Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:15 pm BST

PDB ID	:	3WVR
Title	:	Structure of ATP grasp protein with AMP
Authors	:	Matsui, T.; Noike, M.; Ooya, K.; Sasaki, I.; Hamano, Y.; Maruyama, C.; Ishikawa, J.; Satoh, Y.; Ito, H.; Dairi, T.; Morita, H.
Deposited on	:	2014-06-04
Resolution	:	2.17 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

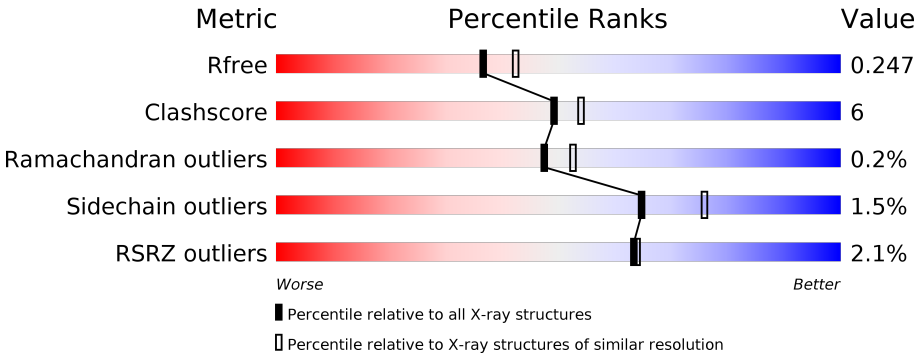
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	447	3% 85% 10%
1	B	447	3% 83% 12%
1	C	447	83% 14%
1	D	447	% 83% 9% 7%

2 Entry composition

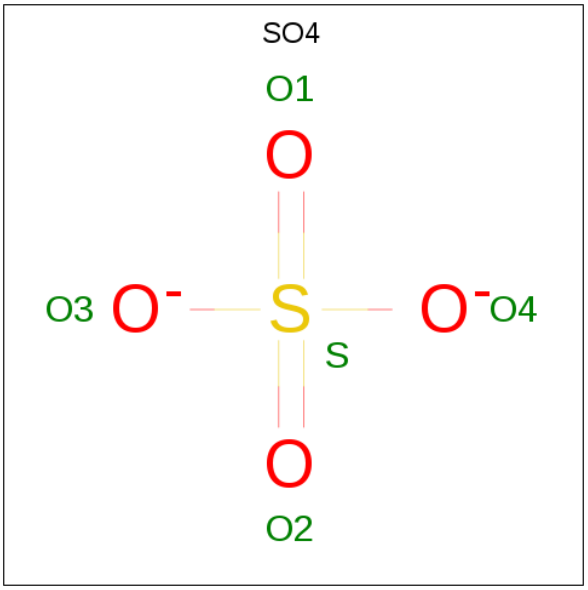
There are 5 unique types of molecules in this entry. The entry contains 13581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PGM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	Se	0	0	0
			3244	2040	594	602	4	4			
1	B	430	Total	C	N	O	S	Se	0	0	0
			3274	2058	603	605	4	4			
1	C	433	Total	C	N	O	S	Se	0	0	0
			3304	2079	609	608	4	4			
1	D	415	Total	C	N	O	S	Se	0	0	0
			3152	1982	580	582	4	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			

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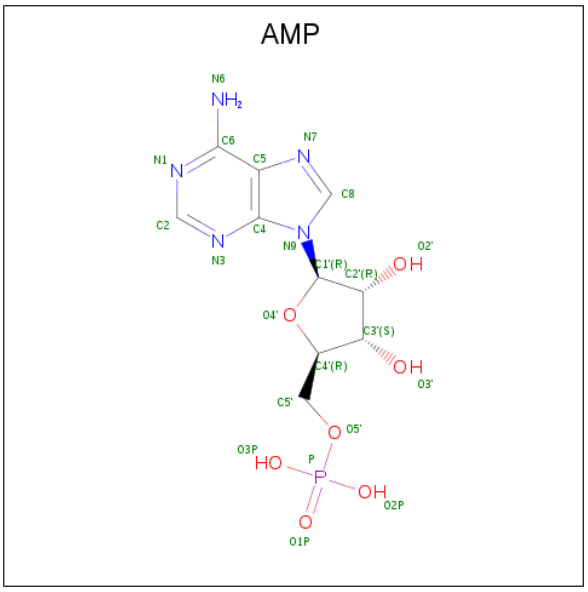
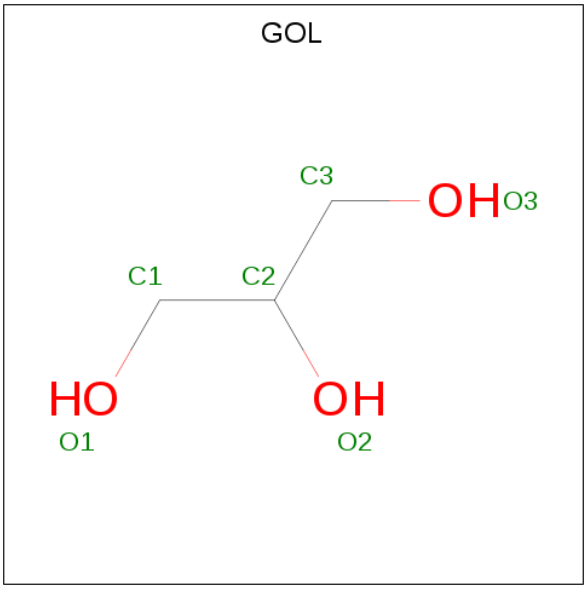
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O		0	0
			6	3	3			

- Molecule 5 is water.

