1:A:340:LEU:N	1:A:341:ARG:HA	2.17	0.58
1:A:742:TYR:O	1:A:744:TYR:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:TYR:HE1	1:A:699:PHE:HE2	1.50	0.58
1:A:343:ARG:HA	1:A:343:ARG:NE	2.18	0.58
1:A:652:HIS:C	1:A:654:ASP:H	2.05	0.58
1:A:379:ALA:HB3	1:A:429:MET:HB2	1.84	0.58
1:A:446:LEU:CB	1:A:448:THR:HG23	2.34	0.58
1:A:675:VAL:HG13	1:A:677:TRP:H	1.69	0.58
1:A:375:GLY:O	1:A:376:LYS:HG2	2.03	0.58
1:A:298:VAL:HG22	2:B:240:LEU:HD21	1.86	0.58
2:B:169:ALA:O	2:B:172:ARG:N	2.37	0.58
1:A:491:LEU:O	1:A:492:SER:OG	2.18	0.57
1:A:440:MET:O	1:A:443:ARG:N	2.38	0.57
1:A:433:PRO:HG3	1:A:485:ILE:HG23	1.87	0.57
1:A:625:ASN:O	1:A:627:GLU:HG3	2.05	0.57
1:A:637:HIS:O	1:A:638:ILE:HG12	2.04	0.56
1:A:421:ASP:OD2	1:A:424:TYR:N	2.26	0.56
1:A:500:PHE:CE2	1:A:502:LYS:HB3	2.41	0.56
1:A:664:ASP:C	1:A:666:ILE:H	2.08	0.56
1:A:584:LEU:HD22	1:A:584:LEU:H	1.71	0.56
1:A:645:LEU:HG	1:A:669:HIS:CD2	2.40	0.56
1:A:687:TYR:HE1	1:A:699:PHE:CE2	2.23	0.55
1:A:749:TYR:N	1:A:749:TYR:CD2	2.73	0.55
1:A:626:PHE:O	1:A:628:GLN:N	2.38	0.55
2:B:240:LEU:HB3	2:B:242:LEU:HD12	1.88	0.55
1:A:675:VAL:HG13	1:A:676:ASP:N	2.22	0.55
1:A:482:LEU:HD21	3:A:801:ANP:H2'	1.89	0.55
1:A:307:ARG:O	1:A:307:ARG:NH1	2.39	0.55
1:A:383:LEU:HD12	1:A:425:LEU:HD12	1.88	0.55
1:A:495:GLY:N	1:A:496:LEU:HA	2.22	0.55
1:A:453:ARG:HH11	1:A:453:ARG:CB	2.16	0.55
1:A:577:TYR:CD2	1:A:577:TYR:N	2.75	0.55
1:A:358:ILE:HD11	1:A:368:LEU:HB2	1.88	0.54
1:A:456:MET:SD	1:A:601:MET:HB2	2.46	0.54
1:A:681:ARG:NH1	1:A:681:ARG:HG2	2.21	0.54
1:A:620:TYR:O	1:A:623:ILE:HG22	2.08	0.54
1:A:414:SER:H	1:A:430:GLU:HG2	1.73	0.54
2:B:116:LEU:HD22	2:B:122:LEU:HD13	1.88	0.54
1:A:696:ASP:OD1	1:A:698:ARG:NE	2.32	0.54
