



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:47 AM UTC

PDB ID : 6OQQ / pdb_00006oqq
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

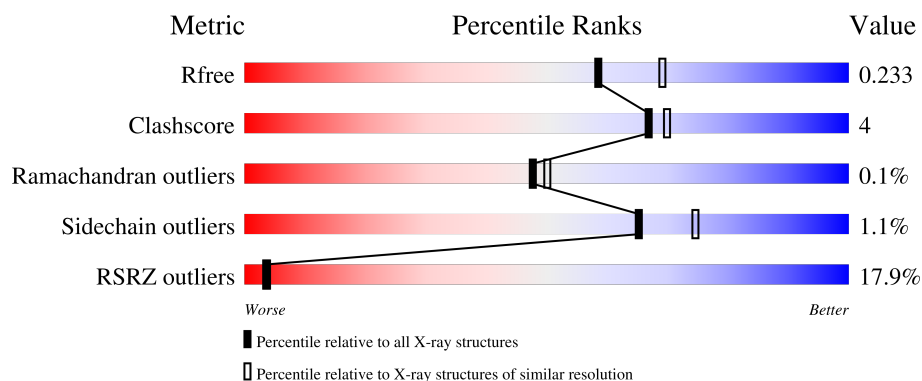
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	
1	C	873	
2	B	147	
2	D	147	

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.

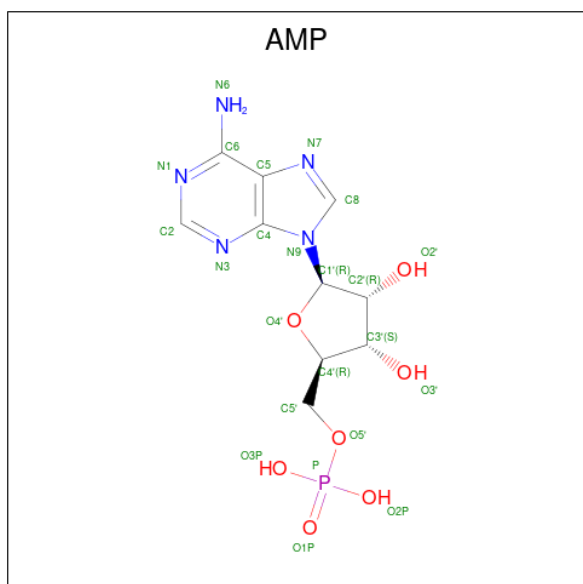
- Molecule 1 is a protein called Legionella pneumophila SidJ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
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.

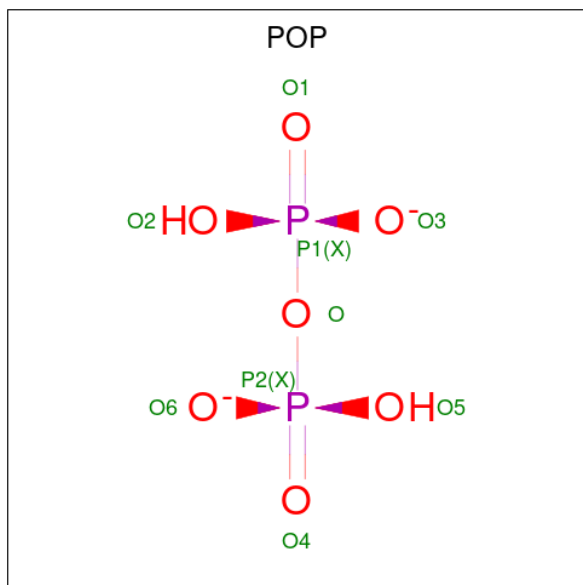
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	133	Total	C	H	N	O	S	0	0	0
			2019	639	991	165	220	4			
2	D	131	Total	C	H	N	O	S	0	0	0
			1986	629	974	162	217	4			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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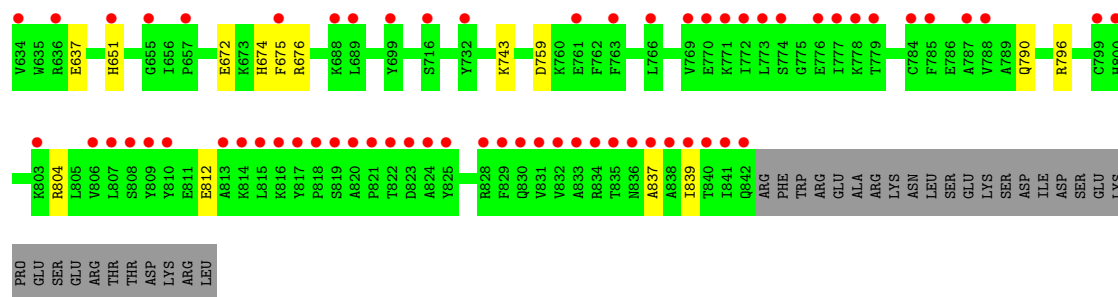
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