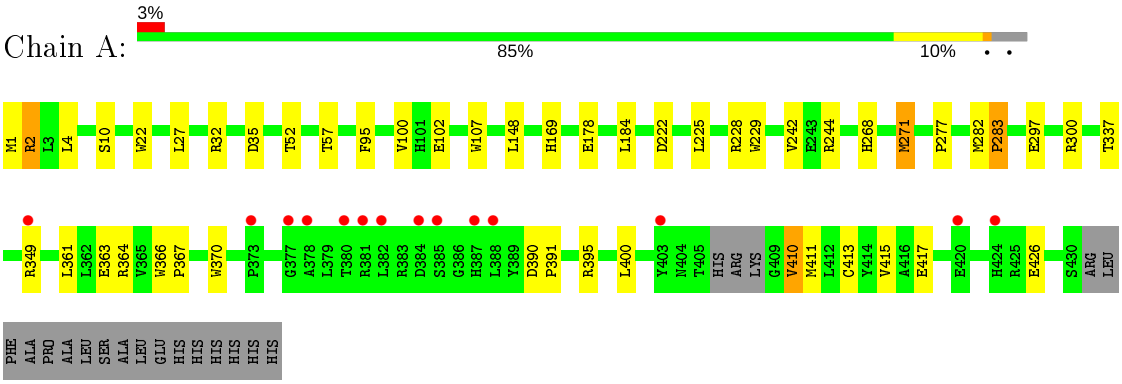
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	106	Total O 106 106	0	0
5	B	107	Total O 107 107	0	0
5	C	120	Total O 120 120	0	0
5	D	114	Total O 114 114	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

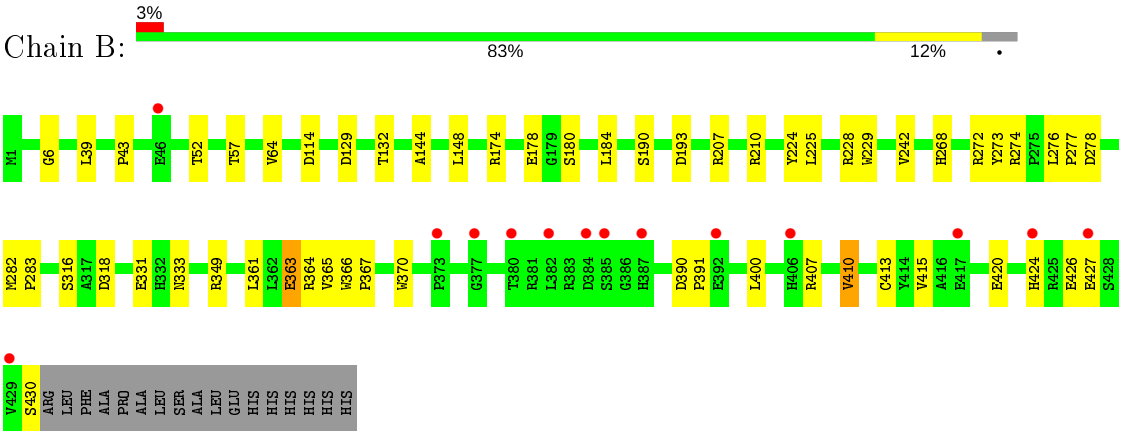
- Molecule 1: PGM1

Chain A:



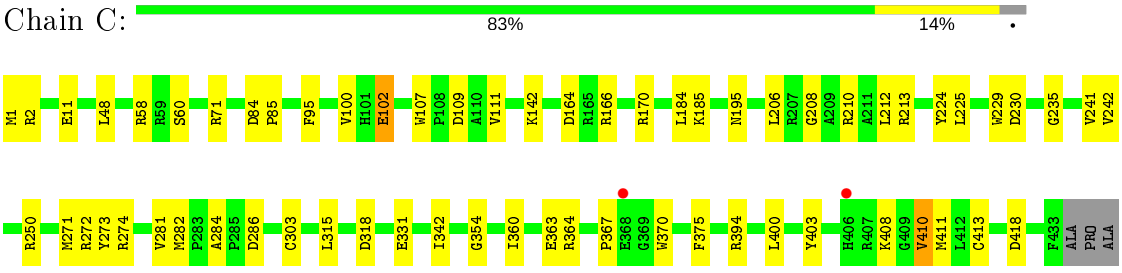
- Molecule 1: PGM1

Chain B:



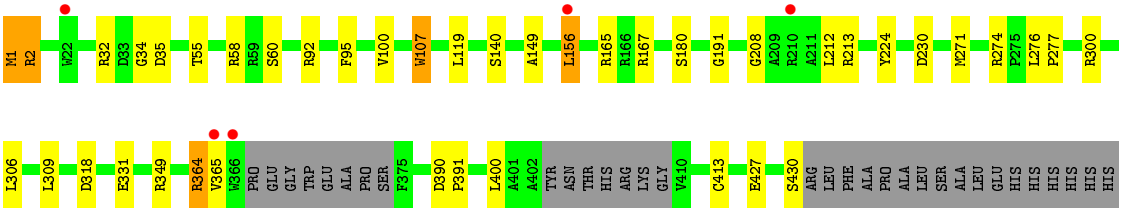
- Molecule 1: PGM1

Chain C:



- Molecule 1: PGM1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.60Å 86.72Å 94.14Å 73.87° 86.06° 68.23°	Depositor
Resolution (Å)	45.18 – 2.17 45.18 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.18-2.17) 97.0 (45.18-2.17)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.246 0.204 , 0.247	Depositor DCC
R_{free} test set	5582 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13581	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.50	1/3315 (0.0%)	0.58	2/4508 (0.0%)
1	B	0.47	0/3347	0.56	1/4551 (0.0%)
1	C	0.48	0/3378	0.57	1/4592 (0.0%)
1	D	0.45	0/3217	0.57	1/4370 (0.0%)
All	All	0.48	1/13257 (0.0%)	0.57	5/18021 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	PRO	N-CD	5.24	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	284	ALA	C-N-CD	5.86	140.70	128.40
1	B	282	MSE	C-N-CD	5.49	139.92	128.40
1	A	271	MSE	N-CA-CB	-5.44	100.81	110.60
1	D	2	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	282	MSE	C-N-CD	5.08	139.07	128.40

There are no chirality outliers.

