



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 01:33 PM EDT

PDB ID : 6K4R  
Title : Crystal structure of SidJ-CaM-AMP ternary complex at 3.11 Å  
Authors : Ouyang, S.Y.  
Deposited on : 2019-05-26  
Resolution : 3.11 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](mailto: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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

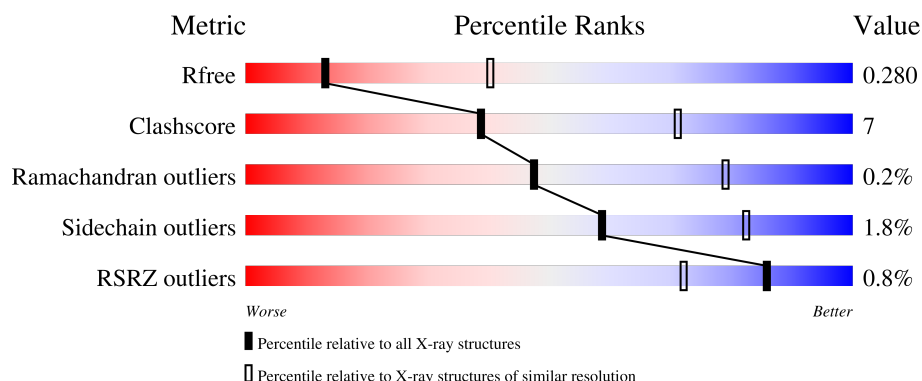
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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  $\geq 3$ , 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	873	
1	B	873	
2	C	149	
2	D	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	A	901	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12715 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.

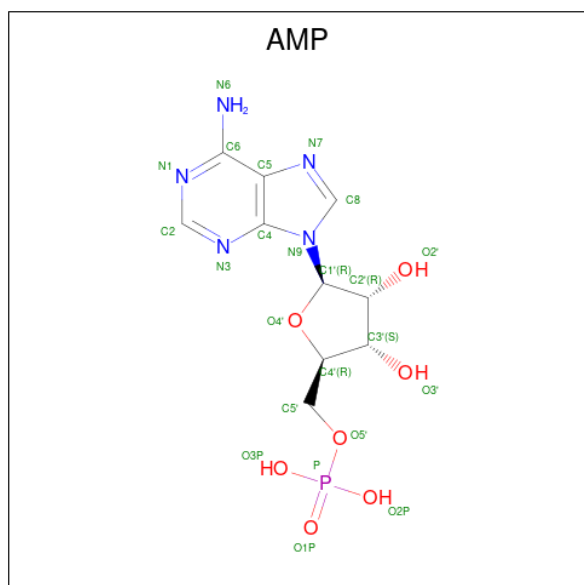
- Molecule 1 is a protein called SidJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	731	Total	C	N	O	S	0	0	0
			5655	3622	949	1070	14			
1	B	738	Total	C	N	O	S	0	0	0
			5734	3672	963	1084	15			

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	116	Total	C	N	O	S	0	0	0
			722	444	125	149	4			
2	D	82	Total	C	N	O	S	0	0	0
			526	323	89	113	1			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ) (labeled as "Ligand of Interest" by depositor).

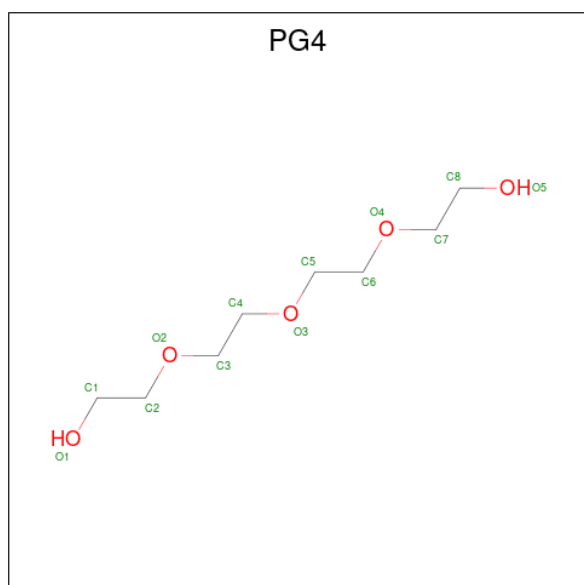


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

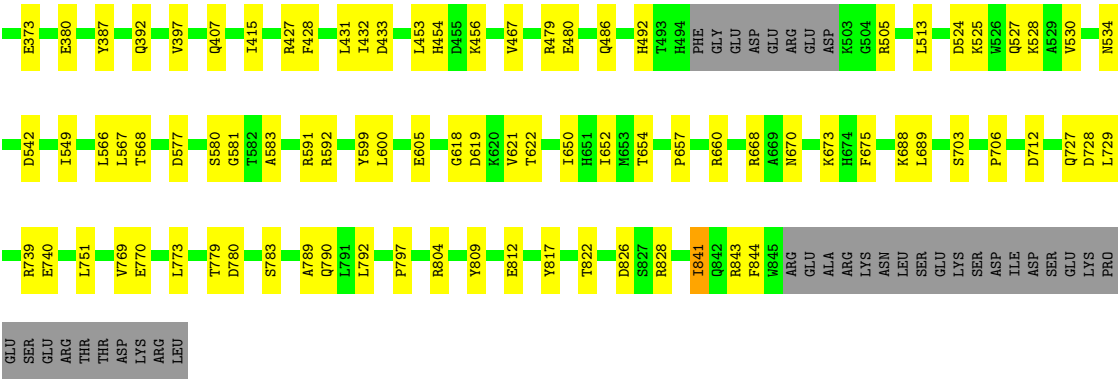
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