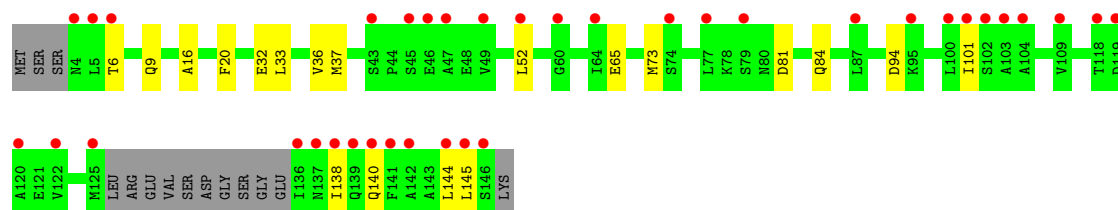
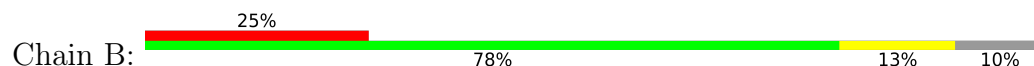
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	D	2	Total	Ca	0	0
			2	2		

- 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		



• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



4 Data and refinement statistics

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)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.234 0.203 , 0.233	Depositor DCC
R_{free} test set	1992 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
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

Xtriage'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, MG, POP, NA, EDO, 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	0.15	0/6242	0.33	0/8439
1	C	0.12	0/6197	0.30	0/8378
2	B	0.09	0/1037	0.28	0/1394
2	D	0.11	0/1021	0.30	0/1372
All	All	0.13	0/14497	0.31	0/19583

There are no bond length outliers.

There are no bond angle outliers.

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	46	0
1	C	6056	6024	6024	27	0
2	B	1028	991	991	17	0
2	D	1012	974	974	18	0
3	A	23	12	12	0	0
3	C	23	12	12	0	0
4	A	9	0	0	0	0
4	C	18	0	0	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	104	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 4.

All (104) 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
2:B:37:MET:HE1	2:B:52:LEU:HD13	1.61	0.82
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:412:LYS:C	1:A:416:LEU:CD1	2.63	0.71
2:B:33:LEU:HG	2:B:37:MET:HE3	1.75	0.69
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
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
1:A:626:MET:HA	1:A:626:MET:HE2	1.80	0.64
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
2:B:37:MET:HE2	2:B:73:MET:HE1	1.83	0.61
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
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)
2:D:63:GLN:C	2:D:64:ILE:HD12	2.29	0.58
1:C:291:MET:HE2	1:C:300:PHE:CE2	2.39	0.58
1:C:548:PRO:HB2	1:C:550:THR:HG22	1.86	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: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
2:D:111:THR:HG22	2:D:111:THR:O	2.09	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:411:LYS:O	1:A:412:LYS:C	2.55	0.50
1:A:412:LYS:C	1:A:416:LEU:HD11	2.37	0.49
1:C:291:MET:HE2	1:C:300:PHE:CD2	2.47	0.49
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
2:B:37:MET:CE	2:B:73:MET:HE1	2.42	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:A:412:LYS:O	1:A:413:SER:C	2.57	0.47
2:B:37:MET:HE1	2:B:52:LEU:CD1	2.37	0.47
1:C:460:LEU:HD21	1:C:637:GLU:HG2	1.96	0.47
1:A:752:ILE:HG22	1:A:756:MET:HE2	1.97	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:C:229:LYS:NZ	1:C:285:ASP:OD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:O	1:A:296:LEU:HB2	2.16	0.46
1:A:341:MET:HE3	1:A:418:ILE:HD13	1.97	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:676:ARG:HB3	1:A:701:ILE:HG22	1.98	0.45
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: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:420:ARG:HA	1:A:425:PHE:CD2	2.55	0.42
1:A:625:MET:HE2	1:A:631:LYS:CG	2.49	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:226:HIS:NE2	7:A:914:EDO:O1	2.48	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
1:C:295:ARG:C	1:C:297:SER:H	2.28	0.41
2:B:37:MET:HE2	2:B:73:MET:CE	2.48	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:C:291:MET:HE1	1:C:743:LYS:NZ	2.35	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%)	36	36
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%)	48	50

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%)	668 (98%)	10 (2%)	57	65
1	C	674/794 (85%)	668 (99%)	6 (1%)	70	78
2	B	115/127 (91%)	114 (99%)	1 (1%)	70	78
2	D	113/127 (89%)	112 (99%)	1 (1%)	70	78
All	All	1580/1842 (86%)	1562 (99%)	18 (1%)	65	74

