Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 04:28 AM EDT

PDB ID	:	1YTM
Title	:	Crystal structure of phosphoenolpyruvate carboxykinase of Anaerobiospirillum succiniciproducens complexed with ATP, oxalate, magnesium and manganese ions
Authors	:	Delbaere, L.T.J.; Cotelesage, J.J.H.
Deposited on	:	2005-02-10
Resolution	:	2.20 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:

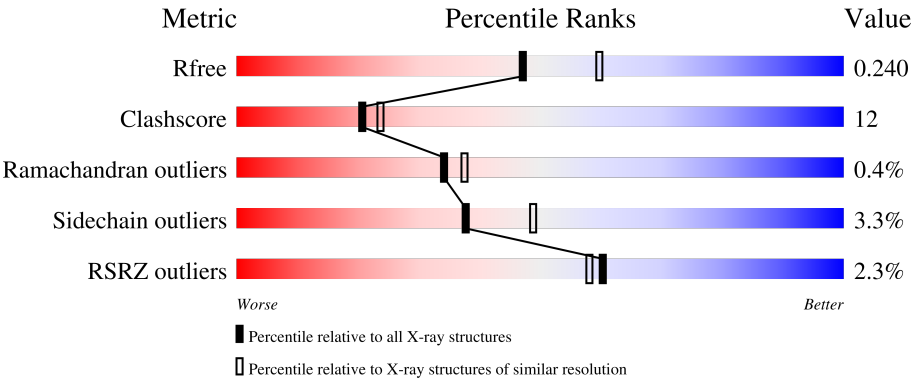
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	532	74% 22%
1	B	532	4% 67% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXD	A	543	-	X	-	-
5	OXD	B	1543	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8462 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 phosphoenolpyruvate carboxykinase [ATP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3992	2555	656	766	15			
1	B	517	Total	C	N	O	S	0	0	0
			4008	2569	662	762	15			

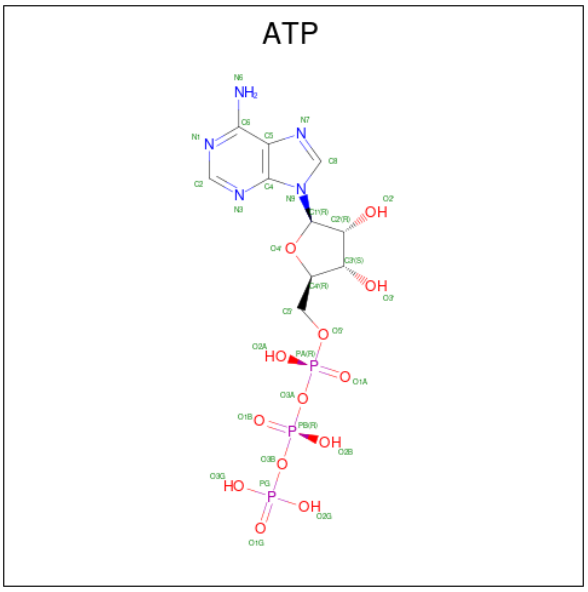
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

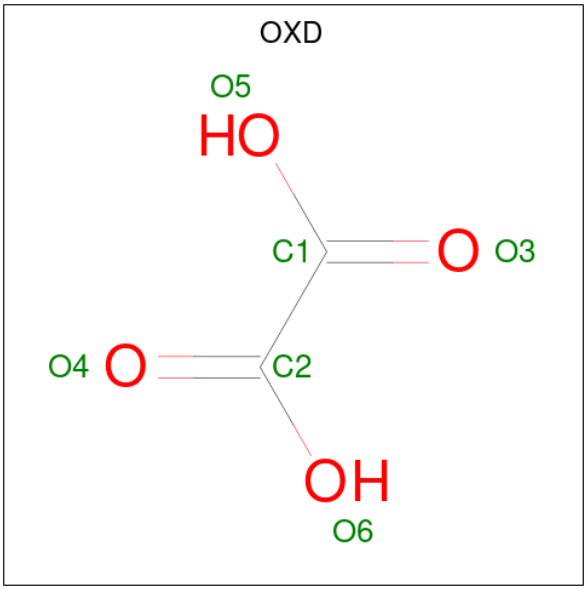
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is OXALIC ACID (three-letter code: OXD) (formula: $C_2H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	2	4		
5	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 6 is water.