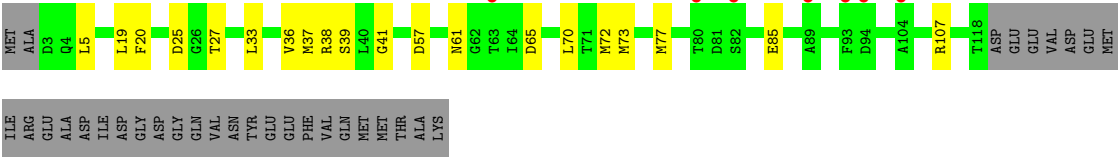
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		

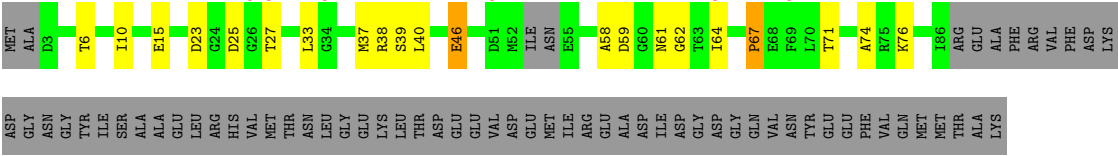




• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.85Å 159.18Å 135.03Å 90.00° 101.78° 90.00°	Depositor
Resolution (Å)	66.09 – 3.11 66.09 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.5 (66.09-3.11) 92.5 (66.09-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.239 , 0.279 0.242 , 0.280	Depositor DCC
$R_{free}$ test set	1981 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PG4, CA, CL, AMP