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

Mol	Chain	Res	Type
1	A	99	VAL
1	A	183	THR
1	A	239	LEU
1	A	294	GLU
1	A	342	SER
1	A	386	ASP
1	A	417	GLU
1	A	420	ARG
1	A	675	PHE
1	A	714	LEU
2	B	65	GLU
1	C	213	ILE
1	C	295	ARG
1	C	296	LEU
1	C	352	ARG
1	C	651	HIS
1	C	675	PHE
2	D	37	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	ASN
1	A	601	ASN
2	B	63	GLN
1	C	141	ASN
1	C	166	GLN
1	C	208	HIS
1	C	259	GLN
1	C	398	HIS

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 [i](#)

There are no oligosaccharides 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
4	POP	C	903	5	6,8,8	0.75	0	12,13,13	0.91	0
3	AMP	A	901	-	25,25,25	1.35	4 (16%)	37,38,38	2.00	10 (27%)
7	EDO	A	914	-	3,3,3	0.41	0	2,2,2	0.30	0
7	EDO	A	908	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	C	908	-	3,3,3	0.45	0	2,2,2	0.31	0
4	POP	C	902	5	6,8,8	0.73	0	12,13,13	0.97	1 (8%)
7	EDO	A	913	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	A	915	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	C	907	-	3,3,3	0.44	0	2,2,2	0.40	0
7	EDO	C	910	-	3,3,3	0.43	0	2,2,2	0.23	0
7	EDO	A	910	-	3,3,3	0.45	0	2,2,2	0.36	0
7	EDO	A	909	-	3,3,3	0.40	0	2,2,2	0.32	0
3	AMP	C	901	5	25,25,25	1.38	4 (16%)	37,38,38	1.93	10 (27%)
7	EDO	A	911	-	3,3,3	0.42	0	2,2,2	0.41	0
7	EDO	A	916	-	3,3,3	0.44	0	2,2,2	0.35	0
4	POP	A	902	5	6,8,8	0.70	0	12,13,13	0.91	0
7	EDO	C	909	-	3,3,3	0.43	0	2,2,2	0.39	0
7	EDO	A	912	-	3,3,3	0.42	0	2,2,2	0.33	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
4	POP	C	903	5	-	1/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	901	-	-	5/10/26/26	0/3/3/3
7	EDO	A	914	-	-	0/1/1/1	-
7	EDO	A	908	-	-	0/1/1/1	-
7	EDO	C	908	-	-	0/1/1/1	-
4	POP	C	902	5	-	3/6/6/6	-
7	EDO	A	913	-	-	0/1/1/1	-
7	EDO	A	915	-	-	1/1/1/1	-
7	EDO	C	907	-	-	0/1/1/1	-
7	EDO	C	910	-	-	0/1/1/1	-
7	EDO	A	910	-	-	1/1/1/1	-
7	EDO	A	909	-	-	1/1/1/1	-
3	AMP	C	901	5	-	1/10/26/26	0/3/3/3
7	EDO	A	911	-	-	0/1/1/1	-
7	EDO	A	916	-	-	0/1/1/1	-
4	POP	A	902	5	-	1/6/6/6	-
7	EDO	C	909	-	-	0/1/1/1	-
7	EDO	A	912	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	AMP	C5-C4	4.53	1.47	1.39
3	A	901	AMP	C5-C4	4.44	1.47	1.39
3	C	901	AMP	C5-C6	2.67	1.48	1.41
3	A	901	AMP	C5-C6	2.56	1.48	1.41
3	C	901	AMP	C8-N7	2.43	1.36	1.31
3	A	901	AMP	C5-N7	-2.31	1.34	1.39
3	A	901	AMP	C8-N7	2.31	1.36	1.31
3	C	901	AMP	C5-N7	-2.19	1.35	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	AMP	C5-C4-N3	-5.96	118.51	126.72
3	C	901	AMP	C5-C4-N3	-5.55	119.08	126.72
3	A	901	AMP	N3-C4-N9	4.87	135.46	127.17
3	C	901	AMP	N3-C4-N9	4.54	134.89	127.17
3	A	901	AMP	C2-N3-C4	4.08	121.79	111.83
3	A	901	AMP	N3-C2-N1	-3.98	122.55	128.58
3	C	901	AMP	N3-C2-N1	-3.86	122.74	128.58
3	C	901	AMP	C2-N3-C4	3.83	121.19	111.83
3	A	901	AMP	C4-C5-N7	-3.32	106.79	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	AMP	C4-C5-N7	-3.26	106.86	110.58
3	C	901	AMP	C4-N9-C8	3.13	109.02	105.74
3	A	901	AMP	C4-N9-C8	3.00	108.89	105.74
3	A	901	AMP	C5-N7-C8	2.78	107.82	103.45
3	C	901	AMP	C5-N7-C8	2.68	107.66	103.45
3	C	901	AMP	N9-C8-N7	-2.47	110.43	113.94
3	A	901	AMP	N9-C8-N7	-2.45	110.47	113.94
3	C	901	AMP	C6-C5-N7	2.24	136.40	132.09
3	C	901	AMP	C2-N1-C6	2.21	122.37	118.73
3	A	901	AMP	C6-C5-N7	2.17	136.27	132.09
3	A	901	AMP	C2-N1-C6	2.03	122.07	118.73
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'
4	C	902	POP	P1-O-P2-O5
3	A	901	AMP	C3'-C4'-C5'-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	910	EDO	O1-C1-C2-O2
7	A	909	EDO	O1-C1-C2-O2
4	C	902	POP	P1-O-P2-O4
4	C	902	POP	P1-O-P2-O6
4	C	903	POP	P1-O-P2-O6

