



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 11:23 PM EST

PDB ID : 6OQQ
Title : Legionella pneumophila SidJ/Saccharomyces cerevisiae calmodulin complex
Authors : Tomchick, D.R.; Tagliabracci, V.S.; Black, M.; Osinski, A.
Deposited on : 2019-04-28
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-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

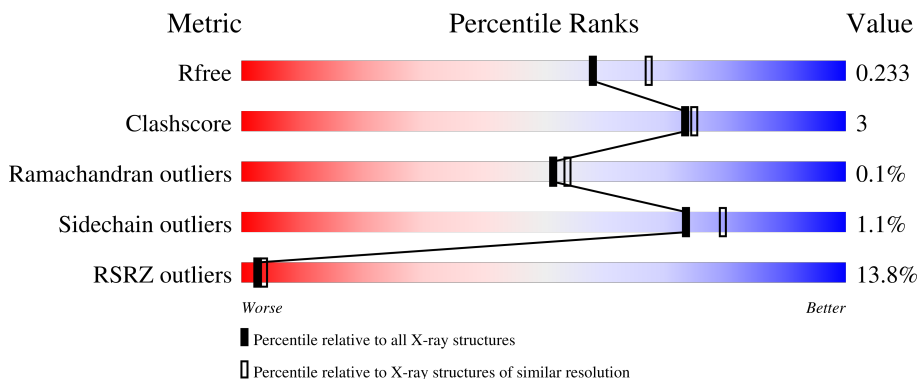
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	873	 3% (Poor fit), 79% (0-3 outliers), 6% (1 outlier), 14% (2+ outliers or not modelled)
1	C	873	 8% (Poor fit), 80% (0-3 outliers), 5% (1 outlier), 15% (2+ outliers or not modelled)
2	B	147	 29% (Poor fit), 79% (0-3 outliers), 12% (1 outlier), 10% (2+ outliers or not modelled)
2	D	147	 67% (Poor fit), 70% (0-3 outliers), 19% (1 outlier), 11% (2+ outliers or not modelled)

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 29179 atoms, of which 14154 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.

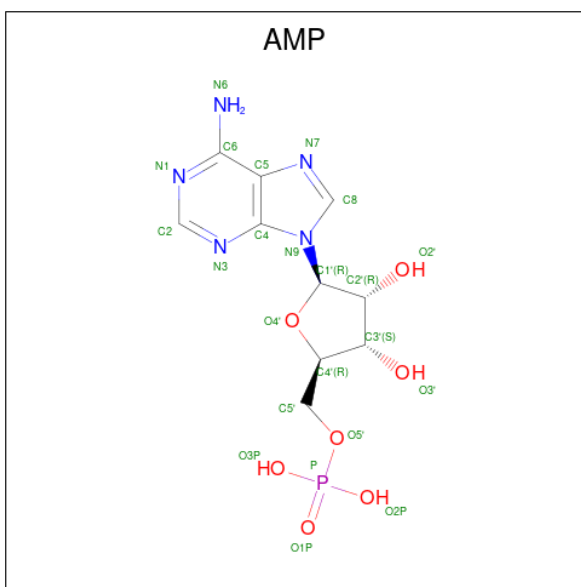
- Molecule 1 is a protein called Legionella pneumophila SidJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	748	Total	C	H	N	O	S	0	0	0
			12164	3903	6063	1033	1150	15			
1	C	743	Total	C	H	N	O	S	0	1	0
			12080	3872	6024	1024	1145	15			

- Molecule 2 is a protein called Calmodulin.

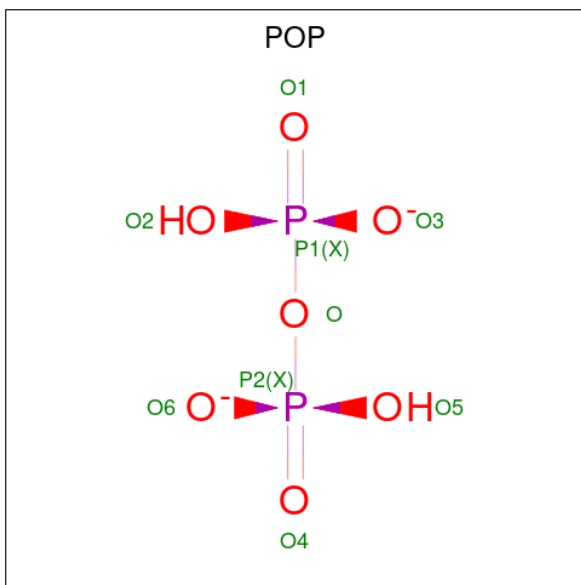
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	133	Total	C	H	N	O	S	0	0	0
			2019	639	991	165	220	4			
2	D	131	Total	C	H	N	O	S	0	0	0
			1986	629	974	162	217	4			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
3	C	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O P	0	0
			9	7 2		
4	C	1	Total	O P	0	0
			9	7 2		
4	C	1	Total	O P	0	0
			9	7 2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mg	0	0
			4	4		
5	C	3	Total	Mg	0	0
			3	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	C	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	D	2	Total	Ca	0	0
			2	2		