1:A:357:VAL:HA	1:A:367:ARG:HG2	1.90	0.53
1:A:484:ASP:OD1	1:A:488:HIS:N	2.41	0.53
1:A:561:ARG:HD2	1:A:608:TRP:CG	2.44	0.53
2:B:248:SER:O	2:B:252:HIS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:TYR:HB3	1:A:596:SER:HB3	1.90	0.53
1:A:321:SER:OG	1:A:322:GLU:N	2.41	0.52
1:A:341:ARG:HH11	1:A:341:ARG:CG	2.14	0.52
1:A:301:ALA:HB1	2:B:245:HIS:CE1	2.44	0.52
1:A:613:SER:HB2	1:A:618:GLU:HB3	1.91	0.52
1:A:583:PHE:HD2	1:A:583:PHE:O	1.92	0.52
1:A:367:ARG:N	1:A:380:MET:O	2.42	0.52
1:A:481:ILE:HG22	1:A:489:ILE:HD12	1.92	0.52
1:A:660:HIS:CE1	1:A:662:GLY:HA3	2.45	0.52
2:B:114:VAL:HB	2:B:256:PHE:HD1	1.74	0.52
1:A:345:THR:HB	2:B:201:THR:HG23	1.91	0.52
1:A:463:ILE:HD11	1:A:476:ILE:HD12	1.91	0.52
1:A:425:LEU:HD22	1:A:426:TYR:H	1.75	0.52
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.76	0.52
1:A:339:PHE:HB3	1:A:341:ARG:HD3	1.90	0.52
1:A:307:ARG:C	1:A:307:ARG:HH11	2.13	0.51
2:B:217:ARG:HA	2:B:220:VAL:HG22	1.91	0.51
1:A:572:VAL:CB	1:A:573:GLY:HA2	2.41	0.51
1:A:611:PHE:CD2	1:A:623:ILE:HB	2.46	0.51
2:B:228:HIS:CE1	2:B:232:HIS:HE1	2.29	0.51
1:A:618:GLU:HG3	1:A:622:LYS:HE2	1.92	0.51
1:A:367:ARG:NH1	1:A:380:MET:HG2	2.26	0.51
2:B:121:ASP:OD1	2:B:123:GLY:N	2.38	0.50
1:A:582:ILE:HG13	1:A:588:TYR:CE1	2.46	0.50
2:B:169:ALA:O	2:B:171:ASN:N	2.44	0.50
2:B:257:ALA:O	2:B:262:ILE:N	2.40	0.50
2:B:148:VAL:HG11	2:B:233:HIS:CD2	2.46	0.50
1:A:317:SER:HB3	1:A:320:TRP:CZ3	2.46	0.50
1:A:383:LEU:O	1:A:424:TYR:HD2	1.93	0.50
1:A:386:SER:HA	1:A:388:MET:H	1.75	0.50
1:A:341:ARG:HG2	1:A:341:ARG:NH1	2.06	0.50
1:A:590:GLN:OE1	1:A:594:TRP:NE1	2.45	0.50
1:A:340:LEU:HG	1:A:341:ARG:O	2.11	0.49