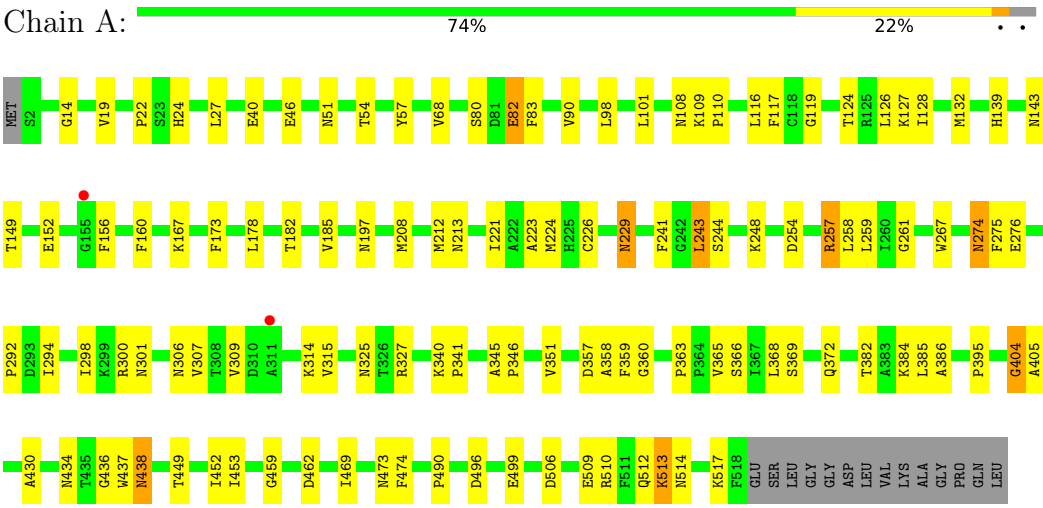
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	225	Total O 225 225	0	0
6	B	159	Total O 159 159	0	0

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.

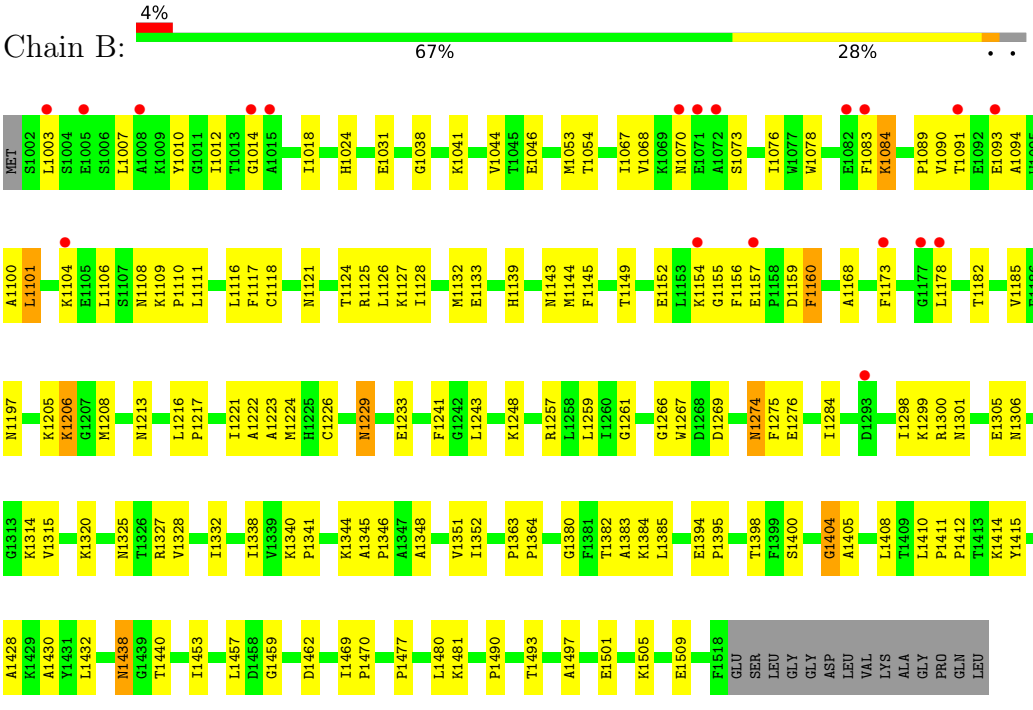
• Molecule 1: phosphoenolpyruvate carboxykinase [ATP]

Chain A:



• Molecule 1: phosphoenolpyruvate carboxykinase [ATP]

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	194.87Å 123.22Å 48.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 45.31 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.20) 95.8 (45.31-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.18Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.251 0.204 , 0.240	Depositor DCC
R_{free} test set	6137 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.9	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	0.94	EDS
Total number of atoms	8462	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7417e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ATP, MG, MN, OXD

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	0.39	0/4081	0.62	0/5536
1	B	0.37	1/4097 (0.0%)	0.59	1/5550 (0.0%)
All	All	0.38	1/8178 (0.0%)	0.60	1/11086 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1299	LYS	CE-NZ	-6.30	1.33	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1299	LYS	CD-CE-NZ	5.46	124.25	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	TYR	Sidechain

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	3992	0	3910	83	0
1	B	4008	0	3968	113	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	225	0	0	2	0
6	B	159	0	0	4	0
All	All	8462	0	7902	196	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 12.