There are no planarity outliers.

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	3244	0	3184	35	0
1	B	3274	0	3218	38	0
1	C	3304	0	3251	52	0
1	D	3152	0	3109	29	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	30	0	0	1	0
2	D	25	0	0	1	0
3	B	23	0	12	0	0
3	C	23	0	12	2	0
3	D	23	0	12	2	0
4	D	6	0	8	0	0
5	A	106	0	0	2	0
5	B	107	0	0	0	0
5	C	120	0	0	1	0
5	D	114	0	0	3	0
All	All	13581	0	12806	153	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 6.

All (153) 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:271:MSE:HE3	1:A:277:PRO:CB	1.74	1.17
1:A:271:MSE:HE3	1:A:277:PRO:HB2	1.14	1.14
1:A:271:MSE:CE	1:A:277:PRO:HB2	1.84	1.08
1:C:1:MSE:HE2	1:C:95:PHE:CD1	1.88	1.07
1:C:1:MSE:CE	1:C:95:PHE:CD1	2.43	1.01
1:C:2:ARG:HG2	1:C:102:GLU:HG2	1.50	0.93
1:C:272:ARG:HD2	1:C:281:VAL:HG23	1.56	0.87
1:D:271:MSE:HE2	1:D:277:PRO:HB2	1.57	0.86
1:C:282:MSE:HE1	1:C:342:ILE:HG21	1.66	0.78
1:C:1:MSE:HE1	1:C:95:PHE:CD1	2.19	0.76
1:C:410:VAL:HG23	1:C:411:MSE:N	2.02	0.75
1:A:271:MSE:HE3	1:A:277:PRO:HB3	1.67	0.75
1:B:366:TRP:O	1:B:407:ARG:NH2	2.21	0.73
1:C:274:ARG:HH21	1:C:364:ARG:HH22	1.37	0.72
1:C:272:ARG:HD2	1:C:281:VAL:CG2	2.21	0.71
1:C:1:MSE:HE2	1:C:95:PHE:HD1	1.48	0.70
1:B:272:ARG:HH12	1:B:274:ARG:HH11	1.41	0.68
1:A:2:ARG:HG2	1:A:102:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:OE2	1:A:300:ARG:NH1	2.27	0.67
1:C:58:ARG:NH1	1:C:60:SER:OG	2.27	0.67
1:D:55:THR:O	1:D:349:ARG:NH2	2.27	0.66
1:D:271:MSE:HE2	1:D:277:PRO:CB	2.26	0.66
1:B:193:ASP:HA	1:B:210:ARG:HG3	1.79	0.65
1:C:410:VAL:HG23	1:C:411:MSE:H	1.62	0.63
1:C:318:ASP:HB2	1:C:331:GLU:HG3	1.80	0.63
1:C:11:GLU:OE2	1:C:71:ARG:NH2	2.26	0.63
1:C:2:ARG:HD2	5:C:678:HOH:O	1.99	0.62
1:B:272:ARG:NH1	1:B:274:ARG:HD3	2.16	0.61
1:B:272:ARG:CZ	1:B:274:ARG:HD3	2.31	0.60
1:D:300:ARG:NE	5:D:625:HOH:O	2.34	0.60
1:C:400:LEU:HD11	1:C:413:CYS:HB2	1.83	0.60
1:A:1:MSE:HE2	1:A:95:PHE:CD1	2.37	0.59
1:A:349:ARG:NH1	5:A:625:HOH:O	2.29	0.58
1:B:400:LEU:HD11	1:B:413:CYS:HB2	1.86	0.57
1:D:58:ARG:NH1	1:D:60:SER:OG	2.38	0.57
1:C:271:MSE:HE3	1:C:273:TYR:CE1	2.40	0.56
1:A:1:MSE:CE	1:A:95:PHE:CD1	2.89	0.55
1:A:2:ARG:CG	1:A:102:GLU:HB3	2.36	0.55
1:C:375:PHE:HB2	1:C:403:TYR:HB2	1.88	0.55
1:A:268:HIS:CE1	1:A:283:PRO:HB2	2.42	0.54
1:A:2:ARG:HB2	1:A:35:ASP:OD1	2.07	0.54
1:D:2:ARG:HH11	1:D:32:ARG:NH2	2.06	0.54
1:D:58:ARG:NH2	5:D:669:HOH:O	2.38	0.53
1:B:193:ASP:HA	1:B:210:ARG:CG	2.38	0.53
1:A:22:TRP:HH2	1:A:411:MSE:CE	2.22	0.53
1:C:184:LEU:HD22	1:C:242:VAL:HG22	1.89	0.52
1:A:364:ARG:HD2	1:A:426:GLU:OE2	2.09	0.52
1:C:282:MSE:CE	1:C:342:ILE:HG21	2.39	0.52
1:D:2:ARG:NH1	1:D:32:ARG:NH2	2.57	0.52
1:D:167:ARG:NH2	5:D:619:HOH:O	2.43	0.52
1:A:349:ARG:HD3	5:A:699:HOH:O	2.10	0.51
1:A:400:LEU:HD11	1:A:413:CYS:HB2	1.90	0.51
1:C:282:MSE:HE1	1:C:342:ILE:CG2	2.36	0.51
1:A:367:PRO:HB2	1:A:370:TRP:CD1	2.46	0.51
1:C:195:ASN:O	1:C:210:ARG:HG2	2.11	0.51
1:C:2:ARG:HG2	1:C:102:GLU:CG	2.34	0.51
1:C:230:ASP:OD1	1:C:235:GLY:HA2	2.11	0.51
1:B:184:LEU:HD22	1:B:242:VAL:HG22	1.93	0.51
1:D:1:MSE:HE2	1:D:95:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:O	1:B:229:TRP:HB2	2.11	0.51
1:D:191:GLY:HA2	3:D:506:AMP:O3P	2.11	0.50
1:C:58:ARG:HG3	2:C:501:SO4:O3	2.11	0.50
1:D:213:ARG:HG3	1:D:224:TYR:CE1	2.46	0.50
1:D:92:ARG:HH21	1:D:119:LEU:HA	1.76	0.50
1:B:367:PRO:HB2	1:B:370:TRP:CD1	2.46	0.49
1:B:318:ASP:HB2	1:B:331:GLU:HG2	1.94	0.49
1:B:364:ARG:HD2	1:B:426:GLU:OE1	2.12	0.49
1:C:225:LEU:O	1:C:229:TRP:HB2	2.12	0.49
1:D:107:TRP:HZ2	1:D:140:SER:HG	1.60	0.48
1:B:274:ARG:NH1	1:B:364:ARG:HH22	2.11	0.48
1:C:1:MSE:CE	1:C:95:PHE:CG	2.95	0.48
1:A:337:THR:HB	2:A:503:SO4:O1	2.12	0.48
1:C:1:MSE:HE1	1:C:100:VAL:HG22	1.96	0.48
1:C:367:PRO:HG2	1:C:370:TRP:CG	2.49	0.48
1:C:354:GLY:HA3	1:C:394:ARG:HH21	1.79	0.47