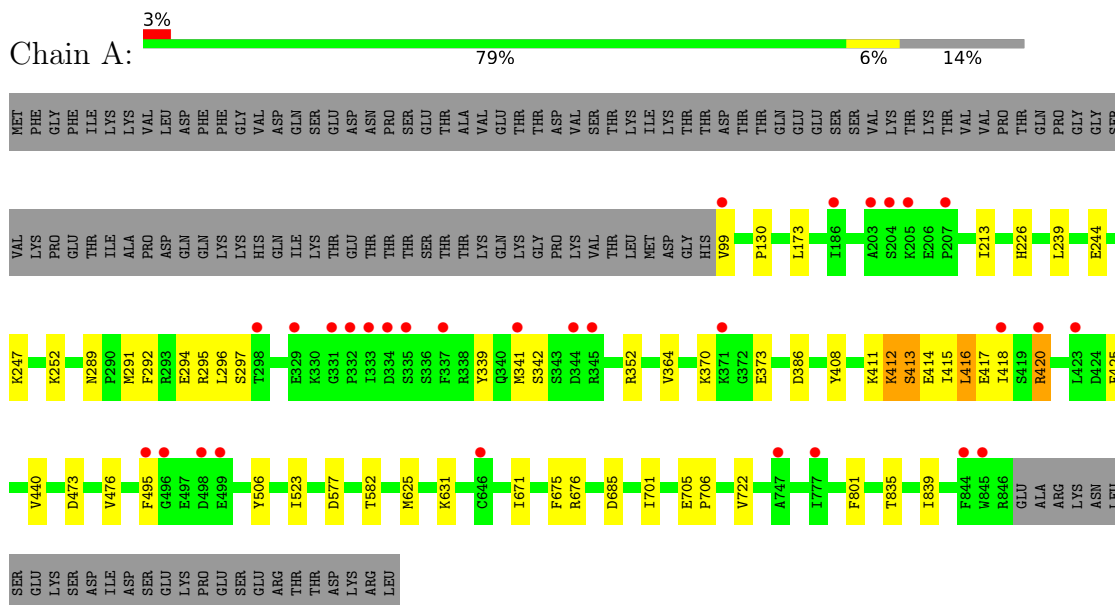
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	398	Total	O	0	0
			398	398		
9	B	37	Total	O	0	0
			37	37		
9	C	246	Total	O	0	0
			246	246		
9	D	9	Total	O	0	0
			9	9		

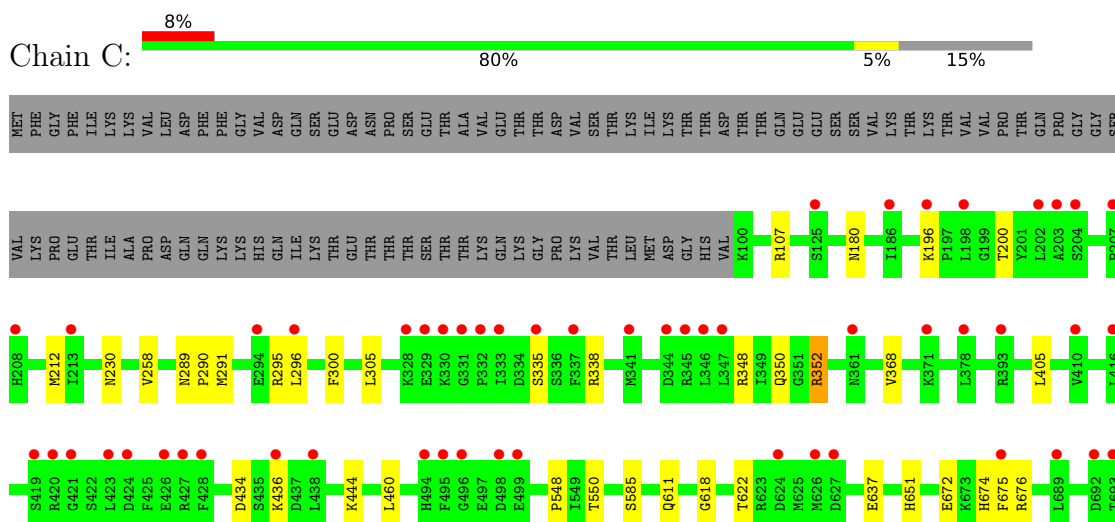
3 Residue-property plots [i](#)

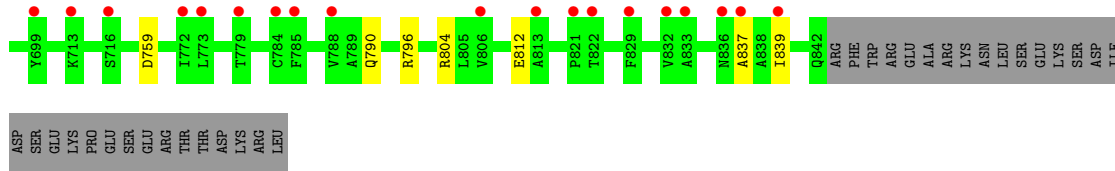
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: *Legionella pneumophila* SidJ

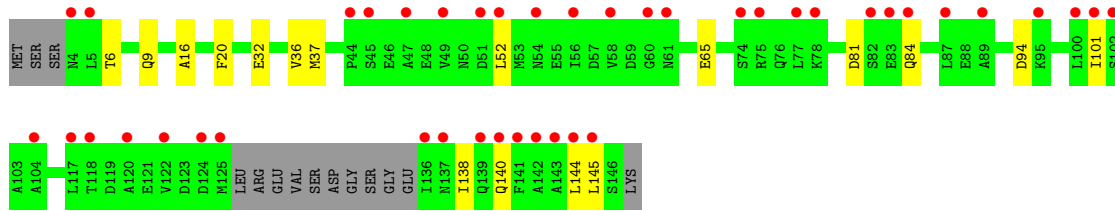
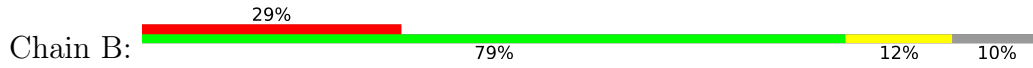


- Molecule 1: *Legionella pneumophila* SidJ

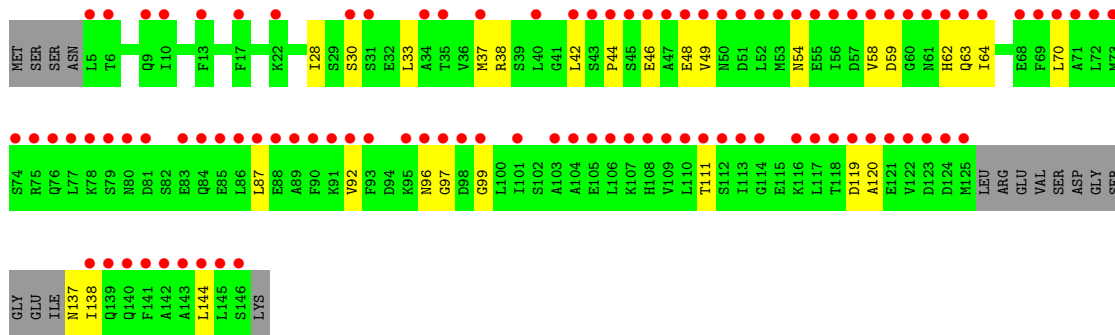




• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.49Å 104.75Å 107.77Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	46.83 – 2.10 46.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.9 (46.83-2.10) 84.9 (46.83-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.10Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.234 0.202 , 0.233	Depositor DCC
R_{free} test set	1992 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29179	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CA, EDO, MG, AMP, POP, NA

