Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 11:37 PM EST

PDB ID	:	4LQP
Title	:	Crystal structure of the Cbk1(T743E)-Mob2 kinase-coactivator complex, in crystal form A
Authors	:	Gogl, G.; Remenyi, A.
Deposited on	:	2013-07-19
Resolution	:	4.50 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:

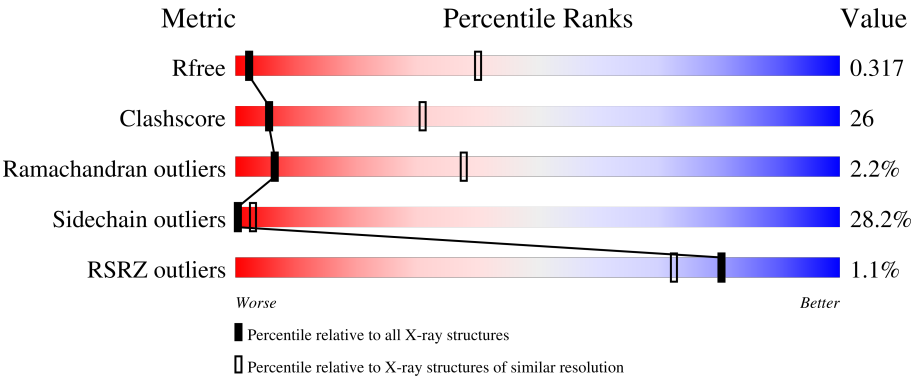
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 <=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	% 32% 31% 12% 25%
2	B	244	% 41% 19% 5% • 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4131 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	383	Total	C	N	O	S	0	0	0
			2954	1888	513	541	12			

There are 4 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
A	743	GLU	THR	engineered mutation	UNP P53894

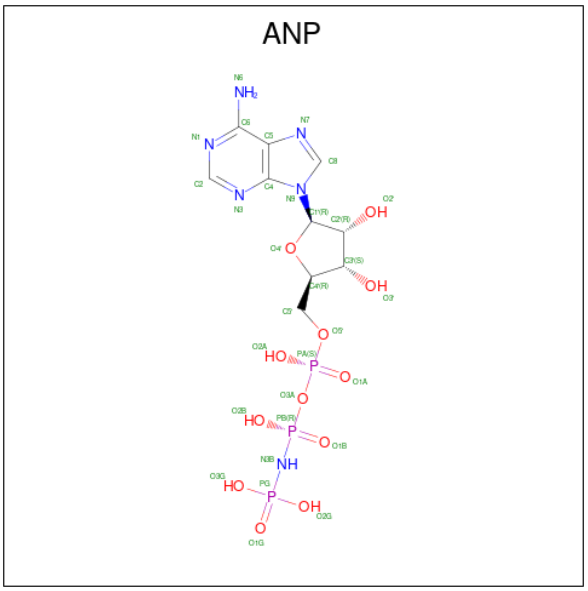
- Molecule 2 is a protein called CBK1 kinase activator protein MOB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	163	Total	C	N	O	S	0	0	0
			1146	749	191	205	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: $C_{10}H_{17}N_6O_{12}P_3$).



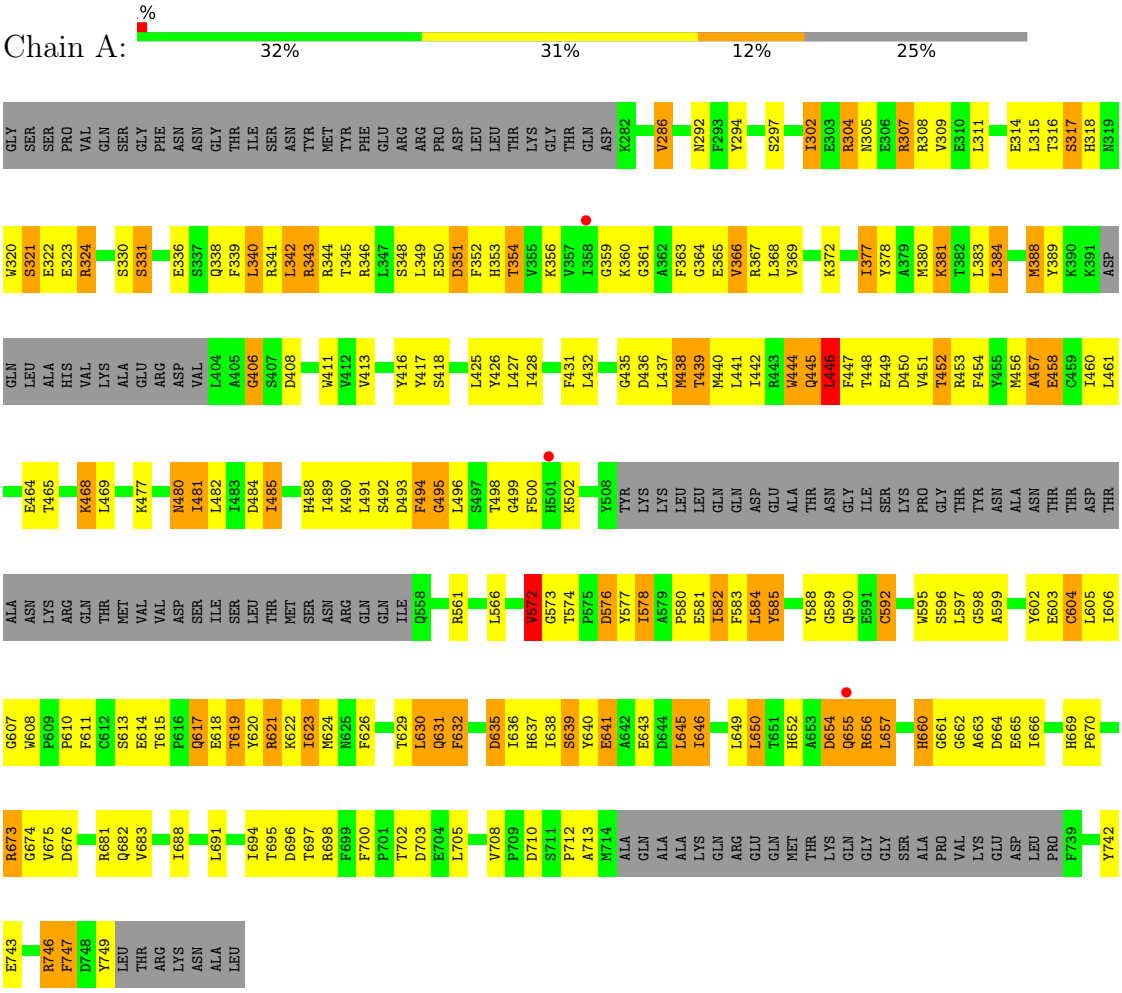
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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.