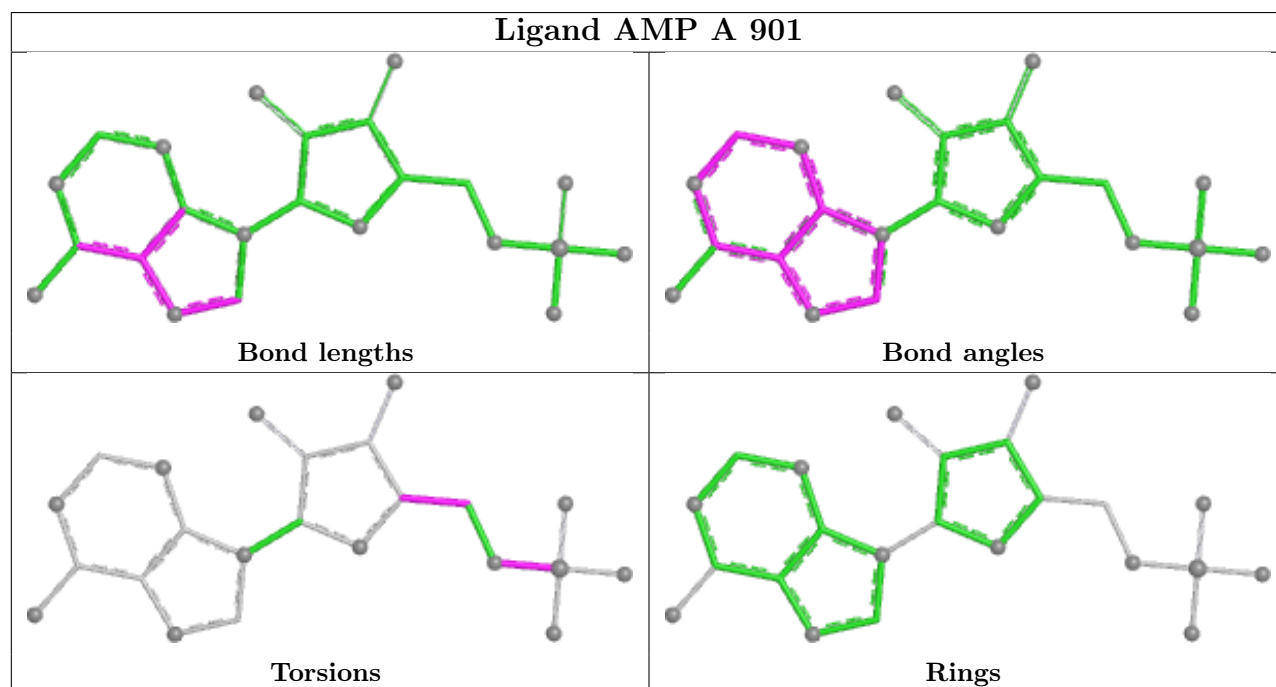
There are no ring outliers.