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	0/6242	0.45	1/8439 (0.0%)
1	C	0.25	0/6197	0.42	0/8378
2	B	0.24	0/1037	0.40	0/1394
2	D	0.24	0/1021	0.40	0/1372
All	All	0.25	0/14497	0.43	1/19583 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LEU	CB-CG-CD2	5.54	120.42	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6101	6063	6061	44	0
1	C	6056	6024	6024	24	0
2	B	1028	991	991	12	0
2	D	1012	974	974	18	0
3	A	23	12	12	0	0
3	C	23	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	0	0
4	C	18	0	0	0	0
5	A	4	0	0	0	0
5	C	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	36	54	54	3	0
7	C	16	24	24	1	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
9	A	398	0	0	0	0
9	B	37	0	0	0	0
9	C	246	0	0	2	0
9	D	9	0	0	0	0
All	All	15025	14154	14152	94	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 3.

All (94) 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:416:LEU:H	1:A:416:LEU:HD12	1.31	0.93
1:A:412:LYS:CG	1:A:416:LEU:HD11	1.99	0.93
1:A:412:LYS:HG2	1:A:416:LEU:HD11	1.64	0.78
1:A:413:SER:HA	1:A:416:LEU:HD13	1.67	0.75
1:A:130:PRO:HG2	1:A:582:THR:HG22	1.73	0.68
1:A:294:GLU:N	1:A:297:SER:O	2.27	0.68
1:A:412:LYS:HG3	1:A:416:LEU:HD11	1.75	0.68
2:B:101:ILE:HG23	2:B:138:ILE:HD11	1.77	0.67
1:A:412:LYS:C	1:A:416:LEU:CD1	2.63	0.66
2:B:32:GLU:O	2:B:36:VAL:HG23	1.96	0.66
1:A:416:LEU:HD12	1:A:416:LEU:N	2.08	0.65
1:C:804:ARG:HH21	1:C:839:ILE:HD11	1.62	0.65
2:D:99:GLY:O	2:D:137:ASN:N	2.33	0.62
1:A:412:LYS:O	1:A:416:LEU:HD12	1.99	0.62
1:A:173:LEU:HD21	1:A:213:ILE:HG23	1.84	0.59
2:B:140:GLN:OE1	2:B:140:GLN:N	2.36	0.59
1:A:495:PHE:HZ	1:A:722:VAL:HG11	1.66	0.59
1:A:226:HIS:HE2	7:A:914:EDO:HO1	1.51	0.59
2:B:6:THR:HG23	2:B:9:GLN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:PRO:HB2	1:C:550:THR:HG22	1.86	0.57
2:B:37:MET:HE1	2:B:52:LEU:HD13	1.87	0.57
2:D:87:LEU:HD11	2:D:138:ILE:CD1	2.36	0.56
1:C:348:ARG:NH1	1:C:350:GLN:OE1	2.39	0.55
1:A:413:SER:CA	1:A:416:LEU:HD13	2.35	0.55
2:D:54:ASN:O	2:D:58:VAL:HG23	2.07	0.55
2:B:20:PHE:CG	2:B:36:VAL:HG22	2.42	0.55
2:D:119:ASP:OD1	2:D:120:ALA:N	2.40	0.54
1:A:412:LYS:O	1:A:414:GLU:N	2.41	0.54
1:A:412:LYS:HG2	1:A:416:LEU:HD21	1.90	0.53
2:D:111:THR:HG22	2:D:111:THR:O	2.09	0.53
2:D:63:GLN:C	2:D:64:ILE:HD12	2.29	0.53
2:D:87:LEU:HD11	2:D:138:ILE:HD12	1.91	0.53
1:A:473:ASP:HA	1:A:476:VAL:HG22	1.92	0.52
1:C:335:SER:O	1:C:338[A]:ARG:NH2	2.42	0.52
1:A:341:MET:SD	1:A:418:ILE:CD1	2.98	0.51
1:C:291:MET:HE1	1:C:300:PHE:HE2	1.75	0.51
1:A:412:LYS:O	1:A:415:ILE:N	2.44	0.51
1:C:196:LYS:O	1:C:200:THR:HG23	2.11	0.51
1:A:495:PHE:CZ	1:A:722:VAL:HG11	2.46	0.51
1:C:837:ALA:HB2	2:D:92:VAL:HG21	1.94	0.50
1:A:412:LYS:HE2	1:A:416:LEU:HD21	1.94	0.49
1:C:230:ASN:OD1	1:C:230:ASN:N	2.45	0.49
1:A:294:GLU:O	1:A:297:SER:N	2.44	0.49
1:A:296:LEU:HD11	1:C:258:VAL:HG12	1.95	0.49
1:A:370:LYS:HB2	1:A:373:GLU:HB2	1.95	0.49
1:A:252:LYS:NZ	1:A:577:ASP:OD1	2.46	0.48
1:A:339:TYR:CE1	1:A:364:VAL:HG11	2.48	0.48
2:D:96:ASN:OD1	2:D:97:GLY:N	2.45	0.48
2:D:30:SER:HA	2:D:33:LEU:HD13	1.95	0.48
1:C:289:ASN:O	1:C:291:MET:N	2.47	0.48
1:C:460:LEU:HD21	1:C:637:GLU:HG2	1.96	0.47
1:C:436:LYS:NZ	9:C:1028:HOH:O	2.48	0.46
1:A:408:TYR:O	1:A:440:VAL:HG22	2.15	0.46
1:A:295:ARG:O	1:A:296:LEU:HB2	2.16	0.46
2:D:46:GLU:HA	2:D:49:VAL:HG12	1.98	0.46
1:C:107:ARG:NE	9:C:1020:HOH:O	2.43	0.45
2:B:101:ILE:CG2	2:B:138:ILE:HD11	2.45	0.45
1:A:411:LYS:O	1:A:412:LYS:C	2.55	0.45
1:A:676:ARG:HB3	1:A:701:ILE:HG22	1.98	0.45
1:A:412:LYS:C	1:A:416:LEU:HD11	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:O	1:A:416:LEU:CD1	2.63	0.45
2:B:94:ASP:HB2	2:B:101:ILE:HG22	1.99	0.45
1:A:705:GLU:HB3	1:A:706:PRO:HD2	1.99	0.44
2:D:70:LEU:O	2:D:70:LEU:HD12	2.17	0.44
2:D:42:LEU:HD12	2:D:42:LEU:O	2.17	0.44
2:D:59:ASP:OD1	2:D:62:HIS:HB2	2.18	0.44
1:C:672:GLU:O	1:C:676:ARG:HG3	2.17	0.43
1:C:291:MET:HE1	1:C:300:PHE:CE2	2.53	0.43
1:A:292:PHE:HE1	7:A:915:EDO:HO1	1.67	0.43
1:C:759:ASP:OD2	1:C:796:ARG:NH2	2.38	0.43
2:D:28:ILE:O	2:D:64:ILE:N	2.49	0.43
1:C:290:PRO:HB3	1:C:305:LEU:HD11	2.01	0.43
2:D:44:PRO:HB2	2:D:48:GLU:HB2	1.99	0.43
1:A:625:MET:HE2	1:A:631:LYS:CG	2.49	0.42
1:A:412:LYS:O	1:A:413:SER:C	2.57	0.42
1:A:420:ARG:HA	1:A:425:PHE:CD2	2.55	0.42
2:D:144:LEU:HD23	2:D:144:LEU:O	2.19	0.42
1:A:244:GLU:O	1:A:247:LYS:HE3	2.20	0.42
2:B:144:LEU:HD12	2:B:145:LEU:N	2.35	0.42
1:C:352:ARG:O	1:C:368:VAL:HG22	2.18	0.42
1:A:416:LEU:H	1:A:416:LEU:CD1	2.16	0.42
1:A:289:ASN:O	1:A:291:MET:N	2.47	0.42
1:A:835:THR:O	1:A:839:ILE:HG12	2.20	0.42
1:A:506:TYR:CE1	1:A:523:ILE:HG12	2.55	0.41
1:A:671:ILE:HG23	7:A:912:EDO:C2	2.50	0.41
1:C:812:GLU:OE1	2:D:38:ARG:NH2	2.38	0.41
1:C:180:ASN:O	1:C:790:GLN:NE2	2.52	0.41
2:B:81:ASP:OD1	2:B:84:GLN:N	2.51	0.41
2:B:101:ILE:HG23	2:B:138:ILE:CD1	2.46	0.41
1:C:611:GLN:OE1	1:C:674:HIS:NE2	2.53	0.41
1:A:801:PHE:CZ	2:B:16:ALA:HA	2.56	0.40
1:C:585:SER:HB2	7:C:910:EDO:H21	2.03	0.40
1:C:405:LEU:HD11	1:C:444:LYS:HB2	2.03	0.40
1:C:618:GLY:O	1:C:622:THR:HG23	2.21	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	746/873 (86%)	724 (97%)	20 (3%)	2 (0%)	41	41
1	C	742/873 (85%)	716 (96%)	26 (4%)	0	100	100
2	B	129/147 (88%)	125 (97%)	4 (3%)	0	100	100
2	D	127/147 (86%)	120 (94%)	7 (6%)	0	100	100
All	All	1744/2040 (86%)	1685 (97%)	57 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	SER
1	A	412	LYS