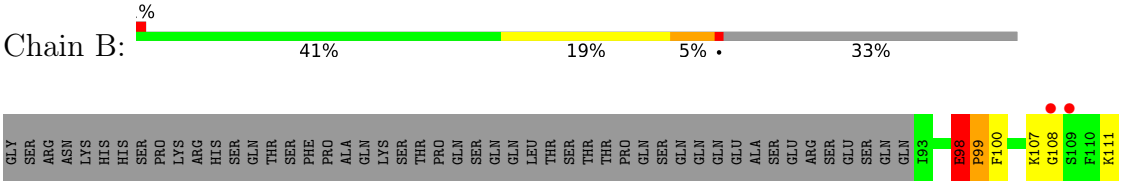
• Molecule 1: Serine/threonine-protein kinase CBK1

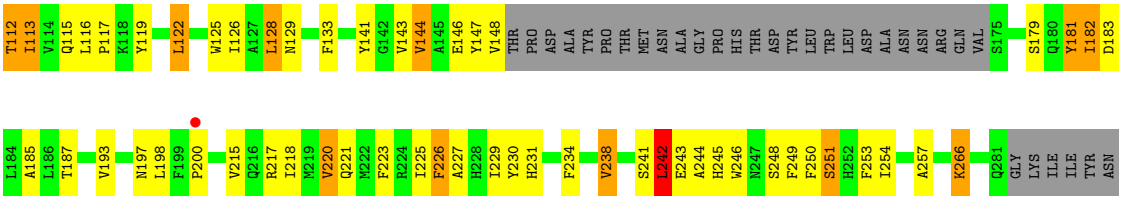
Chain A:



• Molecule 2: CBK1 kinase activator protein MOB2

Chain B:




T112 I113 V114 Q115 L116 P117 K118 Y119 L122 W125 I126 A127 L128 N129 F133 Y141 G142 V143 V144 A145 E146 Y147 V148 THR PRO ASP ALA TYR PRO THR MET ASN ALA GLY PRO HIS THR ASP TYR LEU TRP LEU ASP ALA ASN ASN ARG GLN VAL S175 S179 Q180 Y181 I182 D183
L184 A185 L186 T187 V193 N197 L198 F199 P200 V215 Q216 R217 I218 M219 V220 Q221 M222 F223 R224 I225 F226 A227 H228 I229 Y230 H231 F234 V238 S241 L242 E243 A244 H245 W246 M247 S248 F249 F250 S251 H252 F253 I254 A257 K266 Q281 GLY LYS ILE ILE TYR ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	129.38Å 129.38Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 4.50 49.59 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.59-4.50) 95.0 (49.59-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.288 , 0.310 0.286 , 0.317	Depositor DCC
R_{free} test set	588 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	242.2	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 252.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4131	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.32	0/3024	0.75	7/4100 (0.2%)
2	B	0.34	0/1180	0.75	2/1629 (0.1%)
All	All	0.33	0/4204	0.75	9/5729 (0.2%)

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	2
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	742	TYR	N-CA-C	6.40	128.29	111.00
1	A	495	GLY	N-CA-C	6.09	128.33	113.10
1	A	635	ASP	N-CA-C	-5.78	95.39	111.00
2	B	242	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	446	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	406	GLY	N-CA-C	5.49	126.81	113.10
1	A	583	PHE	N-CA-C	-5.40	96.42	111.00
2	B	108	GLY	N-CA-C	5.29	126.31	113.10
1	A	607	GLY	N-CA-C	5.11	125.86	113.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	VAL	Peptide
1	A	292	ASN	Peptide
1	A	331	SER	Peptide
1	A	406	GLY	Peptide
1	A	572	VAL	Peptide
1	A	582	ILE	Peptide
1	A	619	THR	Peptide
2	B	181	TYR	Peptide
2	B	98	GLU	Peptide

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	2954	0	2727	167	0
2	B	1146	0	921	39	0
3	A	31	0	13	3	0
All	All	4131	0	3661	201	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 26.