1:A:712:PRO:N	1:A:713:ALA:HA	2.27	0.49
1:A:616:PRO:O	1:A:619:THR:O	2.30	0.49
1:A:476:ILE:HG22	1:A:600:ILE:HD12	1.94	0.49
1:A:474:ARG:HG2	1:A:592:CYS:SG	2.53	0.49
1:A:435:GLY:HA2	1:A:700:PHE:CE1	2.48	0.49
1:A:561:ARG:O	1:A:564:ARG:HB2	2.13	0.49
1:A:577:TYR:CG	1:A:578:ILE:N	2.79	0.48
1:A:675:VAL:CG1	1:A:677:TRP:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HB3	1:A:345:THR:CG2	2.42	0.48
1:A:297:SER:HB3	2:B:143:VAL:HG22	1.95	0.48
1:A:566:LEU:HD23	1:A:566:LEU:H	1.79	0.48
1:A:645:LEU:HG	1:A:669:HIS:CG	2.49	0.47
1:A:432:LEU:O	1:A:700:PHE:HZ	1.97	0.47
1:A:379:ALA:HB2	1:A:431:PHE:HA	1.95	0.47
1:A:453:ARG:NE	1:A:673:ARG:HD2	2.30	0.47
1:A:742:TYR:C	1:A:744:TYR:H	2.17	0.47
1:A:664:ASP:OD2	1:A:665:GLU:N	2.46	0.47
1:A:348:SER:OG	1:A:349:LEU:N	2.48	0.47
1:A:477:LYS:HE3	1:A:479:ASP:OD1	2.15	0.47
1:A:498:THR:OG1	1:A:499:GLY:N	2.48	0.47
1:A:297:SER:HB3	2:B:143:VAL:HG13	1.98	0.46
1:A:577:TYR:N	1:A:577:TYR:HD2	2.12	0.46
1:A:308:ARG:HH22	2:B:249:PHE:HD1	1.62	0.46
1:A:595:TRP:HZ2	1:A:611:PHE:HE2	1.64	0.46
1:A:425:LEU:HD22	1:A:426:TYR:N	2.31	0.46
1:A:748:ASP:HA	1:A:749:TYR:HA	1.70	0.46
2:B:181:TYR:HE1	2:B:228:HIS:CD2	2.33	0.46
1:A:339:PHE:HB3	1:A:341:ARG:NE	2.31	0.46
1:A:421:ASP:HB3	1:A:426:TYR:HE2	1.81	0.46
1:A:564:ARG:HG2	1:A:565:ARG:H	1.81	0.45
2:B:182:ILE:HG23	2:B:225:ILE:HG12	1.97	0.45
2:B:116:LEU:HD11	2:B:120:VAL:O	2.17	0.45
2:B:168:ASP:CB	2:B:169:ALA:HA	2.46	0.45
1:A:582:ILE:HA	1:A:588:TYR:HE1	1.81	0.45
2:B:226:PHE:CE1	2:B:250:PHE:HA	2.47	0.45
1:A:711:SER:HB3	1:A:713:ALA:HB2	1.97	0.45
1:A:345:THR:HB	2:B:201:THR:CG2	2.47	0.45
1:A:299:LYS:HA	1:A:302:ILE:HG12	1.97	0.44
1:A:358:ILE:HG23	1:A:700:PHE:CD1	2.52	0.44