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	678/794 (85%)	669 (99%)	9 (1%)	69	75
1	C	674/794 (85%)	667 (99%)	7 (1%)	76	82
2	B	115/127 (91%)	114 (99%)	1 (1%)	78	84
2	D	113/127 (89%)	112 (99%)	1 (1%)	78	84
All	All	1580/1842 (86%)	1562 (99%)	18 (1%)	73	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	239	LEU
1	A	342	SER
1	A	352	ARG
1	A	386	ASP
1	A	417	GLU
1	A	420	ARG
1	A	675	PHE
1	A	685	ASP
2	B	65	GLU
1	C	212	MET
1	C	295	ARG
1	C	296	LEU
1	C	352	ARG
1	C	434	ASP
1	C	651	HIS
1	C	675	PHE
2	D	37	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 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
7	EDO	A	912	-	3,3,3	0.45	0	2,2,2	0.29	0
7	EDO	A	915	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	A	909	-	3,3,3	0.43	0	2,2,2	0.27	0
3	AMP	C	901	5	22,25,25	0.89	1 (4%)	25,38,38	1.27	3 (12%)
4	POP	C	903	5	6,8,8	0.73	0	13,13,13	1.24	1 (7%)
7	EDO	A	914	-	3,3,3	0.44	0	2,2,2	0.25	0
7	EDO	A	916	-	3,3,3	0.47	0	2,2,2	0.31	0
7	EDO	C	910	-	3,3,3	0.46	0	2,2,2	0.18	0
7	EDO	A	911	-	3,3,3	0.45	0	2,2,2	0.37	0
4	POP	C	902	5	6,8,8	0.71	0	13,13,13	1.25	2 (15%)
7	EDO	C	908	-	3,3,3	0.48	0	2,2,2	0.26	0
7	EDO	C	909	-	3,3,3	0.46	0	2,2,2	0.35	0
3	AMP	A	901	-	22,25,25	0.87	1 (4%)	25,38,38	1.25	2 (8%)
7	EDO	A	913	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	A	910	-	3,3,3	0.48	0	2,2,2	0.32	0
4	POP	A	902	5	6,8,8	0.68	0	13,13,13	1.20	1 (7%)
7	EDO	A	908	-	3,3,3	0.48	0	2,2,2	0.30	0
7	EDO	C	907	-	3,3,3	0.48	0	2,2,2	0.35	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
7	EDO	A	912	-	-	0/1/1/1	-
7	EDO	A	915	-	-	1/1/1/1	-
7	EDO	A	909	-	-	1/1/1/1	-
3	AMP	C	901	5	-	1/6/26/26	0/3/3/3
4	POP	C	903	5	-	1/6/6/6	-
7	EDO	A	914	-	-	0/1/1/1	-
7	EDO	A	916	-	-	0/1/1/1	-
7	EDO	C	910	-	-	0/1/1/1	-
7	EDO	A	911	-	-	0/1/1/1	-
4	POP	C	902	5	-	3/6/6/6	-
7	EDO	C	908	-	-	0/1/1/1	-
7	EDO	C	909	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	901	-	-	5/6/26/26	0/3/3/3
7	EDO	A	913	-	-	0/1/1/1	-
7	EDO	A	910	-	-	1/1/1/1	-
4	POP	A	902	5	-	1/6/6/6	-
7	EDO	A	908	-	-	0/1/1/1	-
7	EDO	C	907	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	AMP	C5-C4	2.36	1.47	1.40
3	A	901	AMP	C5-C4	2.30	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	AMP	N3-C2-N1	-3.92	122.55	128.68
3	C	901	AMP	N3-C2-N1	-3.80	122.74	128.68
4	C	903	POP	P2-O-P1	-3.17	121.94	132.83
4	C	902	POP	P2-O-P1	-3.00	122.53	132.83
4	A	902	POP	P2-O-P1	-2.99	122.58	132.83
3	A	901	AMP	C4-C5-N7	-2.50	106.79	109.40
3	C	901	AMP	C4-C5-N7	-2.44	106.86	109.40
3	C	901	AMP	C2-N1-C6	2.11	122.37	118.75
4	C	902	POP	O2-P1-O	2.03	111.45	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	AMP	C5'-O5'-P-O2P
3	A	901	AMP	C5'-O5'-P-O3P
3	A	901	AMP	O4'-C4'-C5'-O5'
3	A	901	AMP	C3'-C4'-C5'-O5'
4	C	902	POP	P1-O-P2-O5
7	A	915	EDO	O1-C1-C2-O2
3	C	901	AMP	C5'-O5'-P-O1P
4	A	902	POP	P1-O-P2-O4
3	A	901	AMP	C5'-O5'-P-O1P
7	A	909	EDO	O1-C1-C2-O2
7	A	910	EDO	O1-C1-C2-O2