All (201) 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:339:PHE:HB3	1:A:341:ARG:HE	1.47	0.80
1:A:356:LYS:HD2	1:A:697:THR:HG21	1.65	0.79
1:A:308:ARG:HH22	2:B:249:PHE:HA	1.47	0.79
1:A:381:LYS:NZ	3:A:801:ANP:O1A	2.16	0.78
2:B:218:ILE:HA	2:B:221:GLN:HG2	1.65	0.78
2:B:183:ASP:O	2:B:187:THR:OG1	2.02	0.77
1:A:477:LYS:HB2	1:A:480:ASN:HB2	1.69	0.74
1:A:343:ARG:HB3	1:A:345:THR:HG23	1.70	0.72
1:A:673:ARG:HD3	1:A:674:GLY:H	1.55	0.71
2:B:181:TYR:O	2:B:183:ASP:N	2.19	0.70
1:A:448:THR:HB	1:A:452:THR:HB	1.74	0.70
1:A:632:PHE:HE1	1:A:643:GLU:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:TYR:HD2	1:A:589:GLY:H	1.39	0.69
1:A:453:ARG:HD3	1:A:673:ARG:HD2	1.74	0.68
2:B:182:ILE:HA	2:B:185:ALA:HB3	1.74	0.68
1:A:613:SER:HB2	1:A:618:GLU:HB3	1.77	0.67
2:B:227:ALA:HA	2:B:230:TYR:HB2	1.76	0.67
1:A:663:ALA:H	1:A:666:ILE:HD12	1.60	0.66
1:A:314:GLU:HA	1:A:317:SER:HB2	1.79	0.65
1:A:610:PRO:HB3	1:A:630:LEU:HD21	1.79	0.64
1:A:708:VAL:O	1:A:710:ASP:N	2.31	0.64
1:A:664:ASP:C	1:A:666:ILE:H	1.99	0.64
1:A:346:ARG:NH1	2:B:193:VAL:O	2.31	0.63
2:B:125:TRP:O	2:B:129:ASN:ND2	2.31	0.63
1:A:598:GLY:HA2	1:A:649:LEU:HD13	1.80	0.63
1:A:618:GLU:O	1:A:621:ARG:HB3	1.99	0.63
1:A:330:SER:OG	1:A:331:SER:N	2.32	0.62
1:A:311:LEU:HD21	2:B:113:ILE:HG21	1.81	0.62
2:B:238:VAL:HA	2:B:243:GLU:HB3	1.82	0.61
1:A:461:LEU:HA	1:A:464:GLU:HB2	1.82	0.60
1:A:348:SER:OG	1:A:349:LEU:O	2.16	0.59
1:A:495:GLY:N	1:A:496:LEU:HA	2.16	0.59
1:A:652:HIS:HB2	1:A:654:ASP:HB3	1.85	0.59
1:A:413:VAL:HG21	1:A:482:LEU:HD12	1.85	0.59
1:A:635:ASP:HB3	1:A:637:HIS:HE1	1.68	0.59
2:B:116:LEU:HD13	2:B:122:LEU:HD13	1.83	0.59
1:A:349:LEU:HD23	1:A:350:GLU:H	1.67	0.59
2:B:179:SER:HA	2:B:181:TYR:CD1	2.38	0.58
1:A:432:LEU:HD21	1:A:490:LYS:HB2	1.84	0.58
1:A:646:ILE:HA	1:A:649:LEU:HD12	1.85	0.58
2:B:116:LEU:HD12	2:B:117:PRO:HD2	1.85	0.58
1:A:604:CYS:SG	1:A:605:LEU:N	2.77	0.58
2:B:215:VAL:HA	2:B:218:ILE:H	1.67	0.58
1:A:366:VAL:HG23	1:A:381:LYS:HG2	1.85	0.58
1:A:603:GLU:HA	1:A:608:TRP:H	1.67	0.57
1:A:353:HIS:HB2	1:A:372:LYS:HG3	1.86	0.57
1:A:377:ILE:H	1:A:377:ILE:HD13	1.68	0.57
1:A:652:HIS:C	1:A:654:ASP:H	2.09	0.56
1:A:577:TYR:CG	1:A:578:ILE:N	2.73	0.56
1:A:366:VAL:HG21	3:A:801:ANP:H8	1.88	0.56
1:A:645:LEU:HG	1:A:669:HIS:CD2	2.42	0.55
1:A:364:GLY:HA3	1:A:383:LEU:HA	1.88	0.55
1:A:494:PHE:C	1:A:496:LEU:HA	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PHE:HE1	1:A:582:ILE:HG22	1.71	0.55
1:A:638:ILE:HG22	1:A:639:SER:O	2.07	0.55
1:A:613:SER:C	1:A:615:THR:H	2.10	0.54
1:A:498:THR:OG1	1:A:499:GLY:N	2.34	0.54
1:A:435:GLY:HA2	1:A:700:PHE:CE1	2.42	0.54
1:A:584:LEU:HD23	1:A:585:TYR:HD2	1.72	0.54
1:A:457:ALA:O	1:A:460:ILE:N	2.40	0.54
1:A:343:ARG:NE	1:A:343:ARG:HA	2.23	0.54
1:A:602:TYR:CG	1:A:610:PRO:HG3	2.43	0.54
1:A:712:PRO:N	1:A:713:ALA:HA	2.23	0.53
1:A:340:LEU:N	1:A:341:ARG:HA	2.24	0.53
2:B:141:TYR:HA	2:B:144:VAL:HG23	1.89	0.53
1:A:361:GLY:N	1:A:364:GLY:O	2.42	0.53
1:A:577:TYR:HD1	1:A:596:SER:HB3	1.72	0.53
1:A:448:THR:HA	1:A:451:VAL:HB	1.90	0.53
1:A:621:ARG:HD3	1:A:622:LYS:H	1.73	0.53