1:A:689:PRO:HB2	1:A:691:LEU:HD21	1.98	0.44
2:B:245:HIS:CD2	2:B:245:HIS:H	2.35	0.44
1:A:307:ARG:NH2	1:A:311:LEU:HD22	2.29	0.44
1:A:696:ASP:HA	1:A:698:ARG:HH21	1.81	0.44
1:A:311:LEU:O	1:A:315:LEU:HD22	2.17	0.44
1:A:698:ARG:HD3	1:A:698:ARG:HA	1.67	0.44
1:A:340:LEU:HD23	1:A:340:LEU:N	2.32	0.44
2:B:111:LYS:HB2	2:B:112:THR:H	1.49	0.44
1:A:746:ARG:NH2	1:A:746:ARG:O	2.51	0.44
1:A:564:ARG:NH2	1:A:603:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:LEU:HD12	2:B:117:PRO:HD2	2.00	0.44
1:A:308:ARG:HH21	2:B:249:PHE:HA	1.82	0.44
1:A:386:SER:HA	1:A:387:GLU:HA	1.64	0.44
1:A:657:LEU:HA	1:A:657:LEU:HD22	1.73	0.44
1:A:386:SER:HA	1:A:388:MET:N	2.33	0.43
2:B:146:GLU:HB3	2:B:147:TYR:H	1.58	0.43
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.34	0.43
2:B:249:PHE:O	2:B:252:HIS:HB3	2.17	0.43
1:A:370:GLN:HG3	1:A:375:GLY:HA2	2.00	0.43
1:A:580:PRO:HB3	1:A:623:ILE:HD13	2.00	0.43
1:A:646:ILE:O	1:A:650:LEU:N	2.43	0.43
2:B:116:LEU:HD22	2:B:122:LEU:HD22	2.01	0.43
1:A:342:LEU:O	1:A:343:ARG:HB2	2.18	0.43
2:B:177:PRO:HB2	2:B:181:TYR:CD1	2.53	0.43
1:A:330:SER:OG	1:A:331:SER:N	2.52	0.43
1:A:437:LEU:O	1:A:437:LEU:HD12	2.19	0.43
1:A:502:LYS:HB2	1:A:503:THR:HA	2.00	0.43
1:A:579:ALA:HA	1:A:595:TRP:CD1	2.54	0.43
1:A:594:TRP:CZ2	1:A:663:ALA:HA	2.53	0.43
1:A:344:ARG:HG2	1:A:344:ARG:H	1.63	0.43
1:A:414:SER:O	1:A:429:MET:HA	2.19	0.43
1:A:582:ILE:HG13	1:A:588:TYR:CD1	2.54	0.42
1:A:699:PHE:N	1:A:699:PHE:CD1	2.87	0.42
1:A:711:SER:HA	1:A:712:PRO:HD3	1.93	0.42
1:A:595:TRP:CZ2	1:A:611:PHE:HE2	2.38	0.42
1:A:602:TYR:HE1	1:A:608:TRP:CZ3	2.38	0.42
1:A:476:ILE:HB	1:A:596:SER:CB	2.50	0.42
1:A:682:GLN:HG2	1:A:682:GLN:H	1.58	0.42