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	0.26	0/5782	0.43	1/7867 (0.0%)
1	B	0.25	0/5864	0.42	1/7972 (0.0%)
2	C	0.27	0/727	0.52	0/993
2	D	0.34	0/530	0.50	0/723
All	All	0.26	0/12903	0.44	2/17555 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	844	PHE	N-CA-CB	6.36	122.05	110.60
1	A	437	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	46	GLU	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	5655	0	5383	93	0
1	B	5734	0	5498	76	0
2	C	722	0	554	14	0
2	D	526	0	405	14	0
3	A	23	0	12	13	0
3	B	23	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	26	0	36	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	12715	0	11900	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (184) 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:542:ASP:OD2	3:A:901:AMP:C1'	1.91	1.19
1:A:542:ASP:OD2	3:A:901:AMP:C4	2.01	1.13
1:A:542:ASP:OD2	3:A:901:AMP:N9	1.99	0.95
1:A:541:ALA:O	1:A:542:ASP:O	1.89	0.90
1:A:542:ASP:OD2	3:A:901:AMP:O4'	1.91	0.87
1:A:542:ASP:OD2	3:A:901:AMP:N3	2.09	0.85
1:B:618:GLY:O	1:B:622:THR:HG22	1.80	0.81
1:A:112:THR:HG22	1:A:114:ASP:H	1.49	0.78
1:A:536:ARG:NH2	3:A:901:AMP:O3'	2.17	0.78
1:A:511:GLN:NE2	1:A:742:GLU:OE2	2.16	0.77
1:B:112:THR:HG23	1:B:592:ARG:HG3	1.65	0.76
1:B:112:THR:HG22	1:B:114:ASP:H	1.51	0.74
2:C:70:LEU:O	2:C:73:MET:SD	2.47	0.72
1:B:352:ARG:NH1	1:B:373:GLU:OE2	2.24	0.71
1:A:542:ASP:OD2	3:A:901:AMP:H1'	1.86	0.70
1:A:137:GLU:OE2	1:A:140:ARG:NH1	2.25	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:ASP:HB2	2:C:61:ASN:HB2	1.74	0.69
1:B:505:ARG:NH2	1:B:605:GLU:OE2	2.27	0.68
1:A:534:ASN:HD21	3:A:901:AMP:H1'	1.57	0.68
1:B:179:ALA:O	1:B:188:LYS:NZ	2.26	0.67
1:A:534:ASN:ND2	3:A:901:AMP:O3'	2.27	0.67
1:B:706:PRO:O	1:B:739:ARG:NH2	2.26	0.67
1:B:534:ASN:ND2	1:B:542:ASP:OD2	2.28	0.67
1:A:804:ARG:NH1	2:C:39:SER:O	2.27	0.66
1:B:527:GLN:NE2	1:B:619:ASP:OD2	2.28	0.66
1:B:173:LEU:HD22	1:B:223:PRO:HB2	1.77	0.66
1:B:660:ARG:NH2	2:D:15:GLU:OE2	2.29	0.66
1:B:137:GLU:OE2	1:B:140:ARG:NH1	2.29	0.65
1:A:112:THR:HG23	1:A:592:ARG:HG3	1.78	0.65
1:B:660:ARG:NH1	1:B:797:PRO:O	2.26	0.64
2:C:25:ASP:OD2	2:C:27:THR:OG1	2.15	0.63
1:A:352:ARG:NE	3:A:901:AMP:O3P	2.25	0.62
1:A:676:ARG:HG2	1:A:701:ILE:HG22	1.80	0.62
1:A:479:ARG:NH1	1:A:652:ILE:O	2.31	0.62
1:B:142:GLU:HB3	1:B:254:GLN:HE21	1.68	0.59
1:B:358:THR:HG22	1:B:360:GLN:H	1.68	0.58
1:B:841:ILE:H	1:B:841:ILE:HD12	1.68	0.58
1:B:657:PRO:HD2	1:B:660:ARG:HH21	1.69	0.57
1:B:354:LEU:HB2	1:B:366:VAL:HG13	1.86	0.57
1:B:568:THR:O	1:B:591:ARG:NH1	2.36	0.57
1:A:342:SER:OG	1:A:344:ASP:OD1	2.23	0.57
2:C:20:PHE:CG	2:C:36:VAL:HG12	2.40	0.57
1:A:466:SER:O	1:A:470:ASN:ND2	2.37	0.56
1:A:173:LEU:HD22	1:A:223:PRO:HB2	1.86	0.56
1:B:804:ARG:NH1	2:D:39:SER:O	2.33	0.56
1:B:222:TYR:OH	1:B:790:GLN:OE1	2.25	0.55
1:B:392:GLN:HG3	1:B:397:VAL:HB	1.88	0.55
1:A:434:ASP:OD1	1:A:435:SER:N	2.37	0.55
1:A:294:GLU:N	1:A:297:SER:O	2.36	0.55
2:D:6:THR:O	2:D:10:ILE:N	2.40	0.55
1:A:348:ARG:HG2	1:A:349:ILE:H	1.73	0.54
1:B:251:THR:HG23	1:B:253:ASN:H	1.72	0.54
1:A:239:LEU:HD13	1:A:258:VAL:HG13	1.90	0.54
1:B:577:ASP:HB3	1:B:580:SER:HB3	1.89	0.54
1:A:522:ARG:NH1	1:A:732:TYR:O	2.39	0.54
1:B:310:LEU:HD11	1:B:600:LEU:HD12	1.89	0.54
1:A:660:ARG:NH1	1:A:797:PRO:O	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:SER:OG	1:B:668:ARG:NH2	2.41	0.54
1:A:296:LEU:HD11	1:B:258:VAL:HG12	1.90	0.54
1:A:102:TYR:O	1:A:394:ARG:NH1	2.36	0.53
1:B:479:ARG:NH1	1:B:652:ILE:O	2.39	0.53
1:B:812:GLU:OE1	2:D:38:ARG:NH2	2.30	0.53
1:A:210:TRP:O	1:A:214:ASN:ND2	2.41	0.53
1:A:252:LYS:HE2	1:A:584:ASN:HB2	1.90	0.52
2:D:58:ALA:O	2:D:61:ASN:N	2.42	0.52
1:A:448:SER:HB2	1:A:538:SER:HB3	1.91	0.52
1:B:112:THR:HG22	1:B:114:ASP:N	2.24	0.52
1:B:387:TYR:OH	1:B:480:GLU:OE2	2.28	0.52
1:A:513:LEU:HD22	1:A:566:LEU:HD22	1.91	0.51
1:A:830:GLN:NE2	2:C:85:GLU:OE2	2.39	0.51
1:B:525:LYS:HB3	1:B:528:LYS:HB2	1.91	0.51
2:C:33:LEU:O	2:C:36:VAL:HG22	2.10	0.51
2:D:58:ALA:O	2:D:62:GLY:N	2.36	0.51
1:A:722:VAL:N	1:A:728:ASP:OD2	2.43	0.51
1:B:210:TRP:O	1:B:214:ASN:ND2	2.43	0.51
2:C:73:MET:O	2:C:73:MET:HG3	2.09	0.51
1:A:99:VAL:HG22	1:A:100:LYS:H	1.75	0.51
1:B:428:PHE:HA	1:B:432:ILE:HD12	1.93	0.51
1:A:112:THR:HG22	1:A:114:ASP:N	2.24	0.51
1:A:251:THR:HG23	1:A:253:ASN:H	1.76	0.51
1:B:110:THR:OG1	1:B:111:SER:N	2.44	0.51
1:B:348:ARG:HG2	1:B:349:ILE:H	1.76	0.51
1:A:222:TYR:OH	1:A:790:GLN:OE1	2.28	0.51
1:A:842:GLN:OE1	2:C:107:ARG:N	2.43	0.50
1:A:110:THR:OG1	1:A:111:SER:N	2.45	0.50
1:A:402:PRO:HB3	1:A:445:ALA:HB2	1.94	0.49
1:B:822:THR:OG1	1:B:826:ASP:OD1	2.29	0.49
1:A:541:ALA:O	1:A:542:ASP:C	2.51	0.49