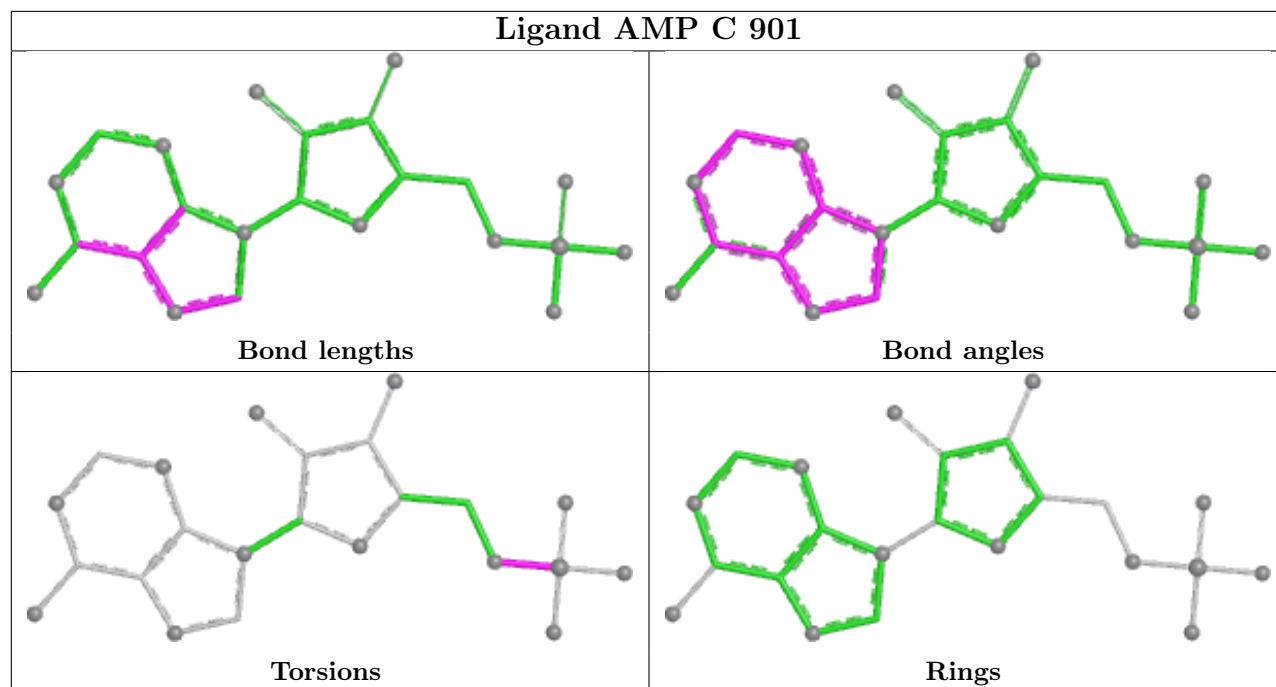
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	914	EDO	1	0
7	C	910	EDO	1	0
7	A	912	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	748/873 (85%)	0.09	50 (6%) 24 25	9, 33, 72, 121	0
1	C	743/873 (85%)	0.88	125 (16%) 4 4	13, 48, 91, 127	1 (0%)
2	B	133/147 (90%)	1.34	37 (27%) 1 1	22, 75, 106, 125	0
2	D	131/147 (89%)	3.21	102 (77%) 0 0	60, 109, 142, 151	0
All	All	1755/2040 (86%)	0.75	314 (17%) 3 4	9, 45, 108, 151	1 (0%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	106	LEU	7.7
1	C	495	PHE	7.2
1	A	495	PHE	7.2
2	D	138	ILE	7.2
2	D	122	VAL	7.1
2	D	141	PHE	6.8
1	A	337	PHE	6.6
2	D	113	ILE	6.4
2	D	109	VAL	6.1
2	D	5	LEU	5.9
2	B	122	VAL	5.9
1	C	785	PHE	5.7
2	D	89	ALA	5.6
1	C	337	PHE	5.5
2	D	42	LEU	5.4
2	D	117	LEU	5.4
2	D	111	THR	5.4
2	D	47	ALA	5.2
2	B	101	ILE	5.1
1	C	815	LEU	5.0
2	D	145	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	331	GLY	4.9
2	D	104	ALA	4.9
2	D	107	LYS	4.9
2	D	56	ILE	4.8
2	D	125	MET	4.8
1	C	813	ALA	4.8
2	D	6	THR	4.6
1	C	423	LEU	4.6
1	C	832	VAL	4.6
1	A	845	TRP	4.6
2	D	105	GLU	4.5
2	D	74	SER	4.5
2	D	93	PHE	4.5
2	D	92	VAL	4.5
1	C	840	THR	4.4
2	D	90	PHE	4.4
2	D	110	LEU	4.4
1	A	332	PRO	4.3
1	C	806	VAL	4.3
1	C	839	ILE	4.3
2	D	44	PRO	4.3
2	D	69	PHE	4.2
2	B	5	LEU	4.2
2	D	53	MET	4.2
1	C	773	LEU	4.2
1	A	335	SER	4.2
2	D	13	PHE	4.2
2	D	95	LYS	4.1
1	C	822	THR	4.1
2	D	118	THR	4.1
1	C	627	ASP	4.1
2	D	100	LEU	4.1
2	D	97	GLY	4.0
2	B	136	ILE	4.0
2	D	137	ASN	4.0
1	C	784	CYS	4.0
1	A	496	GLY	4.0
1	C	296	LEU	4.0
1	C	626	MET	4.0
1	C	496	GLY	4.0
2	D	91	LYS	3.9
1	A	777	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	835	THR	3.9
2	D	43	SER	3.9
2	D	146	SER	3.9
1	C	498	ASP	3.8
2	D	114	GLY	3.8
2	B	125	MET	3.8
2	D	64	ILE	3.8
2	D	101	ILE	3.8
1	A	330	LYS	3.8
2	B	137	ASN	3.7
2	D	17	PHE	3.7
1	C	809	TYR	3.7
2	D	142	ALA	3.7
2	D	49	VAL	3.7
2	D	116	LYS	3.7
2	D	52	LEU	3.6
1	C	494	HIS	3.6
1	C	836	ASN	3.6
2	D	115	GLU	3.6
2	D	22	LYS	3.6
1	C	778	LYS	3.6
2	D	73	MET	3.6
1	C	777	ILE	3.6
2	D	28	ILE	3.6
1	C	183	THR	3.6
2	B	138	ILE	3.5
1	C	208	HIS	3.5
1	C	818	PRO	3.5
1	C	332	PRO	3.5
2	D	9	GLN	3.5
2	D	40	LEU	3.5
1	A	436	LYS	3.5
1	C	633	ALA	3.4
2	D	87	LEU	3.4
2	D	57	ASP	3.4
1	C	817	TYR	3.4
2	D	76	GLN	3.4
1	C	788	VAL	3.4
2	D	37	MET	3.4
2	D	102	SER	3.4
2	D	86	LEU	3.4
2	B	142	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	330	LYS	3.4
1	C	810	TYR	3.3
2	D	103	ALA	3.3
2	D	62	HIS	3.3
1	A	427	ARG	3.3
1	C	624	ASP	3.3
1	C	833	ALA	3.3
1	A	99	VAL	3.3
2	D	16	ALA	3.3
2	D	143	ALA	3.3
1	A	295	ARG	3.3
2	B	52	LEU	3.3
2	D	144	LEU	3.3
1	C	774	SER	3.2
2	B	146	SER	3.2
1	C	820	ALA	3.2
2	D	32	GLU	3.2
1	C	819	SER	3.2
1	C	766	LEU	3.2
2	D	68	GLU	3.2
2	B	4	ASN	3.2
1	C	807	LEU	3.2
1	C	829	PHE	3.2
2	D	120	ALA	3.1
2	D	60	GLY	3.1
2	D	63	GLN	3.1
2	D	71	ALA	3.1
2	D	50	ASN	3.1
2	B	47	ALA	3.1
1	C	655	GLY	3.0
1	A	376	SER	3.0
1	C	186	ILE	3.0
1	C	841	ILE	3.0
1	A	339	TYR	3.0
1	A	334	ASP	3.0
1	C	459	ASP	3.0
2	D	34	ALA	3.0
1	C	209	VAL	3.0
1	C	831	VAL	3.0
2	D	124	ASP	3.0
2	D	108	HIS	3.0
1	C	634	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	72	LEU	3.0
1	C	213	ILE	3.0
2	D	41	GLY	3.0
2	D	35	THR	3.0
2	D	119	ASP	3.0
1	C	808	SER	2.9
1	C	543	LEU	2.9
1	A	498	ASP	2.9
2	D	96	ASN	2.9
2	D	58	VAL	2.9
1	C	816	LYS	2.9
1	C	493	THR	2.9
1	C	716	SER	2.9
2	D	59	ASP	2.8
1	C	770	GLU	2.8
2	D	121	GLU	2.8
1	C	331	GLY	2.8
2	D	78	LYS	2.8
1	C	675	PHE	2.8
1	C	630	LYS	2.8
1	A	435	SER	2.8
2	D	75	ARG	2.8
1	C	830	GLN	2.8
1	A	291	MET	2.8
2	B	104	ALA	2.8
1	A	423	LEU	2.8
1	A	163	ILE	2.8
1	C	163	ILE	2.8