All (196) 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:54:THR:H	1:A:306:ASN:HD21	1.20	0.85
1:A:363:PRO:HB3	1:A:490:PRO:HD3	1.58	0.83
1:B:1363:PRO:HB3	1:B:1490:PRO:HD3	1.62	0.81
1:B:1345:ALA:HB1	1:B:1346:PRO:HD2	1.61	0.81
1:A:369:SER:H	1:A:372:GLN:HE21	1.30	0.79
1:A:51:ASN:ND2	1:A:307:VAL:HG22	1.98	0.78
1:B:1128:ILE:HD13	1:B:1208:MET:HG3	1.68	0.75
1:A:345:ALA:HB1	1:A:346:PRO:HD2	1.68	0.75
1:B:1154:LYS:HG3	1:B:1155:GLY:H	1.51	0.75
1:B:1014:GLY:O	1:B:1108:ASN:HA	1.88	0.74
1:B:1438:ASN:C	1:B:1438:ASN:HD22	1.91	0.74
1:B:1229:ASN:ND2	1:B:1257:ARG:HE	1.85	0.73
1:B:1226:CYS:HA	1:B:1248:LYS:HD2	1.72	0.71
1:A:325:ASN:HD21	1:A:327:ARG:HE	1.38	0.71
1:B:1505:LYS:O	1:B:1509:GLU:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1404:GLY:O	1:B:1408:LEU:HD13	1.91	0.70
1:B:1257:ARG:HD2	1:B:1457:LEU:HD13	1.74	0.69
1:B:1259:LEU:HD12	1:B:1332:ILE:HD11	1.75	0.69
1:A:405:ALA:HA	1:A:408:LEU:HD22	1.76	0.68
1:B:1149:THR:HG22	1:B:1152:GLU:HG3	1.75	0.68
1:A:514:ASN:O	1:A:517:LYS:HG2	1.94	0.68
1:A:274:ASN:HD22	1:A:275:PHE:H	1.41	0.67
1:B:1003:LEU:HD11	1:B:1018:ILE:HG21	1.78	0.66
1:B:1274:ASN:HD22	1:B:1275:PHE:N	1.93	0.66
1:B:1007:LEU:HB3	1:B:1012:ILE:HB	1.78	0.66
1:B:1100:ALA:O	1:B:1104:LYS:HG2	1.96	0.66
1:B:1054:THR:H	1:B:1306:ASN:HD21	1.45	0.64
1:A:109:LYS:HB2	1:A:110:PRO:HD2	1.80	0.64
1:B:1405:ALA:HA	1:B:1408:LEU:HD22	1.79	0.63
1:A:274:ASN:ND2	1:A:276:GLU:H	1.97	0.63
1:A:173:PHE:HB2	1:A:178:LEU:HB2	1.80	0.62
1:A:117:PHE:CE2	1:A:148:PRO:HB3	2.35	0.62
1:A:438:ASN:HD22	1:A:438:ASN:C	2.02	0.62
1:B:1274:ASN:HD22	1:B:1275:PHE:H	1.45	0.62
1:A:274:ASN:HD22	1:A:275:PHE:N	1.98	0.62
1:A:224:MET:HB3	1:A:241:PHE:CE1	2.35	0.61
1:A:229:ASN:ND2	1:A:257:ARG:HH11	1.98	0.61
1:B:1117:PHE:CG	1:B:1125:ARG:HD2	2.35	0.61
1:A:182:THR:HA	1:A:197:ASN:HB3	1.81	0.61
1:A:98:LEU:HD13	1:A:185:VAL:HG21	1.83	0.60
1:A:325:ASN:ND2	1:A:327:ARG:HE	1.98	0.60
1:A:229:ASN:C	1:A:229:ASN:HD22	2.04	0.60
1:A:229:ASN:ND2	1:A:257:ARG:HD3	2.16	0.60
1:A:509:GLU:HA	1:A:512:GLN:HE21	1.66	0.60
1:B:1205:LYS:HE2	1:B:1206:LYS:HE3	1.84	0.60
1:B:1274:ASN:ND2	1:B:1276:GLU:H	2.00	0.59
1:B:1149:THR:HG22	1:B:1152:GLU:CG	2.32	0.59
1:B:1068:VAL:HG12	1:B:1187:ASN:HA	1.84	0.59
1:B:1109:LYS:HE2	1:B:1133:GLU:OE1	2.02	0.59
1:B:1044:VAL:HG12	6:B:167:HOH:O	2.02	0.59
1:A:340:LYS:HB2	1:A:341:PRO:HA	1.84	0.58
1:B:1144:MET:O	1:B:1276:GLU:HB3	2.04	0.58
1:B:1300:ARG:O	1:B:1301:ASN:HB2	2.03	0.58
1:B:1154:LYS:HG3	1:B:1155:GLY:N	2.19	0.58
1:A:404:GLY:O	1:A:408:LEU:HD13	2.04	0.58
1:B:1224:MET:HB3	1:B:1241:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:HIS:HE1	1:A:143:ASN:HD21	1.51	0.56
1:B:1154:LYS:CG	1:B:1155:GLY:H	2.19	0.56
1:B:1173:PHE:HB2	1:B:1178:LEU:HB2	1.87	0.56
1:B:1149:THR:HG23	1:B:1152:GLU:H	1.71	0.56
1:B:1222:ALA:O	1:B:1266:GLY:HA2	2.06	0.56
1:B:1481:LYS:HG3	6:B:282:HOH:O	2.06	0.56
1:B:1382:THR:HG23	1:B:1383:ALA:N	2.22	0.54
1:B:1127:LYS:O	1:B:1159:ASP:HB2	2.08	0.54
1:B:1182:THR:HA	1:B:1197:ASN:HB3	1.90	0.54
1:B:1216:LEU:HB2	1:B:1217:PRO:HD3	1.89	0.54