1:B:370:LYS:HA	1:B:431:LEU:O	2.12	0.49
1:B:454:HIS:NE2	1:B:530:VAL:O	2.46	0.49
1:A:474:LEU:CD1	1:A:540:LEU:HD21	2.43	0.48
1:A:625:MET:O	1:A:627:ASP:N	2.46	0.48
1:A:528:LYS:HA	1:A:531:GLU:HB2	1.95	0.48
1:A:184:ASP:OD1	1:A:187:LYS:HB2	2.14	0.48
1:B:415:ILE:HG22	1:B:427:ARG:HH22	1.78	0.48
1:A:650:ILE:O	1:A:654:THR:OG1	2.28	0.48
1:B:131:LEU:HD23	1:B:583:ALA:HB3	1.94	0.48
1:B:670:ASN:N	1:B:740:GLU:OE1	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:GLU:OE2	1:B:809:TYR:OH	2.32	0.48
1:A:186:ILE:O	1:A:190:GLN:HG2	2.14	0.48
1:B:433:ASP:OD1	1:B:433:ASP:N	2.40	0.48
1:A:358:THR:HG22	1:A:360:GLN:H	1.79	0.47
1:B:456:LYS:HB2	1:B:621:VAL:HG12	1.97	0.47
1:A:801:PHE:HE1	2:C:19:LEU:HD23	1.79	0.47
1:B:841:ILE:CD1	1:B:841:ILE:C	2.83	0.47
1:B:294:GLU:N	1:B:297:SER:O	2.45	0.47
1:A:143:LEU:HD21	1:A:254:GLN:HB3	1.96	0.46
1:A:164:PRO:HG2	1:A:167:GLN:HB2	1.96	0.46
1:A:453:LEU:HD21	1:A:467:VAL:HG22	1.96	0.46
1:B:486:GLN:OE1	3:B:901:AMP:N6	2.49	0.46
1:A:534:ASN:HD21	3:A:901:AMP:C1'	2.26	0.46
1:B:780:ASP:OD1	1:B:780:ASP:N	2.41	0.46
1:A:155:ILE:HD13	1:A:197:PRO:HG2	1.97	0.46
1:A:366:VAL:HG23	1:A:440:VAL:HG13	1.98	0.46
1:A:541:ALA:C	1:A:542:ASP:O	2.54	0.45
1:B:513:LEU:HD22	1:B:566:LEU:HD22	1.98	0.45
1:A:146:ILE:O	1:A:149:THR:HG22	2.16	0.45
1:A:296:LEU:HG	1:B:262:ARG:HE	1.81	0.45
1:B:349:ILE:HD11	1:B:427:ARG:HD3	1.97	0.45
2:D:23:ASP:OD2	2:D:27:THR:N	2.49	0.45
1:A:780:ASP:OD1	1:A:780:ASP:N	2.40	0.45
1:A:808:SER:OG	2:C:38:ARG:NE	2.44	0.45
1:B:143:LEU:HD21	1:B:254:GLN:HB3	1.98	0.45
1:B:325:HIS:HE1	1:B:380:GLU:OE2	2.00	0.45
1:A:769:VAL:O	1:A:773:LEU:HD13	2.16	0.45
1:B:178:LEU:HG	1:B:191:ILE:HD13	1.98	0.45
1:B:729:LEU:HD12	1:B:729:LEU:HA	1.78	0.45
2:C:37:MET:O	2:C:41:GLY:N	2.49	0.45
1:B:492:HIS:CB	1:B:524:ASP:H	2.31	0.44
1:A:542:ASP:CG	3:A:901:AMP:N3	2.70	0.44
1:A:290:PRO:HD2	1:A:668:ARG:HD2	2.00	0.44
1:B:673:LYS:HB2	1:B:740:GLU:HG3	2.00	0.44
1:B:841:ILE:HD12	1:B:841:ILE:O	2.18	0.44
1:A:230:ASN:HD21	1:A:232:ARG:NH1	2.16	0.44
2:C:25:ASP:OD1	2:C:25:ASP:N	2.42	0.44
1:A:360:GLN:N	1:A:360:GLN:OE1	2.51	0.43
1:A:779:THR:HG22	1:A:783:SER:HB3	2.00	0.43
1:A:706:PRO:O	1:A:739:ARG:NH2	2.50	0.43
1:B:769:VAL:O	1:B:773:LEU:HG	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:TYR:H	2:D:25:ASP:HB3	1.84	0.43
1:B:577:ASP:O	1:B:581:GLY:N	2.49	0.43
1:A:282:TYR:CG	1:A:751:LEU:HD21	2.54	0.43
1:A:296:LEU:HD12	1:B:262:ARG:NH2	2.34	0.43
1:A:354:LEU:HB2	1:A:366:VAL:CG1	2.49	0.43
1:B:453:LEU:HD21	1:B:467:VAL:HG22	2.00	0.43
2:D:58:ALA:O	2:D:59:ASP:C	2.55	0.43
1:A:520:LEU:HD13	1:A:742:GLU:HG3	2.01	0.43
1:B:789:ALA:HB1	1:B:828:ARG:HH11	1.83	0.43
1:B:282:TYR:CG	1:B:751:LEU:HD21	2.54	0.43
1:B:668:ARG:HA	1:B:668:ARG:HD3	1.83	0.43
1:A:467:VAL:O	1:A:471:VAL:HG13	2.19	0.42
2:D:67:PRO:O	2:D:71:THR:N	2.36	0.42
1:A:131:LEU:HD23	1:A:583:ALA:HB3	2.00	0.42
1:A:173:LEU:O	1:A:177:SER:OG	2.30	0.42
1:A:382:PHE:CE2	1:A:404:PRO:HB2	2.54	0.42
1:A:668:ARG:HD3	1:A:668:ARG:HA	1.78	0.42
1:A:335:SER:HB3	1:A:407:GLN:H	1.85	0.42
1:A:525:LYS:C	1:A:527:GLN:H	2.23	0.42
1:B:779:THR:O	1:B:817:TYR:OH	2.33	0.42
1:B:804:ARG:NH1	2:D:40:LEU:HA	2.35	0.42
2:D:33:LEU:O	2:D:37:MET:HG3	2.19	0.42
1:A:475:PHE:HE1	1:A:603:ILE:HG23	1.85	0.42
1:B:117:LEU:HD22	1:B:567:LEU:HB3	2.01	0.42
1:B:266:VAL:HG21	1:B:277:TRP:CH2	2.55	0.42
1:A:759:ASP:OD2	1:A:796:ARG:NH2	2.41	0.41
1:A:352:ARG:HD2	1:A:368:VAL:O	2.20	0.41
2:D:64:ILE:H	2:D:64:ILE:HG12	1.71	0.41
1:A:352:ARG:NH2	1:A:367:LYS:HD3	2.35	0.41
1:A:577:ASP:HB3	1:A:580:SER:HB3	2.03	0.41
2:D:74:ALA:O	2:D:76:LYS:N	2.44	0.41
1:A:247:LYS:HE3	1:A:247:LYS:HB3	1.93	0.41
1:A:104:PHE:HB3	1:A:321:SER:HB3	2.01	0.41
1:B:549:ILE:HD11	1:B:599:TYR:HE1	1.86	0.41
1:A:622:THR:HG21	1:A:635:TRP:NE1	2.35	0.41
1:B:727:GLN:HG2	1:B:728:ASP:O	2.21	0.41
1:A:354:LEU:HB2	1:A:366:VAL:HG13	2.03	0.41
1:A:572:HIS:CG	1:A:573:PRO:HD2	2.55	0.41
1:B:688:LYS:O	1:B:689:LEU:HD23	2.19	0.41
2:C:77:MET:O	2:C:77:MET:HG3	2.21	0.41
1:A:185:GLY:O	1:A:189:ASN:ND2	2.32	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:THR:HG22	1:B:783:SER:HB3	2.02	0.41
1:A:294:GLU:O	1:A:296:LEU:N	2.55	0.40
1:A:536:ARG:HH21	3:A:901:AMP:HO3'	1.65	0.40
1:B:650:ILE:O	1:B:654:THR:OG1	2.27	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	723/873 (83%)	682 (94%)	40 (6%)	1 (0%)	51	83
1	B	734/873 (84%)	685 (93%)	49 (7%)	0	100	100
2	C	114/149 (76%)	93 (82%)	21 (18%)	0	100	100
2	D	78/149 (52%)	61 (78%)	15 (19%)	2 (3%)	5	26
All	All	1649/2044 (81%)	1521 (92%)	125 (8%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	ASP
2	D	46	GLU
2	D	67	PRO