1:A:339:PHE:HB3	1:A:341:ARG:NE	2.22	0.52
1:A:577:TYR:HB2	1:A:596:SER:HB3	1.92	0.52
2:B:98:GLU:CB	2:B:99:PRO:HD3	2.39	0.52
1:A:438:MET:O	1:A:442:ILE:HG13	2.09	0.52
1:A:417:TYR:CE1	1:A:428:ILE:HD13	2.45	0.52
1:A:637:HIS:O	1:A:638:ILE:HG12	2.10	0.52
1:A:383:LEU:HB2	1:A:425:LEU:HB3	1.92	0.51
1:A:702:THR:HG23	1:A:703:ASP:H	1.75	0.51
1:A:383:LEU:HD12	1:A:425:LEU:HD12	1.92	0.51
1:A:315:LEU:HG	1:A:318:HIS:NE2	2.26	0.51
2:B:223:PHE:HA	2:B:226:PHE:HB2	1.93	0.51
1:A:342:LEU:HB2	1:A:747:PHE:CZ	2.46	0.51
1:A:477:LYS:HD3	1:A:577:TYR:CE2	2.46	0.51
1:A:620:TYR:HA	1:A:623:ILE:HG22	1.92	0.50
1:A:354:THR:HA	1:A:369:VAL:HG12	1.93	0.50
2:B:229:ILE:O	2:B:234:PHE:N	2.44	0.50
1:A:605:LEU:HD22	1:A:638:ILE:HD12	1.93	0.50
1:A:485:ILE:H	1:A:485:ILE:HD12	1.77	0.50
1:A:582:ILE:HD11	1:A:592:CYS:HB2	1.92	0.50
1:A:660:HIS:N	1:A:661:GLY:HA3	2.27	0.50
1:A:662:GLY:C	1:A:664:ASP:H	2.14	0.49
1:A:304:ARG:HH11	1:A:304:ARG:HB3	1.77	0.49
1:A:305:ASN:O	1:A:309:VAL:HG23	2.11	0.49
1:A:411:TRP:O	1:A:490:LYS:HA	2.12	0.49
1:A:413:VAL:HB	1:A:492:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:OE2	1:A:344:ARG:NH1	2.45	0.49
1:A:584:LEU:HD23	1:A:585:TYR:CD2	2.47	0.49
1:A:349:LEU:C	1:A:351:ASP:H	2.15	0.49
1:A:620:TYR:O	1:A:623:ILE:N	2.46	0.49
1:A:363:PHE:HB3	1:A:383:LEU:HD22	1.95	0.49
1:A:448:THR:OG1	1:A:449:GLU:N	2.45	0.49
1:A:619:THR:HG22	1:A:623:ILE:HB	1.95	0.49
1:A:646:ILE:HG22	1:A:650:LEU:HD22	1.95	0.49
2:B:107:LYS:H	2:B:244:ALA:HB1	1.78	0.48
1:A:367:ARG:HB2	1:A:380:MET:HB3	1.95	0.48
2:B:122:LEU:O	2:B:126:ILE:HG12	2.13	0.48
2:B:179:SER:HA	2:B:181:TYR:HD1	1.74	0.48
3:A:801:ANP:N3B	3:A:801:ANP:O2A	2.46	0.48
1:A:360:LYS:HA	1:A:365:GLU:HA	1.94	0.48
1:A:444:TRP:CD1	1:A:444:TRP:N	2.81	0.48
2:B:226:PHE:CD1	2:B:250:PHE:HD1	2.32	0.48
1:A:669:HIS:HA	1:A:670:PRO:HD2	1.72	0.47
1:A:457:ALA:H	1:A:460:ILE:HD12	1.79	0.47
2:B:98:GLU:CB	2:B:99:PRO:CD	2.91	0.47
1:A:580:PRO:HG3	1:A:626:PHE:HE1	1.78	0.47
2:B:266:LYS:HD3	2:B:266:LYS:H	1.78	0.47
2:B:181:TYR:CG	2:B:182:ILE:N	2.82	0.47
1:A:441:LEU:HD13	1:A:603:GLU:HG2	1.96	0.47
1:A:572:VAL:CB	1:A:573:GLY:HA2	2.45	0.46
1:A:613:SER:CB	1:A:618:GLU:HB3	2.44	0.46
1:A:359:GLY:O	1:A:366:VAL:N	2.42	0.46
1:A:302:ILE:H	1:A:302:ILE:HG12	1.57	0.46
1:A:363:PHE:CZ	1:A:388:MET:HG3	2.50	0.46
1:A:500:PHE:CE2	1:A:502:LYS:HB3	2.51	0.46
1:A:318:HIS:CD2	2:B:117:PRO:HG3	2.51	0.46
1:A:494:PHE:CE2	1:A:496:LEU:HD22	2.50	0.46
1:A:297:SER:HB3	2:B:143:VAL:HG22	1.98	0.46
1:A:458:GLU:OE2	1:A:489:ILE:N	2.46	0.46
2:B:248:SER:HA	2:B:251:SER:HB3	1.98	0.46
1:A:342:LEU:O	1:A:343:ARG:NH2	2.49	0.46
1:A:577:TYR:CD1	1:A:596:SER:HB3	2.51	0.46
1:A:603:GLU:HA	1:A:608:TRP:N	2.30	0.46
1:A:746:ARG:H	1:A:746:ARG:HG3	1.37	0.46
1:A:595:TRP:CD2	1:A:650:LEU:HD12	2.51	0.45
2:B:217:ARG:O	2:B:220:VAL:HG22	2.16	0.45
1:A:321:SER:OG	1:A:322:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ARG:CD	1:A:674:GLY:H	2.24	0.45
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.87	0.45
1:A:574:THR:HG23	1:A:576:ASP:H	1.81	0.45
1:A:576:ASP:O	1:A:599:ALA:HB1	2.17	0.45
1:A:577:TYR:HD2	1:A:577:TYR:H	1.64	0.45