1:A:24:HIS:HE1	1:A:143:ASN:ND2	2.06	0.53
1:A:360:GLY:HA2	1:A:437:TRP:O	2.09	0.53
1:B:1497:ALA:O	1:B:1501:GLU:HG3	2.08	0.53
1:A:116:LEU:HD13	1:A:145:PHE:HB2	1.89	0.53
1:B:1038:GLY:N	1:B:1041:LYS:HE2	2.23	0.53
1:A:226:CYS:HA	1:A:248:LYS:HD2	1.90	0.53
1:B:1438:ASN:C	1:B:1438:ASN:ND2	2.61	0.53
1:B:1067:ILE:O	1:B:1089:PRO:HA	2.10	0.52
1:A:267:TRP:CE2	1:A:422:ARG:HB3	2.44	0.52
1:B:1384:LYS:HG3	1:B:1398:THR:HG21	1.91	0.52
1:A:54:THR:H	1:A:306:ASN:ND2	1.96	0.52
1:A:149:THR:OG1	1:A:152:GLU:HG3	2.10	0.52
1:A:144:MET:O	1:A:276:GLU:HB3	2.10	0.52
1:B:1053:MET:SD	1:B:1306:ASN:HA	2.50	0.52
1:A:300:ARG:O	1:A:301:ASN:HB2	2.10	0.51
1:B:1121:ASN:HD21	1:B:1344:LYS:HD3	1.76	0.51
1:A:496:ASP:O	1:A:499:GLU:HG3	2.11	0.51
1:B:1038:GLY:H	1:B:1041:LYS:HE2	1.75	0.51
1:B:1340:LYS:HB2	1:B:1341:PRO:HA	1.91	0.51
1:B:1084:LYS:HB3	1:B:1084:LYS:NZ	2.26	0.51
1:B:1267:TRP:CE2	1:B:1422:ARG:HB3	2.46	0.51
1:A:68:VAL:HA	1:A:90:VAL:HG23	1.93	0.51
1:A:438:ASN:C	1:A:438:ASN:ND2	2.64	0.51
1:B:1325:ASN:HD21	1:B:1327:ARG:HH21	1.58	0.51
1:B:1257:ARG:HD2	1:B:1457:LEU:CD1	2.39	0.50
1:B:1101:LEU:HD22	1:B:1168:ALA:HB1	1.92	0.50
1:A:24:HIS:HB3	1:A:301:ASN:OD1	2.11	0.50
1:B:1414:LYS:O	1:B:1418:VAL:HG23	2.12	0.50
1:B:1300:ARG:O	1:B:1301:ASN:CB	2.60	0.50
1:B:1453:ILE:O	1:B:1457:LEU:HG	2.12	0.49
1:A:384:LYS:O	1:A:385:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:HD21	1:A:327:ARG:NE	2.08	0.49
1:B:1118:CYS:HB2	1:B:1128:ILE:HD11	1.95	0.49
1:A:243:LEU:HD22	1:A:244:SER:H	1.77	0.49
1:B:1229:ASN:HD22	1:B:1229:ASN:C	2.15	0.49
1:B:1269:ASP:HA	1:B:1422:ARG:HH12	1.78	0.49
1:B:1217:PRO:HB2	1:B:1410:LEU:CD1	2.44	0.48
1:A:126:LEU:HD12	1:A:212:MET:SD	2.54	0.48
1:B:1007:LEU:HA	1:B:1010:TYR:CD2	2.47	0.48
1:B:1116:LEU:HD13	1:B:1145:PHE:HB2	1.96	0.48
1:A:294:ILE:O	1:A:298:ILE:HG13	2.14	0.48
1:B:1310:ASP:OD2	1:B:1314:LYS:HB3	2.13	0.48
1:A:14:GLY:O	1:A:108:ASN:HA	2.14	0.47
1:B:1068:VAL:HG22	1:B:1070:ASN:OD1	2.13	0.47
1:A:27:LEU:HD13	1:A:139:HIS:HA	1.95	0.47
1:B:1352:ILE:N	1:B:1352:ILE:HD12	2.29	0.47
1:B:1091:THR:OG1	1:B:1093:GLU:HG3	2.15	0.47
1:A:259:LEU:HD13	1:A:261:GLY:N	2.29	0.47
1:B:1493:THR:HG23	6:B:29:HOH:O	2.15	0.47
1:B:1003:LEU:CD1	1:B:1018:ILE:HG21	2.43	0.47
1:B:1031:GLU:OE1	1:B:1139:HIS:ND1	2.48	0.47
1:B:1348:ALA:O	1:B:1428:ALA:HB2	2.15	0.47
1:B:1408:LEU:HG	1:B:1415:TYR:CE2	2.50	0.47
1:A:243:LEU:CD2	1:A:244:SER:H	2.27	0.47
1:A:358:ALA:HA	1:A:437:TRP:CE3	2.50	0.46
1:B:1073:SER:HB2	1:B:1076:ILE:HG13	1.97	0.46
1:B:1117:PHE:HB3	1:B:1125:ARG:HD2	1.96	0.46
1:B:1438:ASN:ND2	1:B:1440:THR:H	2.12	0.46
1:A:119:GLY:HA2	1:A:275:PHE:HA	1.97	0.46
1:B:1068:VAL:HA	1:B:1090:VAL:O	2.15	0.46
1:B:1121:ASN:O	1:B:1125:ARG:HB2	2.16	0.46
1:A:80:SER:OG	1:A:82:GLU:HG2	2.16	0.46
1:A:459:GLY:O	1:A:462:ASP:HB2	2.16	0.46
1:A:254:ASP:HB3	1:A:257:ARG:HG3	1.98	0.46
1:B:1217:PRO:HB2	1:B:1410:LEU:HD12	1.98	0.46
1:A:24:HIS:CE1	1:A:143:ASN:HD21	2.34	0.45
1:A:292:PRO:HD2	6:A:1187:HOH:O	2.15	0.45
1:B:1149:THR:CG2	1:B:1152:GLU:H	2.28	0.45