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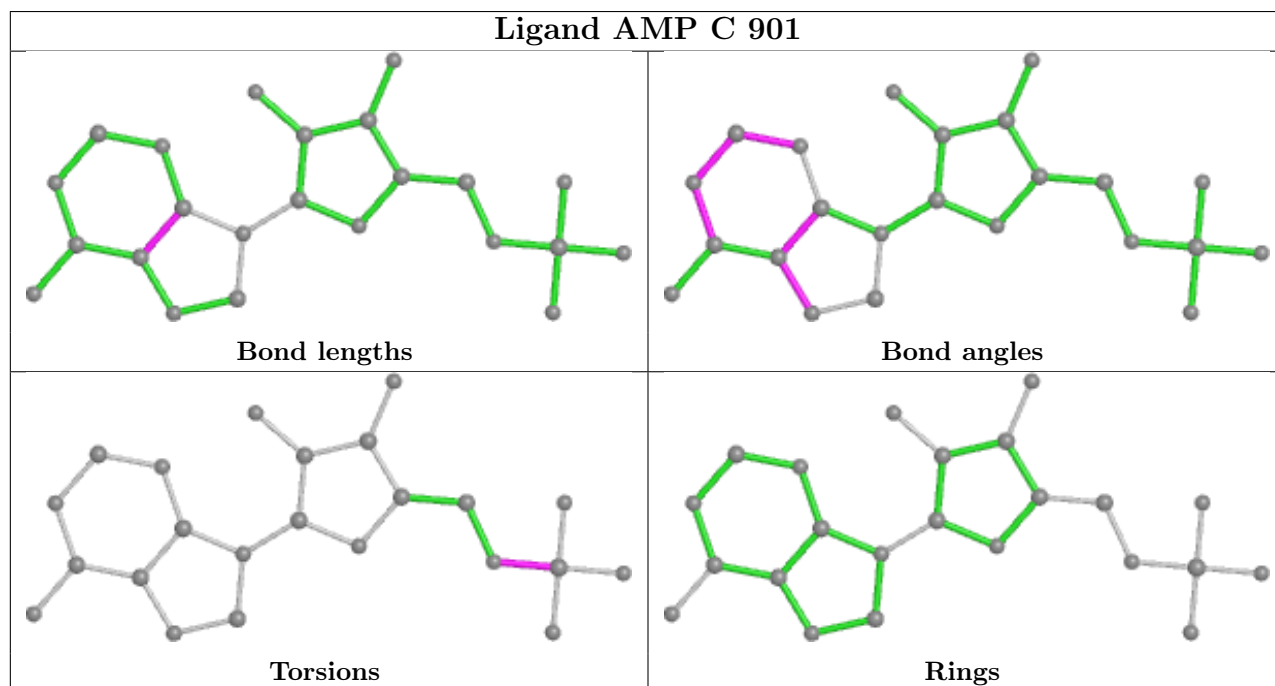
Mol	Chain	Res	Type	Atoms
4	C	902	POP	P1-O-P2-O4
4	C	902	POP	P1-O-P2-O6
4	C	903	POP	P1-O-P2-O6