1:B:361:LEU:HD22	1:B:415:VAL:HG22	1.95	0.47
1:B:424:HIS:HA	1:B:427:GLU:OE1	2.14	0.47
1:C:208:GLY:HA3	3:C:507:AMP:O4'	2.14	0.47
1:B:114:ASP:OD2	1:C:170:ARG:NH2	2.47	0.47
1:C:1:MSE:HE1	1:C:95:PHE:CE1	2.49	0.47
1:A:22:TRP:HH2	1:A:411:MSE:HE3	1.79	0.47
1:B:427:GLU:O	1:B:430:SER:OG	2.31	0.47
1:C:185:LYS:HB2	1:C:241:VAL:HB	1.97	0.46
1:C:213:ARG:HG3	1:C:224:TYR:CE1	2.50	0.46
1:D:1:MSE:HB3	1:D:34:GLY:O	2.15	0.46
1:C:206:LEU:HD21	1:C:212:LEU:HB2	1.96	0.46
1:B:268:HIS:CE1	1:B:283:PRO:HB3	2.50	0.46
1:C:360:ILE:HG12	1:C:418:ASP:HA	1.97	0.46
1:A:225:LEU:O	1:A:229:TRP:HB2	2.15	0.46
1:B:174:ARG:O	1:B:178:GLU:HG3	2.16	0.46
1:A:184:LEU:HD22	1:A:242:VAL:HG22	1.98	0.45
1:A:395:ARG:NH1	1:A:417:GLU:HG3	2.32	0.45
1:D:364:ARG:HG3	1:D:365:VAL:H	1.81	0.45
1:A:361:LEU:CD2	1:A:415:VAL:HG22	2.47	0.45
1:A:22:TRP:CH2	1:A:411:MSE:HE3	2.52	0.45
1:B:420:GLU:H	1:B:420:GLU:CD	2.19	0.45
1:B:272:ARG:NH2	1:B:274:ARG:CD	2.81	0.44
1:C:142:LYS:HD3	1:C:185:LYS:HD3	1.99	0.44
1:D:306:LEU:HD23	1:D:309:LEU:HD21	1.98	0.44
1:B:363:GLU:HG3	1:B:400:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:HG2	1:C:364:ARG:N	2.33	0.44
1:B:316:SER:HB3	1:B:333:ASN:HB2	1.99	0.44
1:D:400:LEU:HD11	1:D:413:CYS:HB2	2.00	0.44
1:D:208:GLY:HA3	3:D:506:AMP:O4'	2.18	0.44
1:B:225:LEU:HA	1:B:225:LEU:HD23	1.84	0.44
1:D:2:ARG:NH1	1:D:32:ARG:CZ	2.81	0.44
1:B:364:ARG:HG2	1:B:365:VAL:O	2.17	0.43
1:B:52:THR:HB	1:B:57:THR:O	2.18	0.43
1:B:390:ASP:HA	1:B:391:PRO:HD3	1.82	0.43
1:D:364:ARG:HG3	1:D:365:VAL:N	2.33	0.43
1:C:331:GLU:OE2	3:C:507:AMP:H5'1	2.19	0.43
1:C:109:ASP:OD2	1:C:111:VAL:HG22	2.19	0.43
1:A:32:ARG:NH1	1:A:349:ARG:HH22	2.16	0.43
1:B:144:ALA:O	1:B:148:LEU:HG	2.18	0.43
1:C:271:MSE:HE3	1:C:273:TYR:CZ	2.53	0.43
1:D:274:ARG:HD3	1:D:274:ARG:HA	1.81	0.43
1:A:1:MSE:HE1	1:A:100:VAL:HG22	2.01	0.43
1:C:408:LYS:HA	1:C:408:LYS:HD2	1.57	0.43
1:C:84:ASP:HA	1:C:85:PRO:HD2	1.87	0.43
1:C:274:ARG:HH21	1:C:364:ARG:NH2	2.11	0.42
1:D:165:ARG:NH2	2:D:501:SO4:O4	2.50	0.42
1:A:4:LEU:HB3	1:A:27:LEU:HD11	2.00	0.42
1:A:10:SER:HB2	1:A:107:TRP:CZ3	2.54	0.42
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.89	0.42
1:B:43:PRO:HD2	1:B:64:VAL:HG11	2.02	0.42
1:C:250:ARG:HH22	1:C:286:ASP:CB	2.33	0.42
1:C:411:MSE:HB2	1:C:411:MSE:HE3	1.73	0.42
1:B:129:ASP:O	1:B:132:THR:OG1	2.31	0.42
1:B:272:ARG:NH2	1:B:274:ARG:HD2	2.35	0.42
1:A:169:HIS:CD2	1:A:222:ASP:OD1	2.73	0.42
1:C:2:ARG:HE	1:C:102:GLU:CD	2.23	0.42
1:A:178:GLU:OE1	1:A:244:ARG:NH2	2.52	0.42
1:B:276:LEU:HD12	1:B:278:ASP:HB3	2.01	0.41
1:B:6:GLY:HA3	1:B:39:LEU:HD23	2.01	0.41
1:A:395:ARG:HH12	1:A:417:GLU:CD	2.24	0.41
1:D:1:MSE:HE1	1:D:100:VAL:HG22	2.02	0.41
1:A:366:TRP:HB2	1:A:410:VAL:O	2.20	0.41
1:B:364:ARG:NH1	1:B:426:GLU:OE2	2.54	0.41
1:C:164:ASP:OD2	1:C:166:ARG:HB3	2.20	0.41
1:A:228:ARG:HA	1:A:228:ARG:HD2	1.95	0.41
1:C:367:PRO:HG2	1:C:370:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TYR:CE1	1:B:228:ARG:HG3	2.56	0.41
1:D:318:ASP:HB2	1:D:331:GLU:HG2	2.02	0.41
1:D:390:ASP:HA	1:D:391:PRO:HD2	1.94	0.41
1:B:207:ARG:HH21	1:B:273:TYR:HB2	1.86	0.41
1:C:274:ARG:NH2	1:C:364:ARG:HH22	2.11	0.41
1:B:276:LEU:CD1	1:B:278:ASP:HB3	2.51	0.40
1:C:303:CYS:SG	1:C:315:LEU:HD12	2.61	0.40
1:B:272:ARG:O	1:B:277:PRO:HA	2.21	0.40
1:D:1:MSE:HB2	1:D:35:ASP:HA	2.02	0.40
1:D:427:GLU:O	1:D:430:SER:HB2	2.22	0.40
1:A:52:THR:HB	1:A:57:THR:O	2.22	0.40
1:D:149:ALA:HB3	1:D:156:LEU:HD23	2.04	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	423/447 (95%)	412 (97%)	10 (2%)	1 (0%)	47	52
1	B	428/447 (96%)	412 (96%)	15 (4%)	1 (0%)	47	52
1	C	431/447 (96%)	418 (97%)	12 (3%)	1 (0%)	47	52
1	D	409/447 (92%)	401 (98%)	8 (2%)	0	100	100
All	All	1691/1788 (95%)	1643 (97%)	45 (3%)	3 (0%)	47	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	410	VAL
1	B	410	VAL
1	A	410	VAL