1:A:584:LEU:HD22	1:A:584:LEU:H	1.81	0.44
2:B:225:ILE:O	2:B:229:ILE:HG13	2.18	0.44
2:B:254:ILE:O	2:B:257:ALA:N	2.50	0.44
1:A:352:PHE:CE2	1:A:428:ILE:HD11	2.52	0.44
1:A:446:LEU:HB2	1:A:448:THR:HG22	2.00	0.44
1:A:324:ARG:HA	1:A:324:ARG:HE	1.82	0.44
1:A:363:PHE:O	1:A:384:LEU:N	2.50	0.44
1:A:574:THR:HG23	1:A:576:ASP:N	2.31	0.44
1:A:464:GLU:O	1:A:468:LYS:HB2	2.18	0.44
2:B:122:LEU:HD13	2:B:122:LEU:HA	1.89	0.44
1:A:448:THR:OG1	1:A:605:LEU:HD23	2.17	0.43
1:A:465:THR:O	1:A:469:LEU:HG	2.18	0.43
1:A:481:ILE:HG23	1:A:489:ILE:HG23	2.00	0.43
1:A:611:PHE:CE1	1:A:626:PHE:HB3	2.54	0.43
1:A:494:PHE:CZ	1:A:496:LEU:HD22	2.53	0.43
1:A:381:LYS:HB2	1:A:427:LEU:HB2	1.99	0.43
1:A:341:ARG:HG3	1:A:342:LEU:HB3	2.00	0.43
1:A:656:ARG:HB2	1:A:657:LEU:H	1.70	0.43
1:A:674:GLY:HA3	1:A:675:VAL:HA	1.72	0.43
1:A:747:PHE:HD1	1:A:747:PHE:HA	1.59	0.43
1:A:447:PHE:CD1	1:A:447:PHE:N	2.85	0.42
1:A:595:TRP:CD1	1:A:595:TRP:C	2.92	0.42
1:A:377:ILE:O	1:A:377:ILE:HG12	2.19	0.42
1:A:451:VAL:O	1:A:454:PHE:HB3	2.20	0.42
1:A:611:PHE:HE1	1:A:626:PHE:HB3	1.84	0.42
2:B:146:GLU:HB3	2:B:147:TYR:H	1.63	0.42
2:B:254:ILE:HD13	2:B:254:ILE:HA	1.91	0.42
1:A:294:TYR:CB	1:A:297:SER:HB2	2.49	0.42
1:A:580:PRO:HG3	1:A:626:PHE:CE1	2.53	0.42
1:A:655:GLN:O	1:A:656:ARG:HG2	2.20	0.42
1:A:675:VAL:HG22	1:A:676:ASP:H	1.85	0.42
2:B:266:LYS:NZ	2:B:266:LYS:HB2	2.35	0.42
1:A:307:ARG:HH12	1:A:311:LEU:HD22	1.83	0.42
1:A:345:THR:HB	1:A:346:ARG:H	1.51	0.42
1:A:611:PHE:CD2	1:A:623:ILE:HG12	2.54	0.42
1:A:359:GLY:N	1:A:366:VAL:HG12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:THR:HA	1:A:620:TYR:C	2.40	0.42
1:A:632:PHE:HD2	1:A:632:PHE:HA	1.71	0.42
1:A:602:TYR:OH	1:A:631:GLN:O	2.32	0.42
1:A:621:ARG:HD3	1:A:622:LYS:N	2.33	0.42
1:A:378:TYR:HE1	1:A:416:TYR:HE2	1.68	0.41
2:B:133:PHE:CZ	2:B:253:PHE:HA	2.55	0.41
1:A:663:ALA:N	1:A:666:ILE:HD12	2.32	0.41
1:A:617:GLN:CD	1:A:617:GLN:H	2.23	0.41
1:A:436:ASP:OD2	1:A:439:THR:HB	2.21	0.41
1:A:484:ASP:OD1	1:A:488:HIS:N	2.52	0.41
1:A:620:TYR:CB	1:A:624:MET:HG2	2.50	0.41
1:A:343:ARG:HA	1:A:343:ARG:CZ	2.51	0.41
1:A:641:GLU:H	1:A:641:GLU:CD	2.17	0.41
1:A:746:ARG:HH21	1:A:747:PHE:HA	1.85	0.41
1:A:359:GLY:H	1:A:366:VAL:HG12	1.86	0.41
1:A:694:ILE:HD12	1:A:694:ILE:HA	1.89	0.41
1:A:343:ARG:NH1	2:B:128:LEU:HD21	2.36	0.41
1:A:425:LEU:HD22	1:A:426:TYR:H	1.86	0.41
1:A:368:LEU:HD13	1:A:431:PHE:CD1	2.56	0.40
1:A:342:LEU:HB2	1:A:747:PHE:HZ	1.86	0.40
1:A:630:LEU:HD23	1:A:630:LEU:HA	1.92	0.40
1:A:439:THR:HA	1:A:442:ILE:HD12	2.02	0.40
2:B:218:ILE:HA	2:B:221:GLN:CG	2.44	0.40
1:A:445:GLN:N	1:A:445:GLN:OE1	2.53	0.40
2:B:242:LEU:HD22	2:B:245:HIS:HB2	2.02	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	375/508 (74%)	291 (78%)	80 (21%)	4 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	159/244 (65%)	127 (80%)	24 (15%)	8 (5%)	2 23
All	All	534/752 (71%)	418 (78%)	104 (20%)	12 (2%)	6 38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLU
2	B	182	ILE
1	A	286	VAL
1	A	572	VAL
2	B	99	PRO
2	B	100	PHE
2	B	111	LYS
2	B	112	THR
1	A	457	ALA
2	B	231	HIS
2	B	200	PRO
1	A	578	ILE