1:B:1205:LYS:HE2	1:B:1206:LYS:CE	2.45	0.45
1:B:1099:LYS:HE2	1:B:1190:GLU:OE2	2.15	0.45
1:A:300:ARG:O	1:A:301:ASN:CB	2.64	0.45
1:B:1091:THR:HG23	1:B:1094:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1305:GLU:O	1:B:1306:ASN:HB2	2.17	0.45
1:A:127:LYS:HB3	1:A:156:PHE:CZ	2.51	0.45
1:B:1298:ILE:HG12	1:B:1328:VAL:HG21	1.99	0.45
1:B:1259:LEU:HB3	1:B:1338:ILE:HG22	1.98	0.45
1:B:1309:VAL:HG22	1:B:1315:VAL:HG22	1.98	0.44
1:A:309:VAL:HG22	1:A:315:VAL:HG22	1.99	0.44
1:A:325:ASN:HD21	1:A:327:ARG:HH21	1.65	0.44
1:B:1046:GLU:OE2	1:B:1314:LYS:HA	2.18	0.44
1:B:1149:THR:CG2	1:B:1152:GLU:HG3	2.46	0.44
1:B:1351:VAL:O	1:B:1430:ALA:HA	2.17	0.44
1:A:19:VAL:HG11	1:A:22:PRO:HB3	1.98	0.44
1:B:1127:LYS:HB3	1:B:1156:PHE:CZ	2.53	0.44
1:A:46:GLU:OE2	1:A:314:LYS:HA	2.17	0.44
1:B:1213:ASN:OD1	1:B:1223:ALA:HB1	2.18	0.44
1:A:128:ILE:HD12	1:A:208:MET:SD	2.58	0.44
1:A:513:LYS:N	1:A:513:LYS:HD2	2.32	0.44
1:A:469:ILE:HB	1:A:474:PHE:HB2	1.99	0.43
1:A:229:ASN:CG	1:A:257:ARG:HD3	2.38	0.43
1:A:283:VAL:O	1:A:286:LEU:HB2	2.18	0.43
1:A:506:ASP:O	1:A:510:ARG:HG3	2.18	0.43
1:A:229:ASN:ND2	1:A:257:ARG:CD	2.80	0.43
1:A:213:ASN:OD1	1:A:223:ALA:HB1	2.18	0.43
1:B:1024:HIS:HE1	1:B:1143:ASN:OD1	2.02	0.43
1:B:1090:VAL:HG22	1:B:1094:ALA:HB3	2.00	0.43
1:A:365:VAL:HB	1:A:452:ILE:HG21	2.00	0.43
1:A:357:ASP:OD1	1:A:359:PHE:HB2	2.19	0.43
1:B:1459:GLY:O	1:B:1462:ASP:HB2	2.19	0.43
1:A:117:PHE:CE1	1:A:127:LYS:HG2	2.54	0.42
1:B:1384:LYS:HA	6:B:137:HOH:O	2.19	0.42
1:A:40:GLU:OE2	1:A:167:LYS:HE2	2.19	0.42
1:A:274:ASN:ND2	1:A:275:PHE:N	2.66	0.42
1:A:512:GLN:HA	6:A:1210:HOH:O	2.18	0.42
1:B:1098:LEU:HD13	1:B:1185:VAL:HG21	2.00	0.42
1:B:1106:LEU:HB3	1:B:1111:LEU:HD21	2.00	0.42
1:A:19:VAL:CG1	1:A:22:PRO:HB3	2.49	0.42
1:A:224:MET:HB3	1:A:241:PHE:CZ	2.54	0.42
1:A:434:ASN:OD1	1:A:436:GLY:N	2.45	0.42
1:B:1243:LEU:HB2	1:B:1382:THR:HG21	2.02	0.41
1:B:1257:ARG:CD	1:B:1457:LEU:HD13	2.48	0.41
1:B:1259:LEU:HD13	1:B:1261:GLY:N	2.35	0.41
1:A:124:THR:HG21	1:A:221:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:O	1:A:430:ALA:HA	2.20	0.41
1:B:1126:LEU:HD21	1:B:1160:PHE:HB2	2.03	0.41
1:A:449:THR:O	1:A:453:ILE:HG12	2.21	0.41
1:B:1154:LYS:CG	1:B:1155:GLY:N	2.80	0.41
1:B:1411:PRO:HA	1:B:1412:PRO:HD3	1.92	0.41
1:B:1477:PRO:HG3	1:B:1480:LEU:HD11	2.03	0.41
1:B:1068:VAL:CG1	1:B:1187:ASN:HA	2.51	0.40
1:B:1394:GLU:HG3	1:B:1395:PRO:HD2	2.03	0.40
1:B:1076:ILE:HB	1:B:1078:TRP:CE2	2.56	0.40
1:A:363:PRO:HG2	1:A:366:SER:OG	2.22	0.40
1:A:385:LEU:HD23	1:A:395:PRO:HA	2.03	0.40
1:B:1110:PRO:O	1:B:1111:LEU:HD12	2.22	0.40
1:B:1124:THR:HG21	1:B:1221:ILE:CD1	2.52	0.40
1:B:1078:TRP:CE3	1:B:1089:PRO:HB3	2.56	0.40
1:B:1380:GLY:HA3	1:B:1400:SER:O	2.21	0.40
1:B:1469:ILE:HA	1:B:1470:PRO:HD3	1.93	0.40
1:B:1284:ILE:HD11	1:B:1320:LYS:HB3	2.03	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	515/532 (97%)	499 (97%)	13 (2%)	3 (1%)	25	26
1	B	515/532 (97%)	490 (95%)	24 (5%)	1 (0%)	47	55
All	All	1030/1064 (97%)	989 (96%)	37 (4%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ALA