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	324/337 (96%)	321 (99%)	3 (1%)	78	87
1	B	327/337 (97%)	322 (98%)	5 (2%)	65	76
1	C	330/337 (98%)	327 (99%)	3 (1%)	78	87
1	D	315/337 (94%)	307 (98%)	8 (2%)	47	57
All	All	1296/1348 (96%)	1277 (98%)	19 (2%)	65	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	148	LEU
1	A	363	GLU
1	B	180	SER
1	B	190	SER
1	B	349	ARG
1	B	363	GLU
1	B	410	VAL
1	C	48	LEU
1	C	102	GLU
1	C	107	TRP
1	D	1	MSE
1	D	107	TRP
1	D	156	LEU
1	D	180	SER
1	D	212	LEU
1	D	230	ASP
1	D	276	LEU
1	D	364	ARG

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

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 carbohydrates in this entry.

5.6 Ligand geometry

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	D	507	-	5,5,5	0.41	0	5,5,5	0.68	0
3	AMP	B	504	-	22,25,25	0.92	2 (9%)	25,38,38	1.23	4 (16%)
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	D	502	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	C	503	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	D	503	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	A	503	-	4,4,4	0.32	0	6,6,6	0.51	0
2	SO4	B	503	-	4,4,4	0.08	0	6,6,6	0.25	0
3	AMP	D	506	-	22,25,25	1.16	2 (9%)	25,38,38	1.36	3 (12%)
2	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.27	0
2	SO4	C	502	-	4,4,4	0.17	0	6,6,6	0.11	0
3	AMP	C	507	-	22,25,25	0.91	2 (9%)	25,38,38	1.27	2 (8%)
2	SO4	C	506	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.35	0
2	SO4	C	501	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	D	505	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	505	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	C	504	-	4,4,4	0.12	0	6,6,6	0.19	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	504	-	-	5/6/26/26	0/3/3/3
3	AMP	D	506	-	-	3/6/26/26	0/3/3/3
3	AMP	C	507	-	-	3/6/26/26	0/3/3/3
4	GOL	D	507	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	507	AMP	C5-C4	2.55	1.47	1.40
3	B	504	AMP	C5-C4	2.46	1.47	1.40
3	D	506	AMP	C5-N7	-2.21	1.31	1.39
3	B	504	AMP	C2-N3	2.20	1.35	1.32
3	D	506	AMP	C4-N3	-2.11	1.32	1.35
3	C	507	AMP	C2-N3	2.04	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	507	AMP	N3-C2-N1	-3.32	123.48	128.68
3	B	504	AMP	N3-C2-N1	-3.13	123.79	128.68
3	C	507	AMP	C4-C5-N7	-2.97	106.30	109.40
3	D	506	AMP	N3-C2-N1	-2.79	124.33	128.68
3	B	504	AMP	C4-C5-N7	-2.51	106.78	109.40
3	D	506	AMP	O3P-P-O2P	2.26	116.29	107.64
3	B	504	AMP	O2P-P-O5'	-2.10	101.16	106.73
3	D	506	AMP	C4-C5-N7	-2.09	107.22	109.40
3	B	504	AMP	O3P-P-O2P	2.01	115.30	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	507	GOL	O1-C1-C2-C3
3	B	504	AMP	C5'-O5'-P-O1P
3	B	504	AMP	C5'-O5'-P-O2P
3	B	504	AMP	C5'-O5'-P-O3P
3	D	506	AMP	C3'-C4'-C5'-O5'
3	C	507	AMP	C3'-C4'-C5'-O5'
3	D	506	AMP	O4'-C4'-C5'-O5'
3	C	507	AMP	O4'-C4'-C5'-O5'
4	D	507	GOL	O1-C1-C2-O2
3	C	507	AMP	C4'-C5'-O5'-P
3	B	504	AMP	C4'-C5'-O5'-P
3	B	504	AMP	O4'-C4'-C5'-O5'
3	D	506	AMP	C4'-C5'-O5'-P