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	285/449 (64%)	197 (69%)	88 (31%)	0 2
2	B	91/223 (41%)	73 (80%)	18 (20%)	1 9
All	All	376/672 (56%)	270 (72%)	106 (28%)	0 3

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ILE
1	A	304	ARG
1	A	307	ARG
1	A	316	THR

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Mol	Chain	Res	Type
1	A	317	SER
1	A	320	TRP
1	A	321	SER
1	A	323	GLU
1	A	324	ARG
1	A	336	GLU
1	A	338	GLN
1	A	340	LEU
1	A	342	LEU
1	A	343	ARG
1	A	351	ASP
1	A	354	THR
1	A	366	VAL
1	A	377	ILE
1	A	381	LYS
1	A	384	LEU
1	A	388	MET
1	A	389	TYR
1	A	408	ASP
1	A	418	SER
1	A	437	LEU
1	A	438	MET
1	A	439	THR
1	A	440	MET
1	A	444	TRP
1	A	445	GLN
1	A	446	LEU
1	A	450	ASP
1	A	452	THR
1	A	456	MET
1	A	458	GLU
1	A	468	LYS
1	A	480	ASN
1	A	481	ILE
1	A	485	ILE
1	A	491	LEU
1	A	493	ASP
1	A	494	PHE
1	A	561	ARG
1	A	566	LEU
1	A	576	ASP
1	A	581	GLU

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Mol	Chain	Res	Type
1	A	584	LEU
1	A	585	TYR
1	A	590	GLN
1	A	592	CYS
1	A	597	LEU
1	A	604	CYS
1	A	606	ILE
1	A	614	GLU
1	A	617	GLN
1	A	621	ARG
1	A	623	ILE
1	A	629	THR
1	A	630	LEU
1	A	631	GLN
1	A	632	PHE
1	A	636	ILE
1	A	639	SER
1	A	640	TYR
1	A	641	GLU
1	A	645	LEU
1	A	646	ILE
1	A	650	LEU
1	A	654	ASP
1	A	655	GLN
1	A	656	ARG
1	A	657	LEU
1	A	660	HIS
1	A	665	GLU
1	A	673	ARG
1	A	681	ARG
1	A	682	GLN
1	A	683	VAL
1	A	688	ILE
1	A	691	LEU
1	A	695	THR
1	A	696	ASP
1	A	698	ARG
1	A	705	LEU
1	A	743	GLU
1	A	746	ARG
1	A	747	PHE
1	A	749	TYR