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Mol	Chain	Res	Type
1	A	382	THR
1	A	404	GLY
1	B	1404	GLY

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	422/443 (95%)	408 (97%)	14 (3%)	38	49
1	B	426/443 (96%)	412 (97%)	14 (3%)	38	49
All	All	848/886 (96%)	820 (97%)	28 (3%)	38	49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	A	83	PHE
1	A	101	LEU
1	A	132	MET
1	A	160	PHE
1	A	229	ASN
1	A	243	LEU
1	A	257	ARG
1	A	258	LEU
1	A	274	ASN
1	A	368	LEU
1	A	438	ASN
1	A	473	ASN
1	A	513	LYS
1	B	1083	PHE
1	B	1084	LYS
1	B	1101	LEU
1	B	1132	MET
1	B	1157	GLU
1	B	1160	PHE

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Mol	Chain	Res	Type
1	B	1206	LYS
1	B	1229	ASN
1	B	1233	GLU
1	B	1274	ASN
1	B	1364	PRO
1	B	1385	LEU
1	B	1432	LEU
1	B	1438	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	51	ASN
1	A	87	ASN
1	A	121	ASN
1	A	137	GLN
1	A	139	HIS
1	A	143	ASN
1	A	179	ASN
1	A	193	GLN
1	A	229	ASN
1	A	236	ASN
1	A	274	ASN
1	A	306	ASN
1	A	325	ASN
1	A	372	GLN
1	A	438	ASN
1	A	512	GLN
1	B	1024	HIS
1	B	1087	ASN
1	B	1121	ASN
1	B	1137	GLN
1	B	1179	ASN
1	B	1193	GLN
1	B	1229	ASN
1	B	1236	ASN
1	B	1274	ASN
1	B	1290	ASN
1	B	1306	ASN
1	B	1312	ASN
1	B	1325	ASN

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Mol	Chain	Res	Type
1	B	1438	ASN
1	B	1492	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	A	541	3,2	26,33,33	1.40	6 (23%)	31,52,52	1.10	1 (3%)
5	OXD	A	543	3	5,5,5	2.74	2 (40%)	6,6,6	6.78	5 (83%)
5	OXD	B	1543	3	5,5,5	2.78	2 (40%)	6,6,6	6.86	5 (83%)
4	ATP	B	1541	3,2	26,33,33	1.25	3 (11%)	31,52,52	1.17	2 (6%)

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	ATP	A	541	3,2	-	2/18/38/38	0/3/3/3
5	OXD	A	543	3	-	0/4/4/4	-
5	OXD	B	1543	3	-	0/4/4/4	-
4	ATP	B	1541	3,2	-	3/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1543	OXD	O4-C2	4.83	1.35	1.22
5	A	543	OXD	O4-C2	4.75	1.35	1.22
5	B	1543	OXD	O3-C1	3.54	1.32	1.22
5	A	543	OXD	O3-C1	3.36	1.31	1.22
4	A	541	ATP	O4'-C1'	3.21	1.45	1.41
4	A	541	ATP	C2'-C1'	-2.63	1.49	1.53
4	B	1541	ATP	PG-O3G	-2.60	1.44	1.54
4	A	541	ATP	C4-N3	2.37	1.38	1.35
4	A	541	ATP	C8-N7	-2.35	1.30	1.34
4	B	1541	ATP	PG-O2G	-2.19	1.46	1.54
4	A	541	ATP	C2-N3	2.17	1.35	1.32
4	B	1541	ATP	O4'-C1'	2.14	1.44	1.41
4	A	541	ATP	PB-O2B	-2.03	1.45	1.55