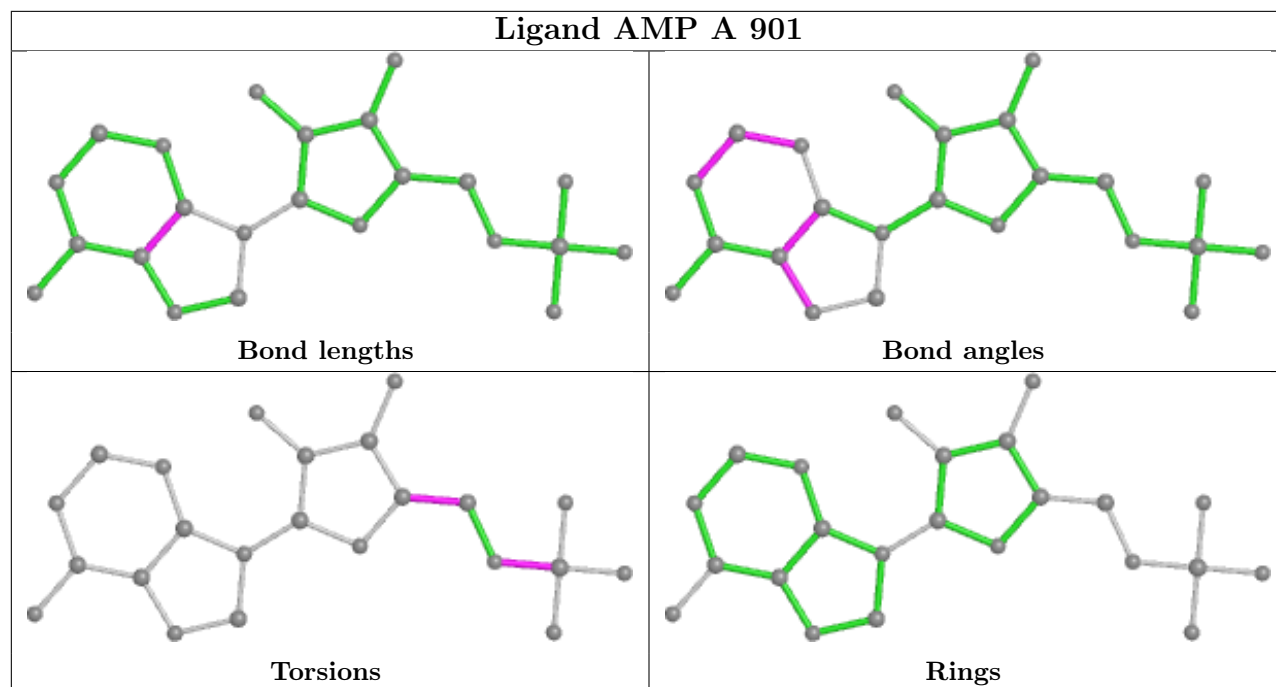
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	912	EDO	1	0
7	A	915	EDO	1	0
7	A	914	EDO	1	0
7	C	910	EDO	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 [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	748/873 (85%)	0.24	30 (4%) 38 44	8, 30, 66, 111	0
1	C	743/873 (85%)	0.64	72 (9%) 7 10	12, 44, 83, 112	0
2	B	133/147 (90%)	1.43	42 (31%) 0 0	20, 67, 97, 112	0
2	D	131/147 (89%)	3.68	98 (74%) 0 0	54, 100, 130, 138	0
All	All	1755/2040 (86%)	0.76	242 (13%) 2 4	8, 41, 98, 138	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	122	VAL	12.3
2	D	106	LEU	10.2
2	D	47	ALA	9.9
2	D	49	VAL	9.5
2	D	145	LEU	9.3
2	D	138	ILE	9.3
2	D	58	VAL	9.1
2	D	60	GLY	8.7
1	C	423	LEU	8.5
2	D	44	PRO	8.5
1	C	495	PHE	8.5
2	D	56	ILE	8.4
2	D	141	PHE	8.2
2	D	125	MET	7.8
2	D	87	LEU	7.7
2	B	122	VAL	7.0
2	D	89	ALA	6.8
1	A	495	PHE	6.6
2	B	101	ILE	6.5
2	D	142	ALA	6.3
2	D	42	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	143	ALA	6.1
2	D	61	ASN	6.0
2	D	75	ARG	5.8
2	D	121	GLU	5.7
2	D	91	LYS	5.5
2	B	58	VAL	5.5
2	D	46	GLU	5.4
2	D	104	ALA	5.4
1	C	186	ILE	5.3
2	D	52	LEU	5.3
2	D	110	LEU	5.2
2	D	92	VAL	5.0
2	B	144	LEU	5.0
2	D	144	LEU	5.0
2	D	71	ALA	4.8
2	B	5	LEU	4.8
2	D	84	GLN	4.8
1	A	844	PHE	4.7
1	A	331	GLY	4.7
1	C	125	SER	4.7
2	D	53	MET	4.7
2	D	114	GLY	4.7
2	D	69	PHE	4.6
2	D	101	ILE	4.6
2	D	73	MET	4.6
1	C	624	ASP	4.5
2	D	51	ASP	4.5
2	D	59	ASP	4.5
2	B	137	ASN	4.4
2	B	143	ALA	4.4
2	D	117	LEU	4.4
2	D	50	ASN	4.3
2	D	57	ASP	4.3
2	B	104	ALA	4.3
1	A	845	TRP	4.1
2	D	81	ASP	4.1
2	D	105	GLU	4.1
1	C	427	ARG	4.0
1	C	689	LEU	4.0
2	D	5	LEU	4.0
2	D	139	GLN	4.0
1	A	337	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	141	PHE	4.0
2	D	13	PHE	4.0
2	D	77	LEU	4.0
1	C	208	HIS	4.0
2	D	109	VAL	3.9
2	D	45	SER	3.9
2	D	113	ILE	3.9
2	D	108	HIS	3.9
2	D	95	LYS	3.9
2	D	43	SER	3.9
2	D	80	ASN	3.9
2	D	119	ASP	3.8
1	C	420	ARG	3.8
2	B	49	VAL	3.8
2	D	118	THR	3.8
1	A	332	PRO	3.8
2	D	64	ILE	3.8
2	D	17	PHE	3.8
2	D	54	ASN	3.7
2	D	103	ALA	3.7
2	D	124	ASP	3.7
1	C	832	VAL	3.7
2	D	63	GLN	3.6
2	D	30	SER	3.6
2	D	31	SER	3.6
2	B	145	LEU	3.6
2	B	51	ASP	3.6
1	C	337	PHE	3.5
2	D	10	ILE	3.5
2	B	100	LEU	3.5
1	C	498	ASP	3.5
2	D	37	MET	3.5
2	D	55	GLU	3.5
2	B	4	ASN	3.5
1	C	296	LEU	3.5
2	D	74	SER	3.5
2	D	6	THR	3.4
2	D	93	PHE	3.4
2	D	99	GLY	3.4
1	C	822	THR	3.4
1	C	207	PRO	3.4
2	B	52	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	34	ALA	3.3
1	C	626	MET	3.3
2	B	140	GLN	3.3
2	B	47	ALA	3.3
2	D	79	SER	3.3
1	C	331	GLY	3.2
2	B	87	LEU	3.2
2	D	85	GLU	3.2
2	D	9	GLN	3.2
2	D	62	HIS	3.2
1	C	494	HIS	3.2
1	C	785	PHE	3.2
1	C	839	ILE	3.2
2	D	76	GLN	3.1
2	B	136	ILE	3.1
1	A	498	ASP	3.1
2	D	116	LYS	3.1
1	A	203	ALA	3.1
1	C	378	LEU	3.1
2	D	98	ASP	3.1
2	D	111	THR	3.1
1	C	772	ILE	3.1
2	D	107	LYS	3.0
1	A	335	SER	3.0
2	B	61	ASN	3.0
2	D	140	GLN	3.0
2	B	142	ALA	3.0
2	B	120	ALA	3.0
2	D	78	LYS	3.0
1	C	496	GLY	3.0
1	C	294	GLU	2.9
2	B	60	GLY	2.9
2	B	95	LYS	2.9
2	B	102	SER	2.9
1	C	837	ALA	2.9
1	C	424	ASP	2.9
2	D	86	LEU	2.9
1	C	333	ILE	2.9
2	B	77	LEU	2.9
2	D	72	LEU	2.9
1	C	419	SER	2.9
1	C	784	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	499	GLU	2.8
2	D	88	GLU	2.8
1	C	347	LEU	2.8
1	C	438	LEU	2.8
2	B	139	GLN	2.8
1	C	813	ALA	2.8
2	B	124	ASP	2.8
2	D	123	ASP	2.8
1	A	334	ASP	2.7
1	A	423	LEU	2.7
1	C	332	PRO	2.7
1	A	344	ASP	2.7
1	A	205	LYS	2.7
1	C	421	GLY	2.7
1	C	393	ARG	2.7
1	C	203	ALA	2.7
1	A	333	ILE	2.7
2	D	48	GLU	2.6
1	A	345	ARG	2.6
1	A	499	GLU	2.6
1	C	329	GLU	2.6
2	D	83	GLU	2.6
1	C	410	VAL	2.6
2	D	120	ALA	2.6
2	D	35	THR	2.6
1	C	361	ASN	2.6
2	B	54	ASN	2.6
2	B	83	GLU	2.6
1	C	806	VAL	2.5
1	C	693	THR	2.5
2	D	40	LEU	2.5
1	C	204	SER	2.5
2	B	45	SER	2.5
2	D	96	ASN	2.5
1	C	788	VAL	2.4
1	C	328	LYS	2.4
2	D	68	GLU	2.4
1	C	699	TYR	2.4
1	A	371	LYS	2.4
1	C	213	ILE	2.4
2	B	74	SER	2.4
1	C	426	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	713	LYS	2.3
2	D	146	SER	2.3
1	C	675	PHE	2.3
1	A	496	GLY	2.3
2	B	118	THR	2.3
1	C	416	LEU	2.3
2	B	117	LEU	2.3
1	C	330	LYS	2.3
1	A	777	ILE	2.3
1	C	344	ASP	2.3
1	C	692	ASP	2.3
2	D	112	SER	2.3
1	C	345	ARG	2.3
1	C	335	SER	2.3
1	A	341	MET	2.2
1	C	627	ASP	2.2
1	C	716	SER	2.2
1	C	371	LYS	2.2
2	B	56	ILE	2.2
2	B	84	GLN	2.2
1	A	207	PRO	2.2
1	A	329	GLU	2.2
1	A	298	THR	2.2
1	C	198	LEU	2.2
1	C	773	LEU	2.2
2	D	22	LYS	2.2
2	D	70	LEU	2.2
2	B	89	ALA	2.2
1	C	196	LYS	2.2
1	A	186	ILE	2.1
2	B	78	LYS	2.1
2	B	125	MET	2.1
1	C	833	ALA	2.1
1	A	99	VAL	2.1
2	B	75	ARG	2.1
1	A	204	SER	2.1
1	A	418	ILE	2.1
1	C	346	LEU	2.1
1	C	436	LYS	2.1
2	D	97	GLY	2.1
2	B	44	PRO	2.1
1	A	646	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	341	MET	2.0
1	C	428	PHE	2.0
1	A	420	ARG	2.0
1	C	836	ASN	2.0
2	B	82	SER	2.0
1	C	202	LEU	2.0
1	A	747	ALA	2.0
1	C	829	PHE	2.0
2	D	90	PHE	2.0
1	C	821	PRO	2.0
1	C	779	THR	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, 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(Å ²)	Q<0.9
5	MG	A	903	1/1	0.63	0.16	46,46,46,46	0
8	CA	D	201	1/1	0.69	0.11	81,81,81,81	0
7	EDO	A	915	4/4	0.75	0.24	55,66,76,82	0
7	EDO	A	910	4/4	0.75	0.25	41,57,68,68	0
6	NA	B	203	1/1	0.76	0.18	49,49,49,49	0
8	CA	D	202	1/1	0.76	0.11	104,104,104,104	0
4	POP	C	903	9/9	0.78	0.25	56,66,82,91	0
7	EDO	A	914	4/4	0.81	0.24	40,53,64,69	0
7	EDO	C	908	4/4	0.84	0.21	37,45,53,59	0
8	CA	B	202	1/1	0.84	0.17	101,101,101,101	0
5	MG	A	906	1/1	0.85	0.42	76,76,76,76	0
5	MG	C	904	1/1	0.86	0.10	41,41,41,41	0