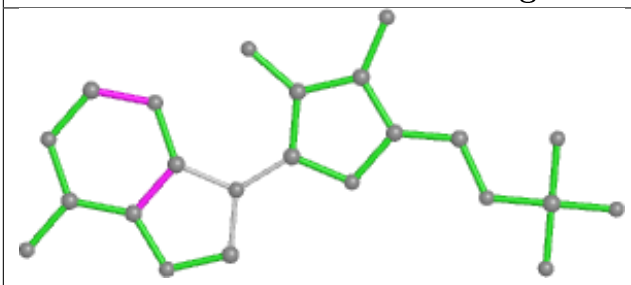
There are no ring outliers.

5 monomers are involved in 7 short contacts:

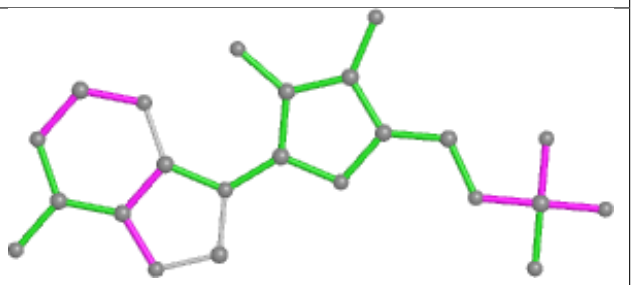
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	SO4	1	0
3	D	506	AMP	2	0
3	C	507	AMP	2	0
2	C	501	SO4	1	0
2	D	501	SO4	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