1:A:620:TYR:O	1:A:621:ARG:C	2.59	0.41
1:A:626:PHE:O	1:A:627:GLU:C	2.59	0.41
1:A:650:LEU:HA	1:A:650:LEU:HD12	1.78	0.41
2:B:184:LEU:HA	2:B:187:THR:OG1	2.20	0.41
1:A:349:LEU:C	1:A:351:ASP:H	2.23	0.41
1:A:383:LEU:HB2	1:A:425:LEU:HB3	2.01	0.41
1:A:440:MET:SD	1:A:455:TYR:OH	2.72	0.41
1:A:476:ILE:HB	1:A:596:SER:HB3	2.02	0.41
2:B:188:TRP:O	2:B:192:LYS:N	2.52	0.41
1:A:323:GLU:OE1	1:A:324:ARG:N	2.32	0.41
1:A:339:PHE:HB3	1:A:341:ARG:CD	2.49	0.41
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.75	0.41
1:A:694:ILE:HD12	1:A:694:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:HZ3	1:A:373:ASP:HB3	1.86	0.41
1:A:431:PHE:CZ	1:A:433:PRO:HA	2.55	0.41
1:A:692:SER:N	1:A:696:ASP:OD2	2.38	0.41
1:A:638:ILE:HG22	1:A:639:SER:O	2.21	0.41
2:B:198:LEU:O	2:B:200:PRO:HD3	2.20	0.41
1:A:583:PHE:CD2	1:A:583:PHE:O	2.73	0.41
1:A:619:THR:HA	1:A:620:TYR:O	2.20	0.41
1:A:457:ALA:O	1:A:460:ILE:N	2.54	0.40
1:A:655:GLN:O	1:A:656:ARG:HG2	2.20	0.40
2:B:140:PHE:HA	2:B:140:PHE:HD1	1.73	0.40
1:A:472:ILE:HG22	1:A:590:GLN:HA	2.03	0.40
1:A:448:THR:HB	1:A:449:GLU:H	1.43	0.40
1:A:473:HIS:CE1	1:A:475:ALA:O	2.73	0.40
1:A:415:LEU:HD21	1:A:427:LEU:HD22	2.03	0.40
1:A:664:ASP:C	1:A:666:ILE:N	2.74	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	364/508 (72%)	279 (77%)	78 (21%)	7 (2%)	8	34
2	B	152/244 (62%)	130 (86%)	20 (13%)	2 (1%)	12	40
All	All	516/752 (69%)	409 (79%)	98 (19%)	9 (2%)	9	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	743	THR
1	A	744	TYR
2	B	182	ILE

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Mol	Chain	Res	Type
1	A	572	VAL
1	A	457	ALA
2	B	180	GLN
1	A	373	ASP
1	A	578	ILE
1	A	675	VAL