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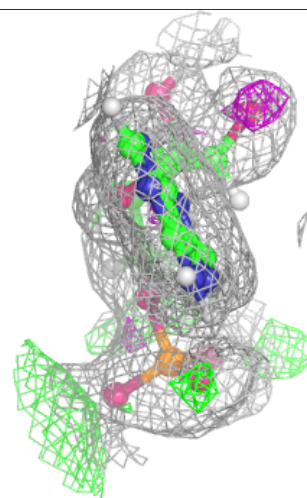
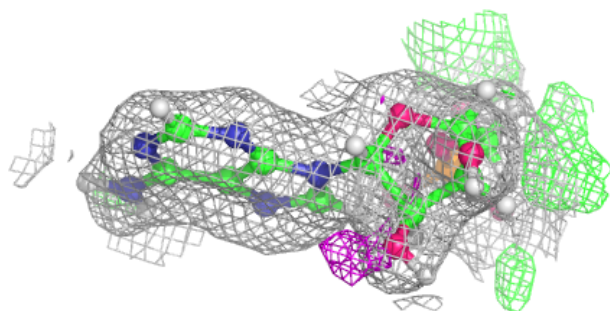
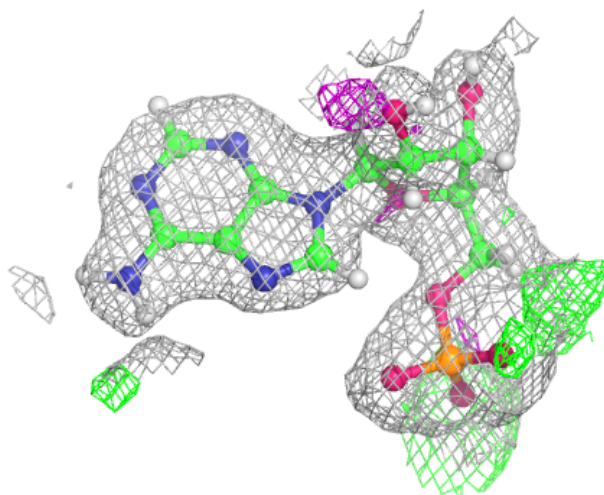
Continued from previous page...