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	543	OXD	O6-C2-C1	9.89	142.54	113.16
5	B	1543	OXD	O6-C2-C1	9.87	142.49	113.16
5	B	1543	OXD	O5-C1-O3	-8.91	103.23	123.61
5	A	543	OXD	O6-C2-O4	-8.46	104.25	123.61
5	A	543	OXD	O5-C1-O3	-8.45	104.27	123.61
5	B	1543	OXD	O6-C2-O4	-8.07	105.14	123.61
5	B	1543	OXD	O3-C1-C2	5.56	138.64	120.78
5	A	543	OXD	O3-C1-C2	5.16	137.34	120.78
4	B	1541	ATP	PA-O3A-PB	-3.21	121.80	132.83
4	A	541	ATP	PA-O3A-PB	-2.90	122.88	132.83
5	B	1543	OXD	O4-C2-C1	-2.62	112.37	120.78
5	A	543	OXD	O4-C2-C1	-2.36	113.22	120.78
4	B	1541	ATP	O2G-PG-O3B	-2.03	97.81	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

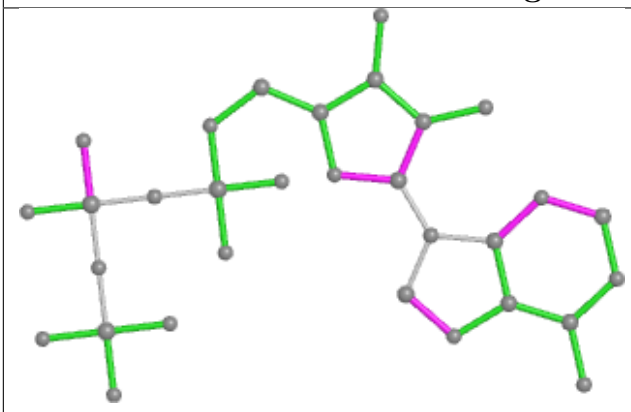
Mol	Chain	Res	Type	Atoms
4	B	1541	ATP	PA-O3A-PB-O2B
4	A	541	ATP	PA-O3A-PB-O2B
4	A	541	ATP	O4'-C4'-C5'-O5'
4	B	1541	ATP	O4'-C4'-C5'-O5'
4	B	1541	ATP	PA-O3A-PB-O1B

There are no ring outliers.

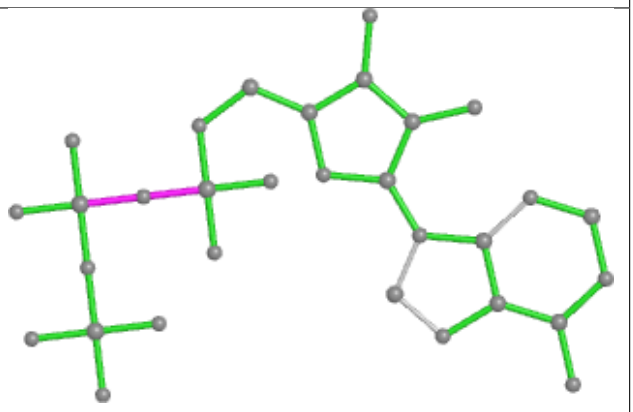
No monomer is involved in short contacts.

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.