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	287/449 (64%)	202 (70%)	85 (30%)	0	1
2	B	92/223 (41%)	76 (83%)	16 (17%)	2	8
All	All	379/672 (56%)	278 (73%)	101 (27%)	0	1

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	TYR
1	A	298	VAL
1	A	304	ARG
1	A	314	GLU
1	A	315	LEU
1	A	316	THR
1	A	321	SER
1	A	323	GLU
1	A	324	ARG
1	A	337	SER
1	A	338	GLN
1	A	340	LEU
1	A	341	ARG
1	A	343	ARG
1	A	344	ARG
1	A	349	LEU
1	A	354	THR

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Mol	Chain	Res	Type
1	A	365	GLU
1	A	367	ARG
1	A	374	THR
1	A	377	ILE
1	A	380	MET
1	A	381	LYS
1	A	382	THR
1	A	384	LEU
1	A	386	SER
1	A	387	GLU
1	A	388	MET
1	A	389	TYR
1	A	421	ASP
1	A	444	TRP
1	A	445	GLN
1	A	448	THR
1	A	452	THR
1	A	453	ARG
1	A	456	MET
1	A	465	THR
1	A	468	LYS
1	A	477	LYS
1	A	480	ASN
1	A	483	ILE
1	A	485	ILE
1	A	486	ARG
1	A	488	HIS
1	A	490	LYS
1	A	491	LEU
1	A	493	ASP
1	A	494	PHE
1	A	566	LEU
1	A	577	TYR
1	A	583	PHE
1	A	584	LEU
1	A	585	TYR
1	A	588	TYR
1	A	591	GLU
1	A	596	SER
1	A	597	LEU
1	A	601	MET
1	A	604	CYS

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Mol	Chain	Res	Type
1	A	608	TRP
1	A	614	GLU
1	A	615	THR
1	A	619	THR
1	A	621	ARG
1	A	623	ILE
1	A	628	GLN
1	A	630	LEU
1	A	637	HIS
1	A	639	SER
1	A	645	LEU
1	A	650	LEU
1	A	654	ASP
1	A	656	ARG
1	A	657	LEU
1	A	665	GLU
1	A	673	ARG
1	A	675	VAL
1	A	681	ARG
1	A	682	GLN
1	A	696	ASP
1	A	698	ARG
1	A	705	LEU
1	A	746	ARG
1	A	747	PHE
1	A	749	TYR
2	B	112	THR
2	B	121	ASP
2	B	122	LEU
2	B	137	LEU
2	B	140	PHE
2	B	181	TYR
2	B	183	ASP
2	B	201	THR
2	B	210	GLN
2	B	226	PHE
2	B	228	HIS
2	B	230	TYR
2	B	238	VAL
2	B	242	LEU
2	B	250	PHE
2	B	266	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	228	HIS