### 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	589/794 (74%)	579 (98%)	10 (2%)	60	83
1	B	602/794 (76%)	592 (98%)	10 (2%)	60	83
2	C	48/127 (38%)	45 (94%)	3 (6%)	18	48
2	D	39/127 (31%)	39 (100%)	0	100	100
All	All	1278/1842 (69%)	1255 (98%)	23 (2%)	59	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	A	166	GLN
1	A	252	LYS
1	A	344	ASP
1	A	357	SER
1	A	398	HIS
1	A	407	GLN
1	A	675	PHE
1	A	712	ASP
1	A	792	LEU
1	B	124	LEU
1	B	166	GLN
1	B	346	LEU
1	B	407	GLN
1	B	675	PHE
1	B	703	SER
1	B	712	ASP
1	B	792	LEU
1	B	841	ILE
1	B	843	ARG
2	C	5	LEU
2	C	65	ASP
2	C	72	MET

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

Mol	Chain	Res	Type
1	A	534	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 ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	AMP	B	901	-	21,25,25	0.78	0	23,38,38	1.21	2 (8%)
5	PG4	B	903	-	12,12,12	0.54	0	11,11,11	0.23	0
3	AMP	A	901	-	21,25,25	0.78	0	23,38,38	1.22	2 (8%)
5	PG4	B	902	-	12,12,12	0.54	0	11,11,11	0.22	0

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	AMP	B	901	-	-	5/6/26/26	0/3/3/3
5	PG4	B	903	-	-	3/10/10/10	-
3	AMP	A	901	-	-	4/6/26/26	0/3/3/3
5	PG4	B	902	-	-	2/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	AMP	N3-C2-N1	-3.82	123.48	128.67
3	B	901	AMP	N3-C2-N1	-3.59	123.80	128.67
3	B	901	AMP	C4-C5-N7	-2.76	106.43	109.34
3	A	901	AMP	C4-C5-N7	-2.75	106.43	109.34

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	AMP	C5'-O5'-P-O1P
3	A	901	AMP	C5'-O5'-P-O2P
3	A	901	AMP	C5'-O5'-P-O3P
3	B	901	AMP	C5'-O5'-P-O2P
3	B	901	AMP	C5'-O5'-P-O3P
3	B	901	AMP	O4'-C4'-C5'-O5'
3	B	901	AMP	C3'-C4'-C5'-O5'
5	B	902	PG4	O3-C5-C6-O4
3	B	901	AMP	C5'-O5'-P-O1P
3	A	901	AMP	C4'-C5'-O5'-P
5	B	902	PG4	O2-C3-C4-O3
5	B	903	PG4	C1-C2-O2-C3
5	B	903	PG4	C5-C6-O4-C7
5	B	903	PG4	O3-C5-C6-O4