1	C	651	HIS	2.7
1	C	803	LYS	2.7
1	A	203	ALA	2.7
1	A	844	PHE	2.7
1	C	689	LEU	2.7
1	C	657	PRO	2.7
1	A	208	HIS	2.7
2	D	70	LEU	2.7
1	C	761	GLU	2.7
1	C	776	GLU	2.6
2	B	103	ALA	2.6
2	D	139	GLN	2.6
1	C	294	GLU	2.6
2	B	43	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	699	TYR	2.6
2	D	99	GLY	2.6
2	B	120	ALA	2.6
2	B	144	LEU	2.6
1	A	352	ARG	2.6
1	C	427	ARG	2.6
1	C	629	PRO	2.6
2	D	45	SER	2.6
2	D	15	GLU	2.5
1	C	291	MET	2.5
1	C	842	GLN	2.5
2	D	11	ALA	2.5
2	D	112	SER	2.5
2	D	140	GLN	2.5
1	A	294	GLU	2.5
2	B	141	PHE	2.5
1	A	350	GLN	2.5
2	D	46	GLU	2.5
1	C	125	SER	2.5
2	B	74	SER	2.5
2	B	102	SER	2.5
2	D	30	SER	2.5
1	C	824	ALA	2.5
1	A	160	LEU	2.5
1	A	434	ASP	2.4
2	B	46	GLU	2.4
1	C	799	CYS	2.4
1	C	295	ARG	2.4
1	C	425	PHE	2.4
1	C	499	GLU	2.4
2	B	109	VAL	2.4
1	C	821	PRO	2.4
1	A	494	HIS	2.4
2	D	77	LEU	2.4
2	B	118	THR	2.4
1	C	347	LEU	2.4
1	C	614	LEU	2.4
1	C	161	ASN	2.4
2	B	60	GLY	2.4
2	D	66	PHE	2.4
1	A	333	ILE	2.4
1	C	333	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	772	ILE	2.4
1	C	341	MET	2.4
1	C	628	LYS	2.4
1	A	372	GLY	2.3
1	C	106	ARG	2.3
1	C	763	PHE	2.3
1	A	343	SER	2.3
1	A	703	SER	2.3
2	B	45	SER	2.3
2	D	7	GLU	2.3
1	C	837	ALA	2.3
2	B	77	LEU	2.3
2	D	51	ASP	2.3
1	A	341	MET	2.3
2	D	20	PHE	2.3
2	B	64	ILE	2.3
1	C	621	VAL	2.3
1	A	183	THR	2.3
1	A	340	GLN	2.3
1	C	359	PRO	2.3
1	C	360	GLN	2.3
1	C	424	ASP	2.3
1	C	437	ASP	2.3
2	B	139	GLN	2.3
2	B	100	LEU	2.3
1	C	800	HIS	2.2
1	A	418	ILE	2.2
1	A	209	VAL	2.2
1	C	828	ARG	2.2
1	C	160	LEU	2.2
1	C	834	ARG	2.2
1	A	205	LYS	2.2
1	C	625	MET	2.2
1	C	501	GLU	2.2
1	A	296	LEU	2.2
2	B	140	GLN	2.2
1	A	336	SER	2.2
1	A	393	ARG	2.2
1	C	361	ASN	2.2
1	C	779	THR	2.2
1	A	347	LEU	2.2
1	C	378	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	617	TYR	2.2
1	C	732	TYR	2.2
1	C	825	TYR	2.2
1	C	371	LYS	2.2
1	A	424	ASP	2.2
2	D	12	GLU	2.1
1	C	203	ALA	2.1
1	C	838	ALA	2.1
1	C	636	ARG	2.1
1	C	434	ASP	2.1
1	C	823	ASP	2.1
1	A	377	THR	2.1
1	A	839	ILE	2.1
2	D	10	ILE	2.1
1	C	769	VAL	2.1
1	A	778	LYS	2.1
1	C	336	SER	2.1
2	B	87	LEU	2.1
2	D	33	LEU	2.1
1	C	340	GLN	2.1
1	A	428	PHE	2.1
1	C	688	LYS	2.1
2	B	119	ASP	2.1
2	D	98	ASP	2.1
1	C	339	TYR	2.1
2	B	6	THR	2.1
1	C	814	LYS	2.1
2	B	95	LYS	2.1
1	C	410	VAL	2.1
1	C	284	GLU	2.0
1	C	787	ALA	2.1
2	B	79	SER	2.1
2	D	82	SER	2.1
1	C	458	GLN	2.0
2	B	49	VAL	2.0
2	D	55	GLU	2.0
1	C	343	SER	2.0
2	B	145	LEU	2.0
1	C	344	ASP	2.0
1	A	127	ARG	2.0
1	C	771	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	915	4/4	0.69	0.23	55,66,76,82	0
4	POP	C	903	9/9	0.70	0.13	56,66,82,91	0
7	EDO	A	910	4/4	0.72	0.25	41,57,68,68	0
7	EDO	A	914	4/4	0.73	0.25	40,53,64,69	0
6	NA	B	203	1/1	0.73	0.15	49,49,49,49	0
8	CA	D	202	1/1	0.74	0.13	104,104,104,104	0
4	POP	A	902	9/9	0.78	0.14	48,59,70,77	0
8	CA	B	202	1/1	0.78	0.11	101,101,101,101	0
4	POP	C	902	9/9	0.78	0.13	54,63,81,81	0
8	CA	D	201	1/1	0.80	0.11	81,81,81,81	0
5	MG	A	903	1/1	0.82	0.12	46,46,46,46	0
5	MG	A	906	1/1	0.83	0.56	76,76,76,76	0
7	EDO	C	908	4/4	0.86	0.20	37,45,53,59	0
7	EDO	A	911	4/4	0.89	0.14	32,49,64,64	0
3	AMP	A	901	23/23	0.90	0.12	8,23,68,75	0
7	EDO	A	912	4/4	0.90	0.12	32,46,60,72	0
7	EDO	A	916	4/4	0.91	0.11	26,43,52,56	0
7	EDO	C	909	4/4	0.91	0.10	38,54,58,65	0
7	EDO	C	910	4/4	0.91	0.12	9,31,41,50	0
7	EDO	A	913	4/4	0.92	0.10	27,49,67,67	0
6	NA	A	907	1/1	0.92	0.24	39,39,39,39	0
5	MG	C	904	1/1	0.93	0.11	41,41,41,41	0
5	MG	A	904	1/1	0.93	0.09	35,35,35,35	0
7	EDO	C	907	4/4	0.93	0.07	22,30,36,38	0
3	AMP	C	901	23/23	0.94	0.09	7,31,55,89	0
7	EDO	A	908	4/4	0.94	0.07	23,28,35,42	0
5	MG	A	905	1/1	0.95	0.09	50,50,50,50	0