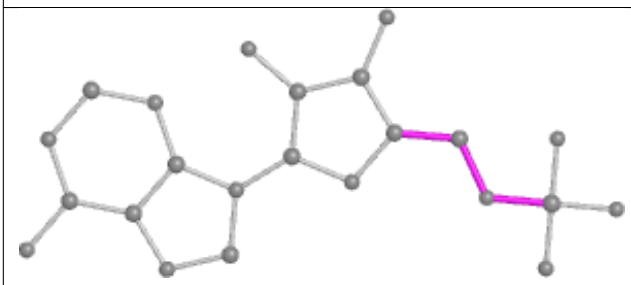
Ligand AMP B 504



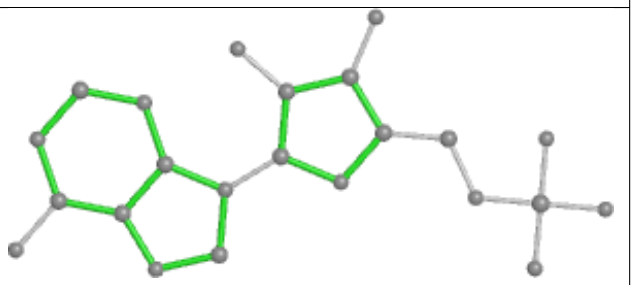
Bond lengths



Bond angles

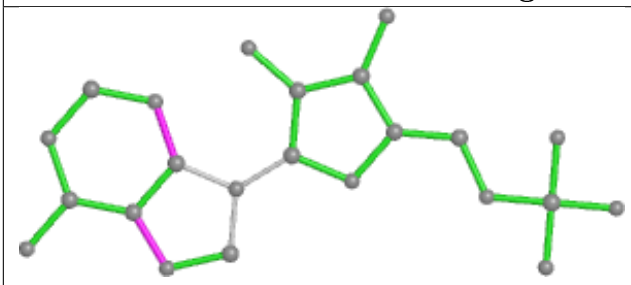


Torsions

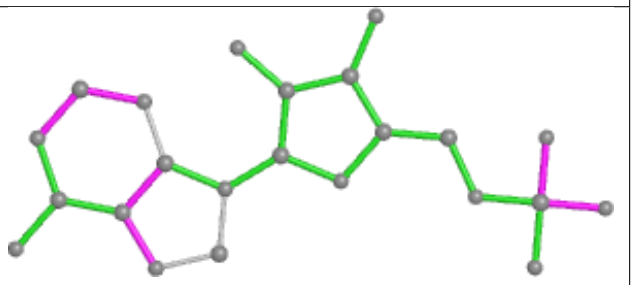


Rings

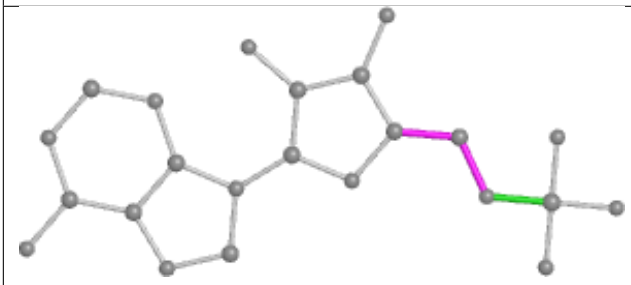
Ligand AMP D 506



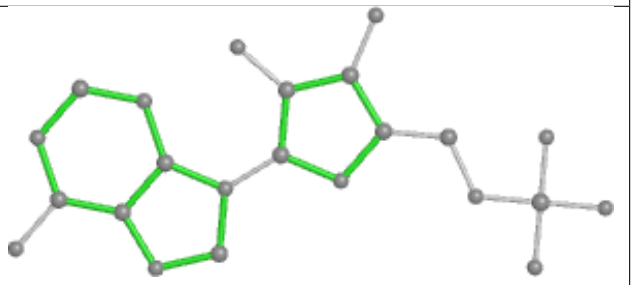
Bond lengths



Bond angles

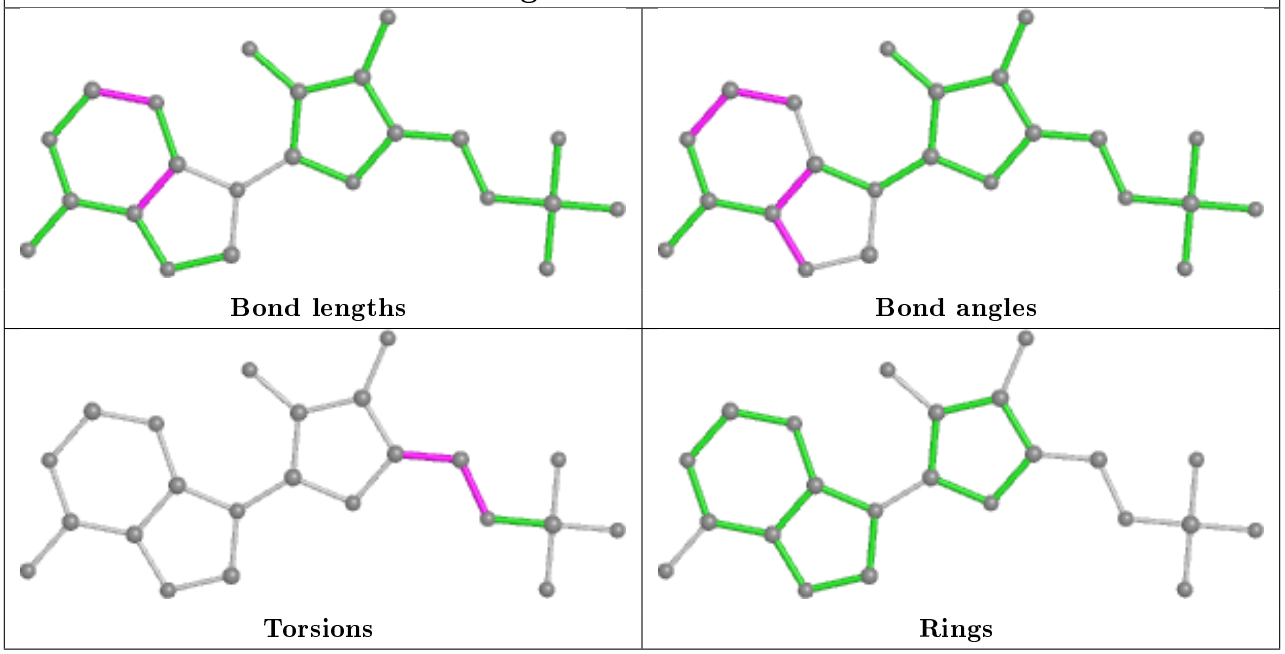


Torsions



Rings

Ligand AMP C 507



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	423/447 (94%)	0.21	14 (3%) 46 47	20, 34, 63, 84	0
1	B	426/447 (95%)	0.21	14 (3%) 46 47	24, 39, 68, 93	0
1	C	429/447 (95%)	0.07	2 (0%) 91 91	22, 35, 53, 79	0
1	D	411/447 (91%)	0.16	5 (1%) 79 79	24, 37, 54, 77	0
All	All	1689/1788 (94%)	0.16	35 (2%) 63 64	20, 36, 61, 93	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLY	4.4
1	B	429	VAL	4.1
1	A	424	HIS	4.0
1	D	366	TRP	4.0
1	B	384	ASP	3.9
1	A	377	GLY	3.7
1	D	22	TRP	3.5
1	A	380	THR	3.4
1	B	424	HIS	3.2
1	A	382	LEU	3.2
1	D	210	ARG	2.9
1	D	365	VAL	2.7
1	B	427	GLU	2.7
1	A	387	HIS	2.7
1	C	368	GLU	2.7
1	B	392	GLU	2.6
1	A	378	ALA	2.6
1	B	387	HIS	2.5
1	B	373	PRO	2.5
1	B	385	SER	2.4
1	B	406	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	406	HIS	2.4
1	B	380	THR	2.3
1	A	384	ASP	2.3
1	A	385	SER	2.2
1	A	403	TYR	2.2
1	A	373	PRO	2.2
1	A	349	ARG	2.2
1	A	420	GLU	2.1
1	B	46	GLU	2.1
1	A	381	ARG	2.1
1	A	388	LEU	2.0
1	B	382	LEU	2.0
1	D	156	LEU	2.0
1	B	417	GLU	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AMP	B	504	23/23	0.90	0.14	29,52,81,83	0
3	AMP	C	507	23/23	0.91	0.14	30,55,69,70	0
2	SO4	C	501	5/5	0.92	0.13	66,66,71,71	0
3	AMP	D	506	23/23	0.93	0.17	32,53,72,73	0
2	SO4	A	503	5/5	0.94	0.14	68,69,73,76	0
4	GOL	D	507	6/6	0.95	0.14	30,39,41,48	0
2	SO4	B	501	5/5	0.95	0.12	59,59,64,68	0
2	SO4	D	505	5/5	0.95	0.11	65,66,69,71	0
2	SO4	C	505	5/5	0.95	0.12	57,61,64,71	0