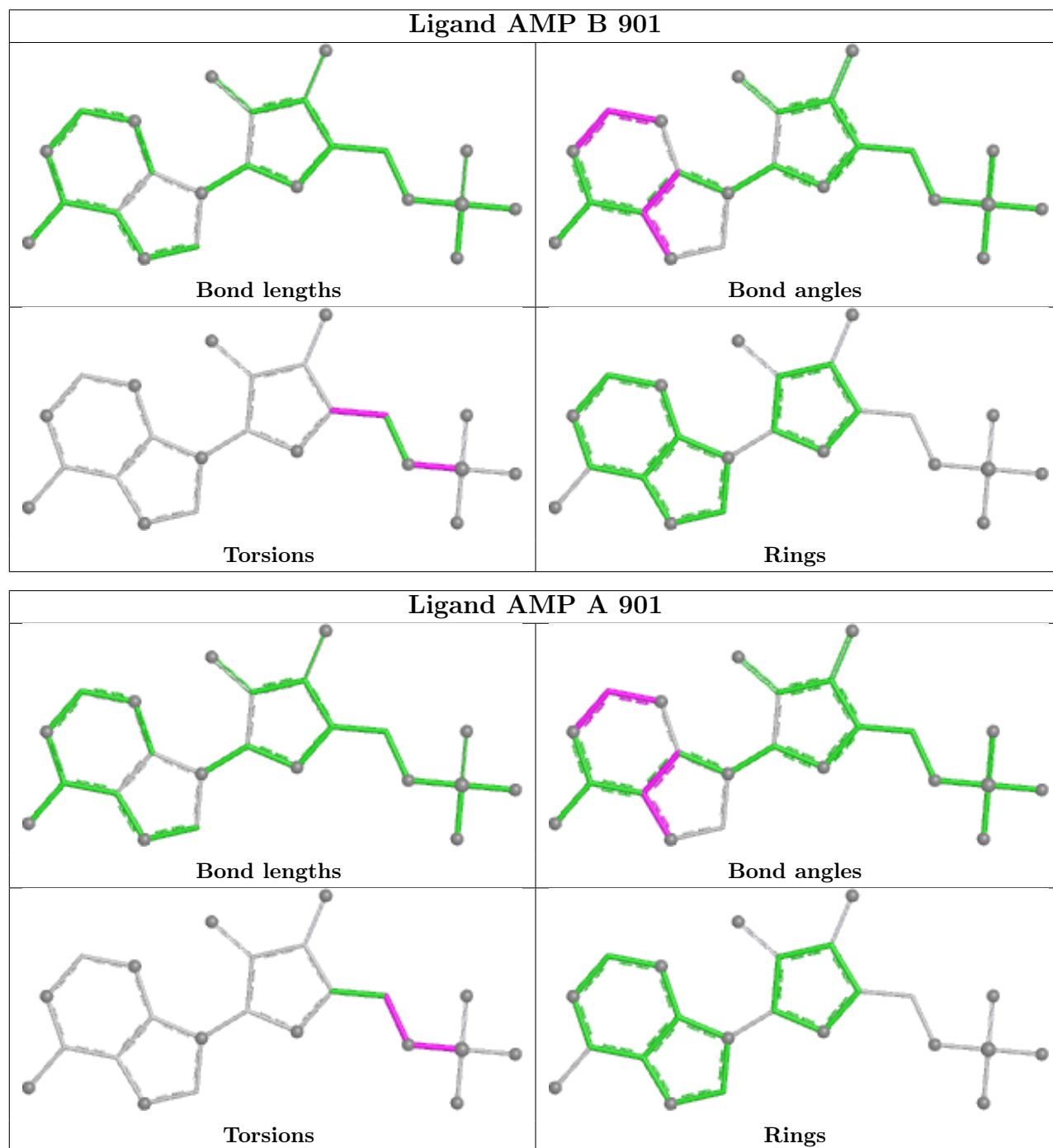
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	AMP	1	0
3	A	901	AMP	13	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	731/873 (83%)	-0.26	0	100 100	44, 64, 89, 102	0
1	B	738/873 (84%)	-0.29	0	100 100	43, 61, 84, 113	0
2	C	116/149 (77%)	0.14	7 (6%)	21 10	63, 97, 123, 129	0
2	D	82/149 (55%)	0.24	6 (7%)	15 6	60, 82, 119, 123	0
All	All	1667/2044 (81%)	-0.22	13 (0%)	86 72	43, 64, 99, 129	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	93	PHE	4.3
2	D	27	THR	3.8
2	C	63	THR	3.3
2	C	104	ALA	3.3
2	C	80	THR	2.9
2	D	51	ASP	2.4
2	D	34	GLY	2.4
2	C	89	ALA	2.3
2	D	69	PHE	2.2
2	C	94	ASP	2.1
2	D	26	GLY	2.0
2	C	82	SER	2.0
2	D	64	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

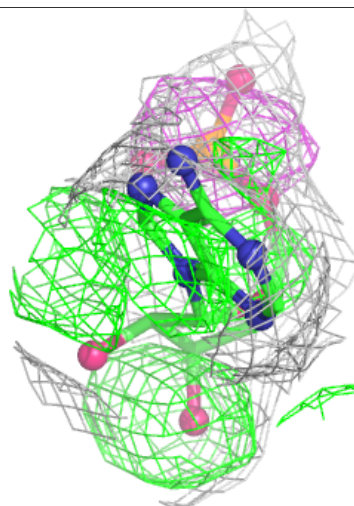
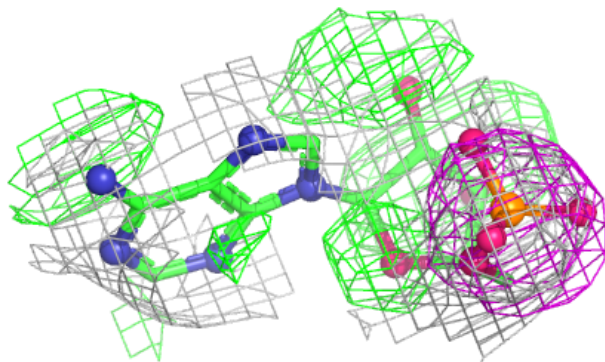
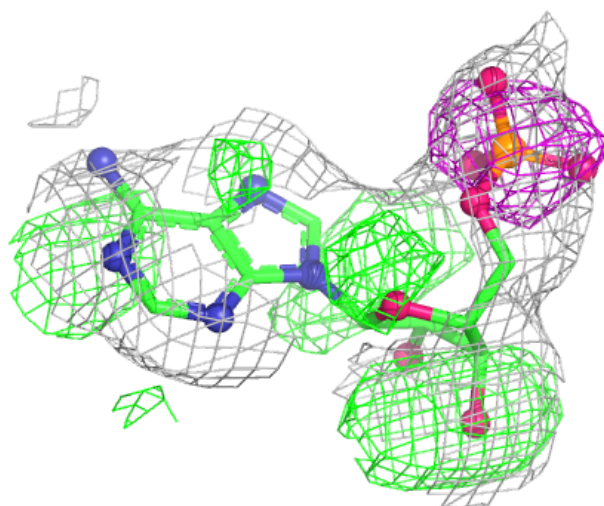
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	PG4	B	903	13/13	0.63	0.15	77,80,90,91	0
3	AMP	B	901	23/23	0.70	0.26	66,72,81,89	0
5	PG4	B	902	13/13	0.82	0.20	68,71,77,78	0
3	AMP	A	901	23/23	0.84	0.20	64,71,75,76	0
4	CL	A	903	1/1	0.84	0.27	80,80,80,80	0
6	CA	D	201	1/1	0.92	0.11	73,73,73,73	0
4	CL	B	904	1/1	0.93	0.12	61,61,61,61	0
4	CL	B	905	1/1	0.94	0.11	57,57,57,57	0
4	CL	A	902	1/1	0.95	0.14	57,57,57,57	0
6	CA	C	201	1/1	0.98	0.10	71,71,71,71	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 AMP B 901:**