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Mol	Chain	Res	Type
2	B	112	THR
2	B	113	ILE
2	B	115	GLN
2	B	119	TYR
2	B	122	LEU
2	B	128	LEU
2	B	144	VAL
2	B	148	VAL
2	B	197	ASN
2	B	198	LEU
2	B	220	VAL
2	B	226	PHE
2	B	238	VAL
2	B	241	SER
2	B	242	LEU
2	B	246	TRP
2	B	251	SER
2	B	266	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	2.60	8 (27%)	31,52,52	2.67	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	-	-	2/14/38/38	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	8.84	1.60	1.46
3	A	801	ANP	PB-N3B	4.66	1.75	1.63
3	A	801	ANP	C2'-C1'	-4.35	1.47	1.53
3	A	801	ANP	C2'-C3'	-4.28	1.41	1.53
3	A	801	ANP	PG-O1G	3.50	1.51	1.46
3	A	801	ANP	O4'-C4'	-3.04	1.38	1.45
3	A	801	ANP	C6-N6	2.85	1.44	1.34
3	A	801	ANP	C3'-C4'	-2.11	1.47	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	ANP	O1B-PB-N3B	-10.91	95.70	111.77
3	A	801	ANP	O2B-PB-O1B	4.86	120.11	109.92
3	A	801	ANP	N3-C2-N1	-4.65	121.41	128.68
3	A	801	ANP	O2B-PB-O3A	4.35	119.16	104.64
3	A	801	ANP	O5'-C5'-C4'	2.91	119.00	108.99
3	A	801	ANP	PB-O3A-PA	-2.86	122.54	132.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

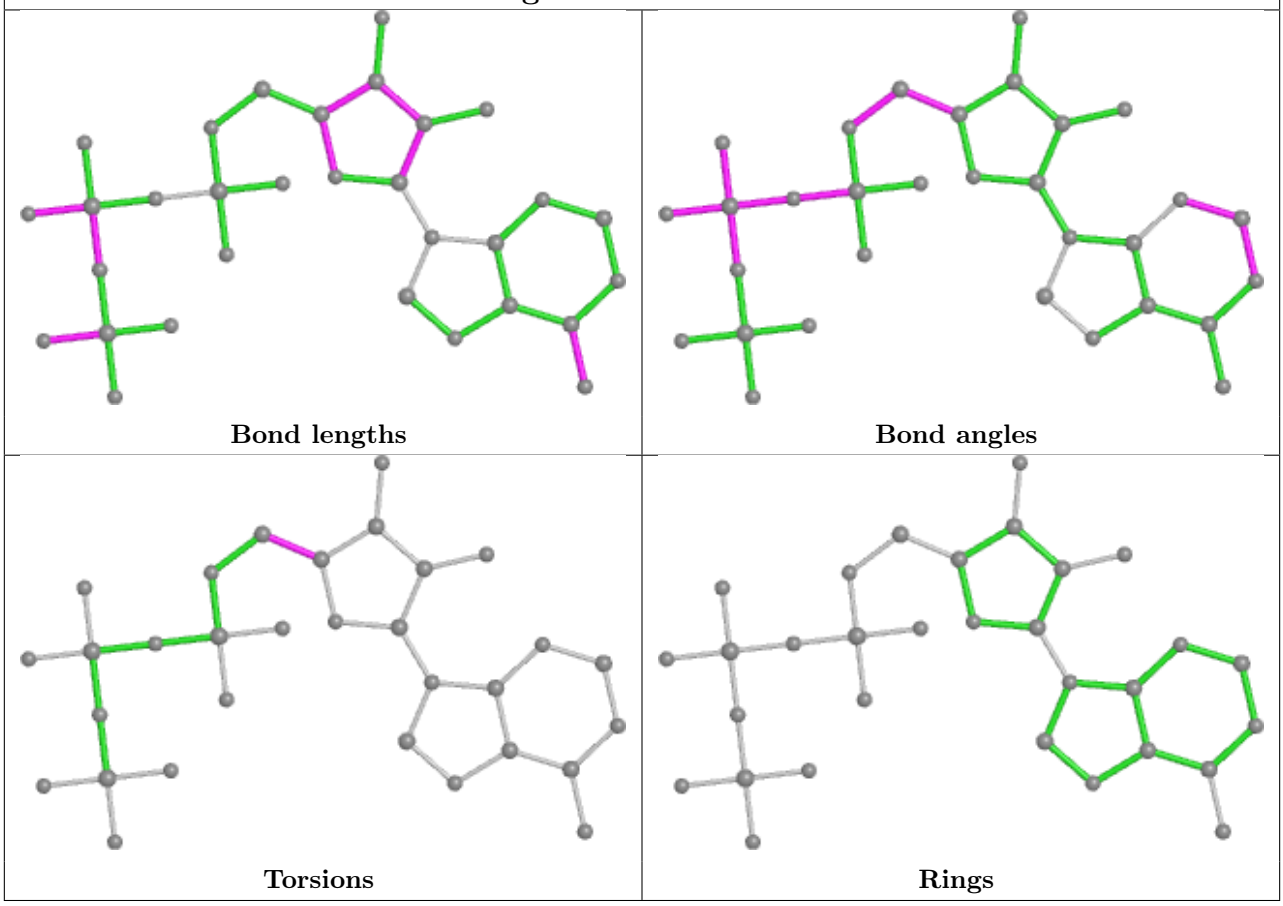
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	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 then 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.