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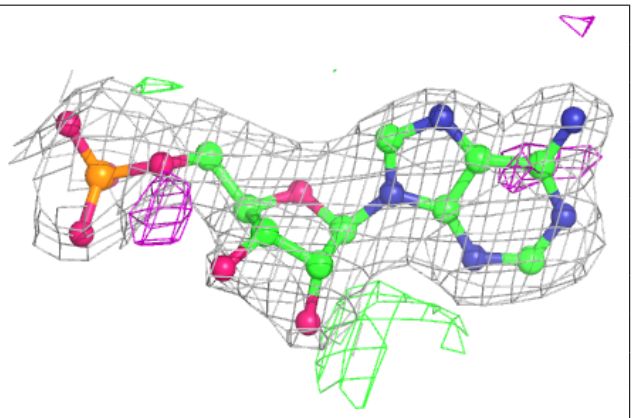
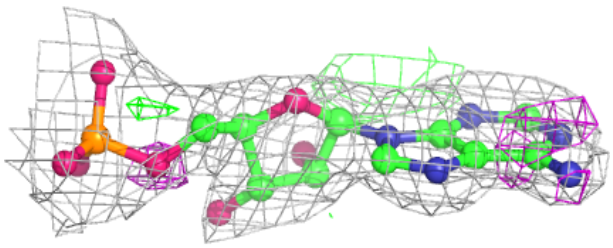
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	501	5/5	0.95	0.12	65,66,72,74	0
2	SO4	C	502	5/5	0.96	0.07	51,57,61,63	0
2	SO4	C	506	5/5	0.96	0.09	61,62,66,66	0
2	SO4	B	502	5/5	0.96	0.14	70,72,74,76	0
2	SO4	A	501	5/5	0.97	0.13	42,45,54,54	0
2	SO4	B	503	5/5	0.97	0.10	55,57,62,64	0
2	SO4	C	503	5/5	0.98	0.08	42,43,48,55	0
2	SO4	D	503	5/5	0.98	0.10	55,57,64,64	0
2	SO4	D	502	5/5	0.99	0.08	48,49,50,58	0
2	SO4	D	504	5/5	0.99	0.11	47,48,55,58	0
2	SO4	A	502	5/5	0.99	0.08	55,55,60,63	0
2	SO4	C	504	5/5	0.99	0.11	37,42,50,50	0

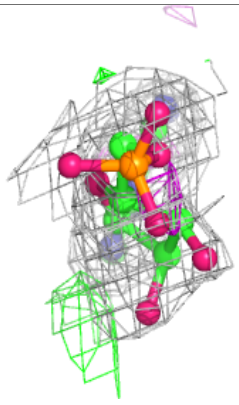
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMP B 504:

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

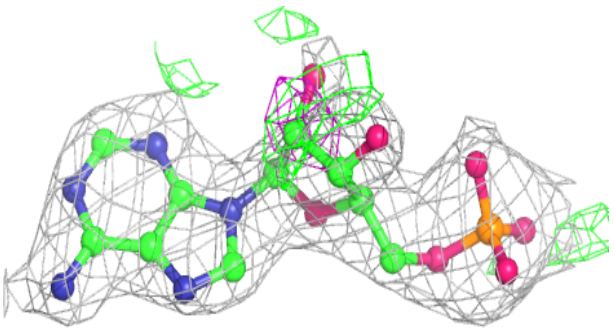


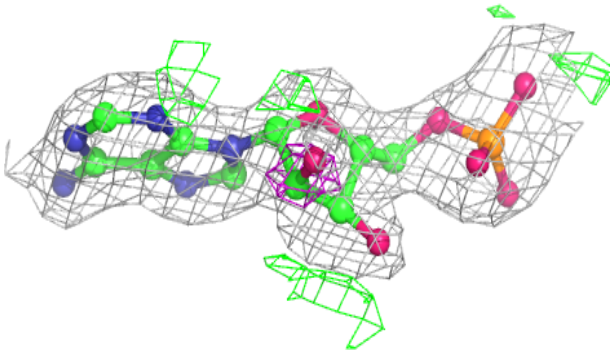


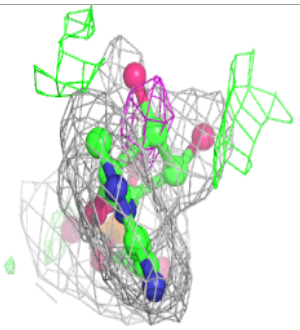


Electron density around AMP C 507:

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

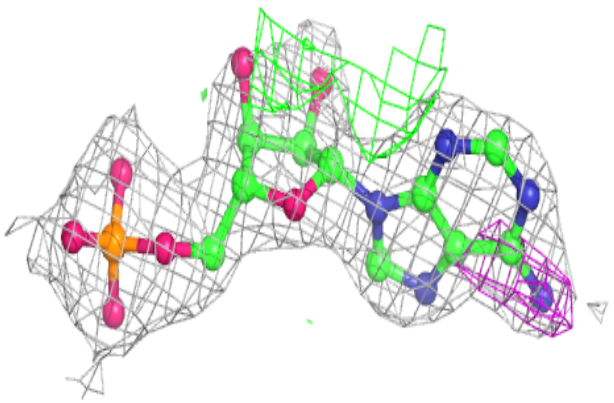


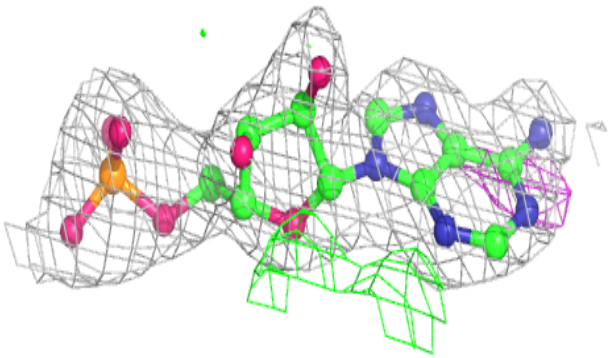


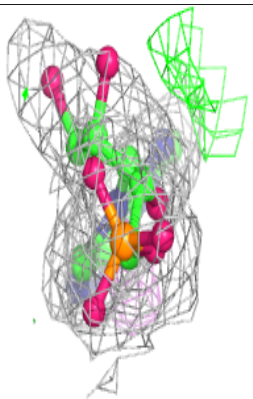


Electron density around AMP D 506:

$2mF_o$-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.