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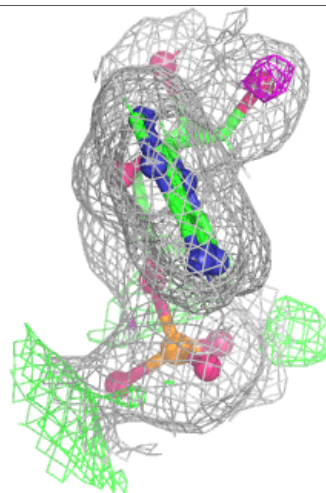
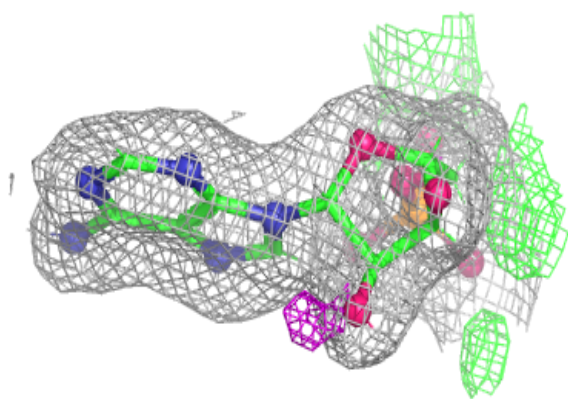
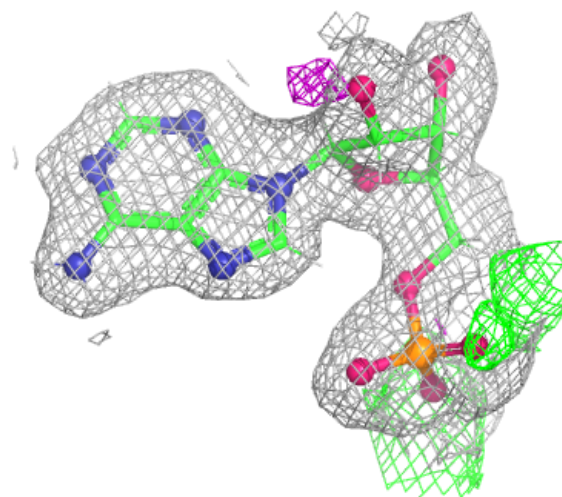
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	909	4/4	0.95	0.12	23,32,49,59	0
5	MG	C	906	1/1	0.96	0.19	50,50,50,50	0
8	CA	B	201	1/1	0.97	0.07	55,55,55,55	0
5	MG	C	905	1/1	0.97	0.09	45,45,45,45	0