Ligand ANP A 801



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, 95^{th} 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	383/508 (75%)	-0.25	3 (0%)	86	79	79, 147, 221, 293	0
2	B	163/244 (66%)	-0.30	3 (1%)	68	59	84, 136, 200, 240	0
All	All	546/752 (72%)	-0.27	6 (1%)	80	72	79, 145, 216, 293	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	HIS	3.0
1	A	655	GLN	2.9
2	B	108	GLY	2.7
2	B	109	SER	2.7
2	B	200	PRO	2.2
1	A	358	ILE	2.1

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 monosaccharides in this entry.

6.4 Ligands

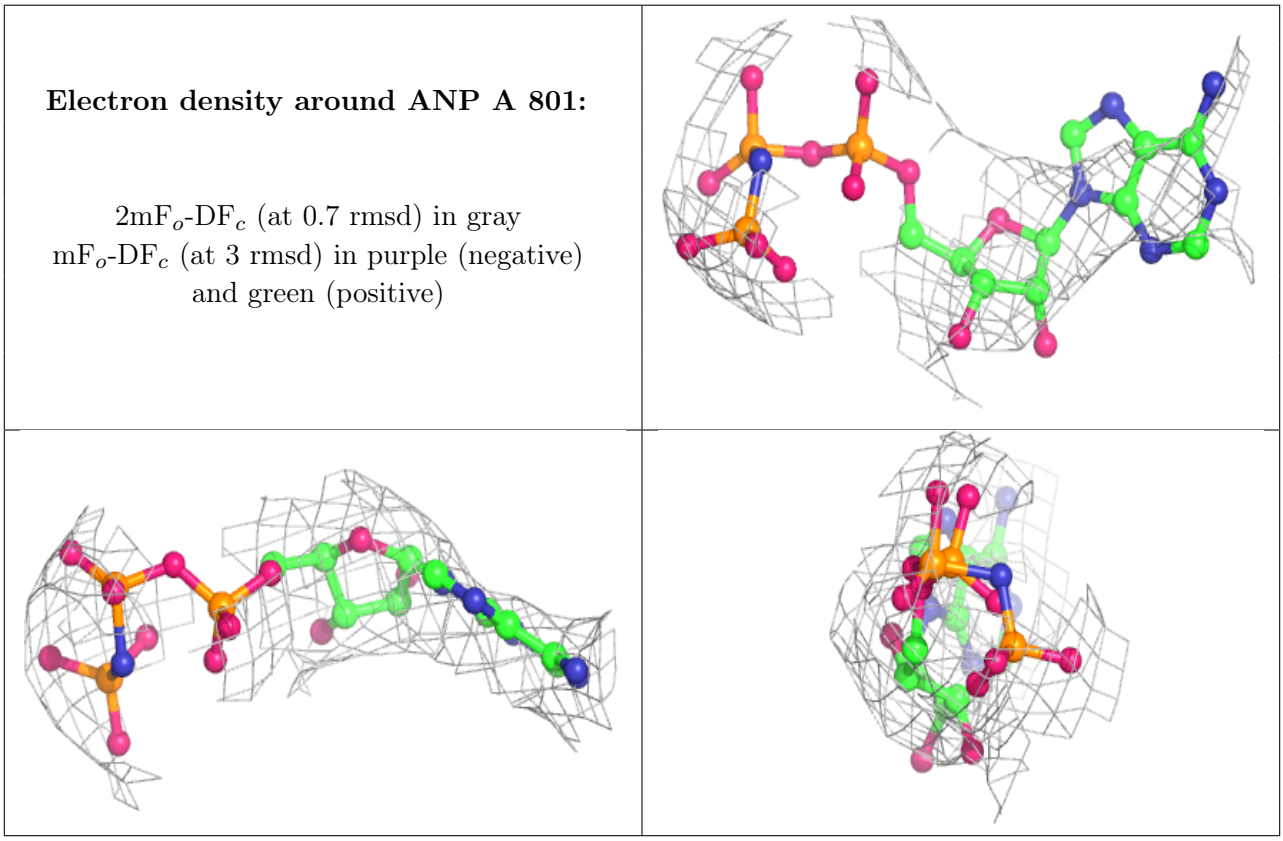
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	801	31/31	0.82	0.36	134,163,204,223	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.

Electron density around ANP A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.