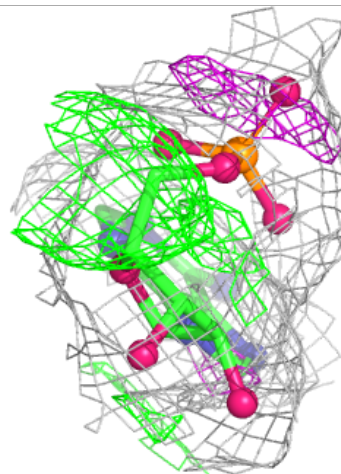
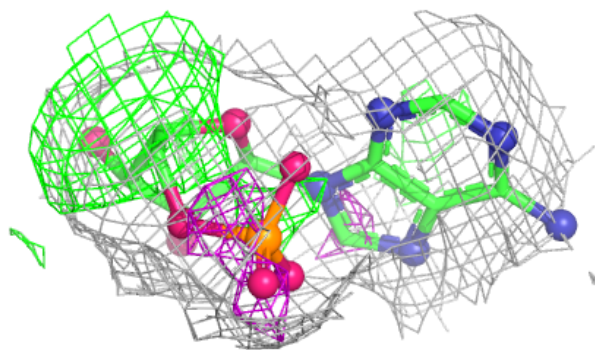
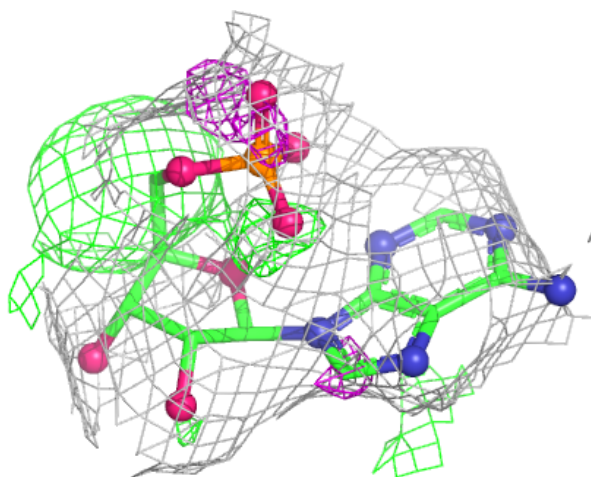
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