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.

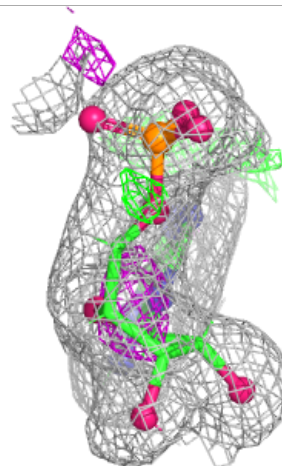
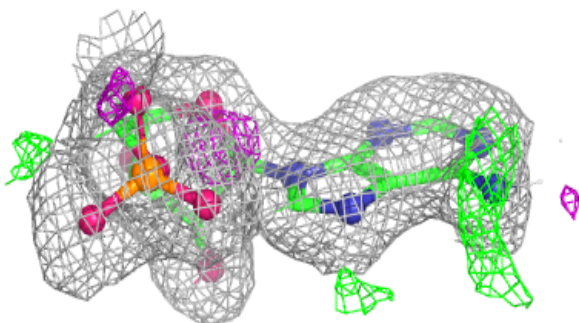
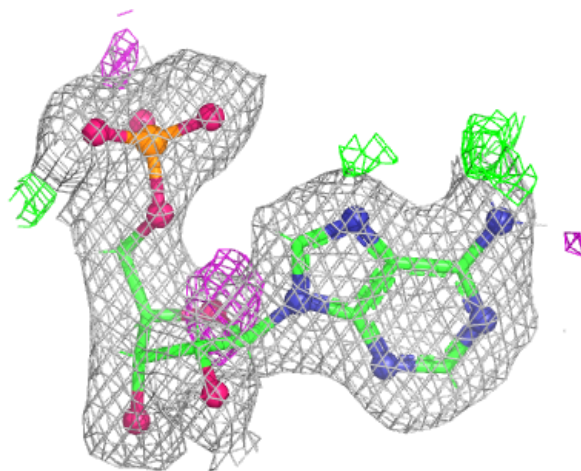
Electron density around AMP A 901:

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



Electron density around AMP C 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.