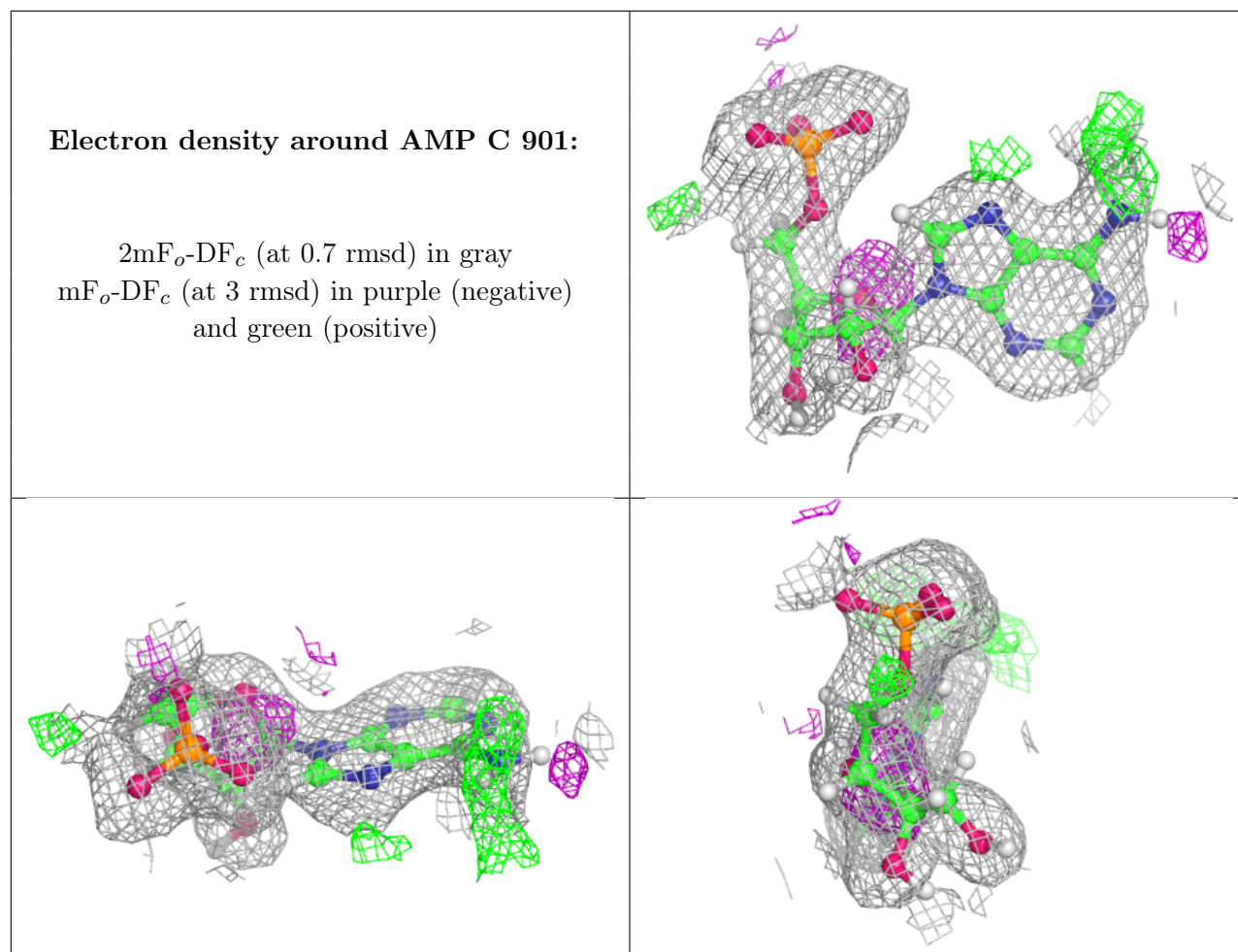
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	906	1/1	0.87	0.20	50,50,50,50	0
7	EDO	A	913	4/4	0.90	0.15	27,49,67,67	0
4	POP	A	902	9/9	0.90	0.14	48,59,70,77	0
7	EDO	C	909	4/4	0.90	0.12	38,54,58,65	0
5	MG	A	905	1/1	0.91	0.09	50,50,50,50	0
7	EDO	C	910	4/4	0.92	0.18	9,31,41,50	0
4	POP	C	902	9/9	0.92	0.16	54,63,81,81	0
3	AMP	A	901	23/23	0.93	0.14	8,23,68,75	0
3	AMP	C	901	23/23	0.93	0.13	7,31,55,89	0
5	MG	A	904	1/1	0.93	0.16	35,35,35,35	0
7	EDO	A	916	4/4	0.93	0.15	26,43,52,56	0
7	EDO	A	912	4/4	0.93	0.15	32,46,60,72	0
7	EDO	A	911	4/4	0.95	0.24	32,49,64,64	0
7	EDO	A	909	4/4	0.96	0.20	23,32,49,59	0
7	EDO	A	908	4/4	0.96	0.12	23,28,35,42	0
7	EDO	C	907	4/4	0.96	0.13	22,30,36,38	0
8	CA	B	201	1/1	0.97	0.07	55,55,55,55	0
6	NA	A	907	1/1	0.97	0.26	39,39,39,39	0
5	MG	C	905	1/1	0.98	0.06	45,45,45,45	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 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.