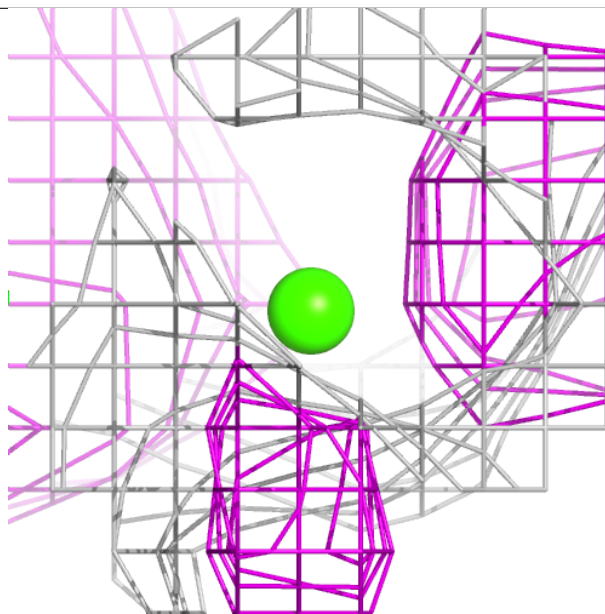
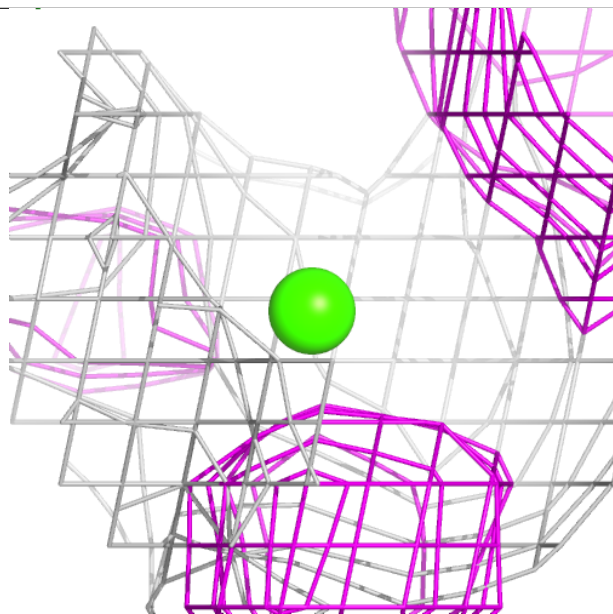
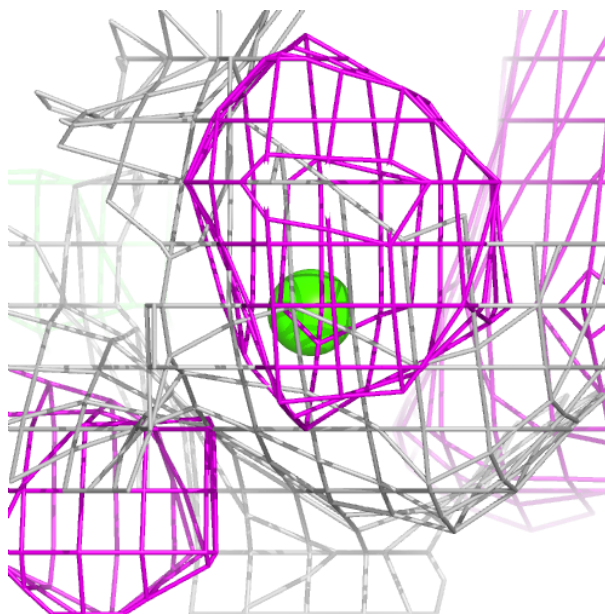
**Electron density around AMP A 901:**

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



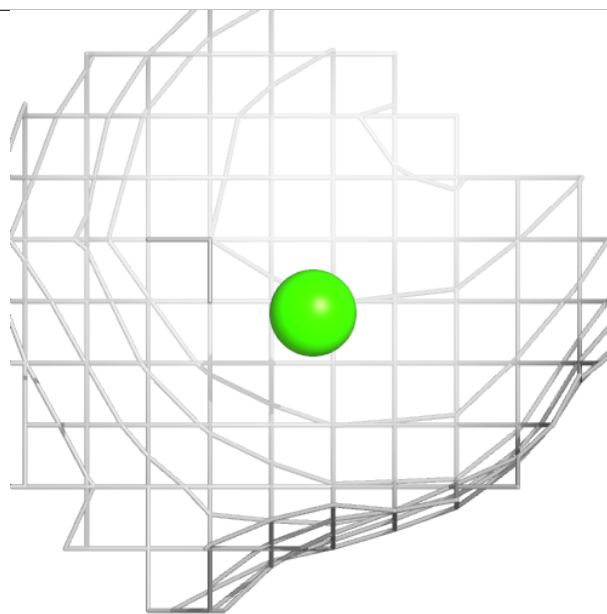
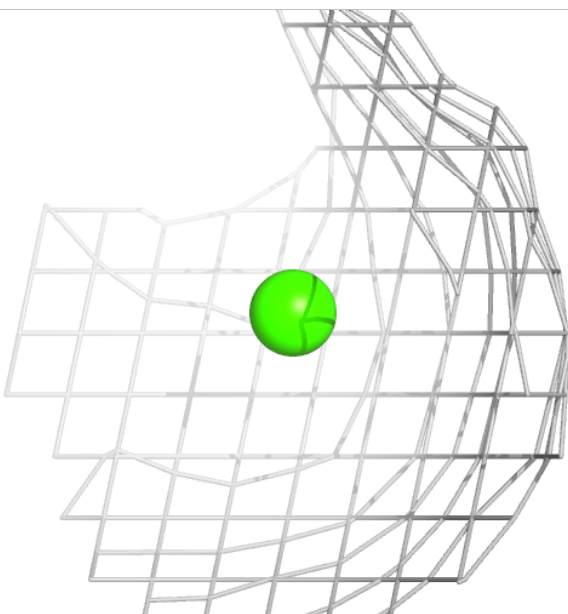
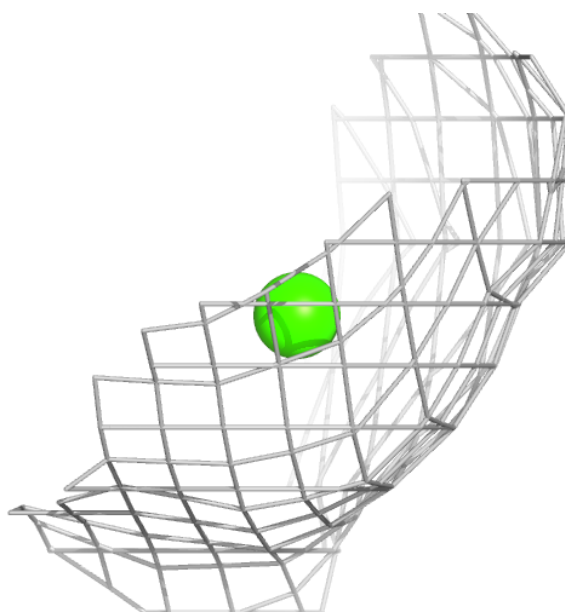
**Electron density around CA D 201:**

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



**Electron density around CA C 201:**

$2mF_o-DF_c$  (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.