2	B	232	HIS
2	B	233	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ANP	A	801	-	29,33,33	2.59	8 (27%)	31,52,52	2.54	6 (19%)

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	801	-	-	3/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	PB-O1B	8.77	1.60	1.46
3	A	801	ANP	C2'-C3'	-4.32	1.41	1.53
3	A	801	ANP	C2'-C1'	-4.29	1.47	1.53
3	A	801	ANP	PB-N3B	4.00	1.73	1.63
3	A	801	ANP	PG-O1G	3.90	1.52	1.46
3	A	801	ANP	C6-N6	3.01	1.45	1.34
3	A	801	ANP	O4'-C4'	-2.70	1.39	1.45
3	A	801	ANP	O3'-C3'	-2.25	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	O1B-PB-N3B	-10.21	96.74	111.77
3	A	801	ANP	O2B-PB-O1B	5.02	120.44	109.92
3	A	801	ANP	O2B-PB-O3A	4.92	121.05	104.64
3	A	801	ANP	N3-C2-N1	-4.00	122.42	128.68
3	A	801	ANP	O3A-PB-N3B	-2.88	98.60	106.59
3	A	801	ANP	O5'-C5'-C4'	2.41	117.28	108.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ANP	PB-N3B-PG-O1G
3	A	801	ANP	O4'-C4'-C5'-O5'
3	A	801	ANP	C3'-C4'-C5'-O5'

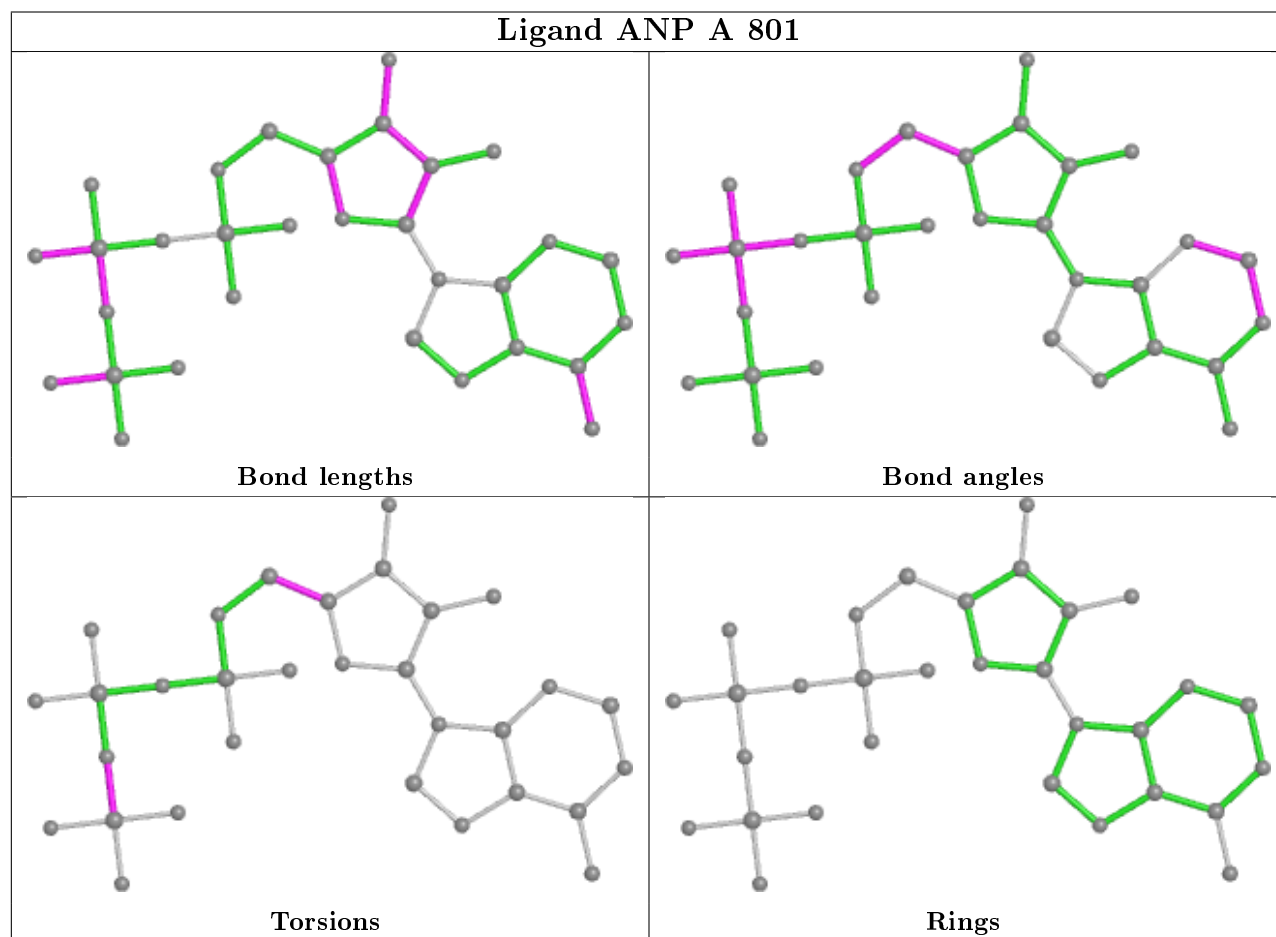
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	372/508 (73%)	-0.36	2 (0%) 91 91	35, 82, 151, 206	0
2	B	156/244 (63%)	-0.16	4 (2%) 56 53	87, 152, 238, 325	0
All	All	528/752 (70%)	-0.30	6 (1%) 80 81	35, 97, 191, 325	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	SER	3.5
1	A	658	GLY	2.7
2	B	168	ASP	2.6
2	B	275	ILE	2.5
2	B	242	LEU	2.3
2	B	264	ASP	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](#)

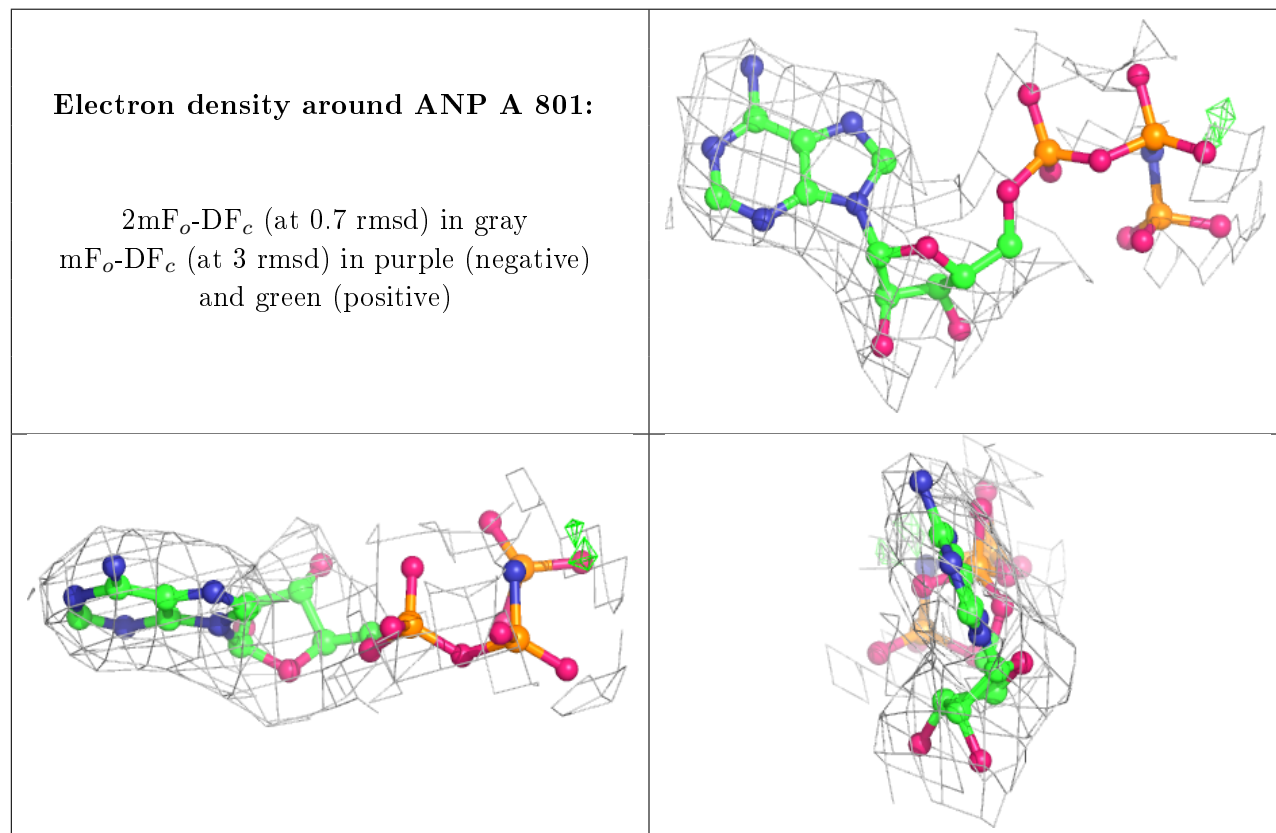
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
3	ANP	A	801	31/31	0.92	0.18	65,78,166,195	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.