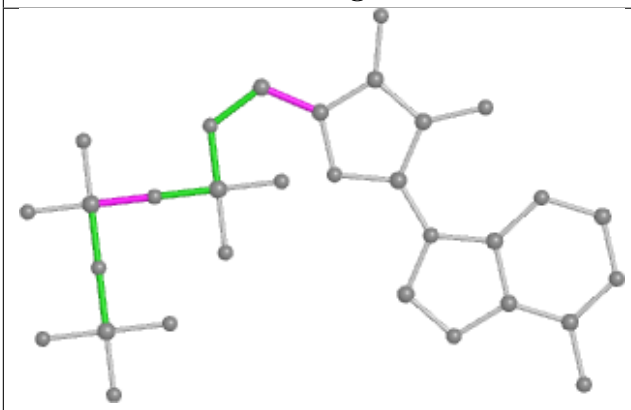
Ligand ATP A 541



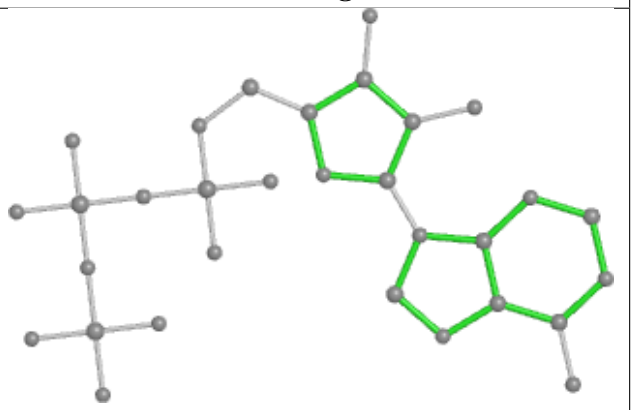
Bond lengths



Bond angles

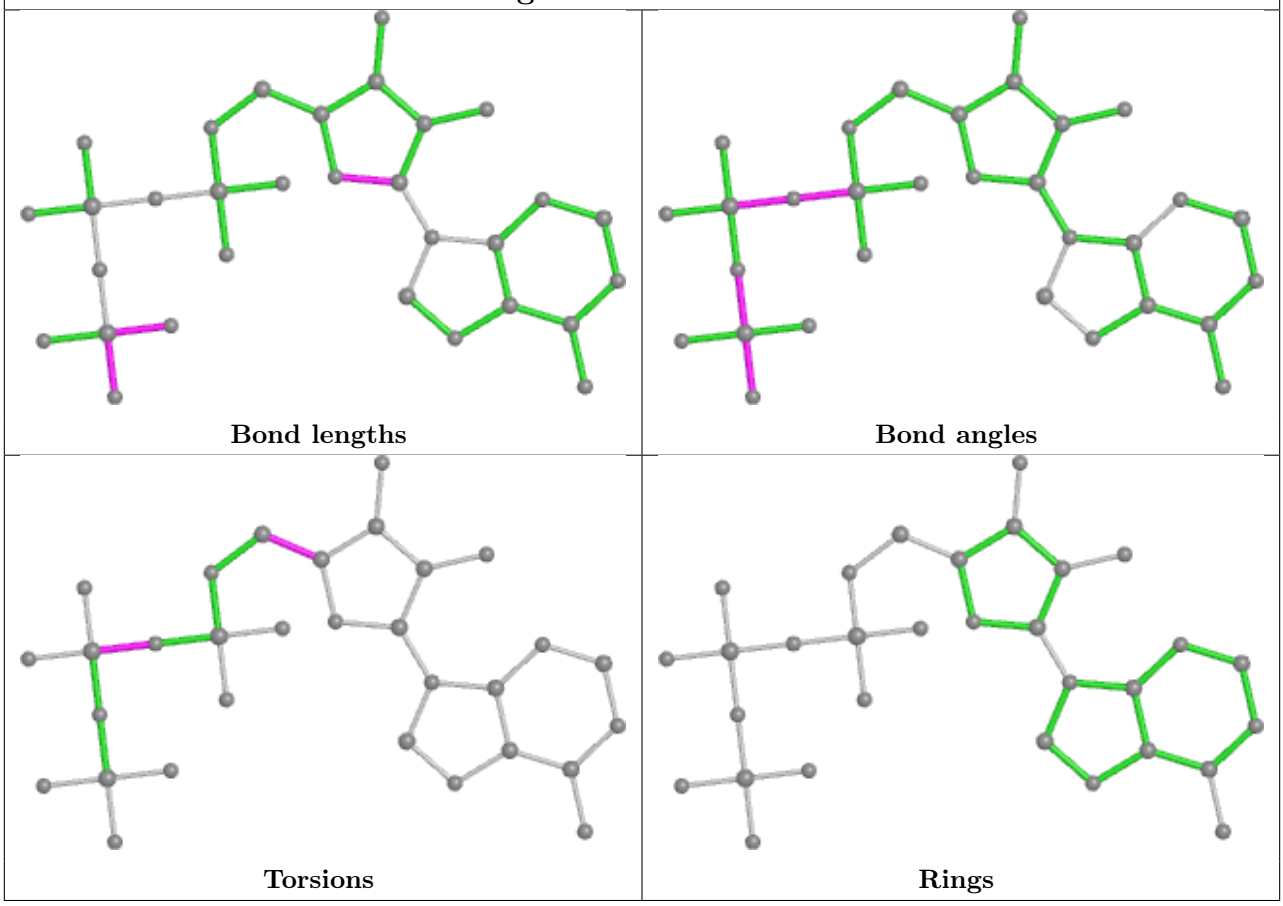


Torsions



Rings

Ligand ATP B 1541



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	517/532 (97%)	-0.17	2 (0%)	92	91	18, 26, 40, 50	0
1	B	517/532 (97%)	0.19	22 (4%)	35	33	18, 33, 55, 79	0
All	All	1034/1064 (97%)	0.01	24 (2%)	60	58	18, 29, 50, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1003	LEU	3.6
1	B	1091	THR	3.5
1	B	1005	GLU	3.3
1	B	1096	ALA	3.3
1	B	1312	ASN	3.1
1	B	1072	ALA	3.0
1	B	1015	ALA	2.8
1	B	1071	GLU	2.8
1	B	1154	LYS	2.8
1	B	1014	GLY	2.7
1	B	1293	ASP	2.7
1	A	155	GLY	2.7
1	B	1173	PHE	2.4
1	B	1157	GLU	2.4
1	A	311	ALA	2.4
1	B	1177	GLY	2.3
1	B	1178	LEU	2.2
1	B	1104	LYS	2.2
1	B	1082	GLU	2.1
1	B	1008	ALA	2.1
1	B	1070	ASN	2.1
1	B	1311	ALA	2.1
1	B	1093	GLU	2.0
1	B	1083	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

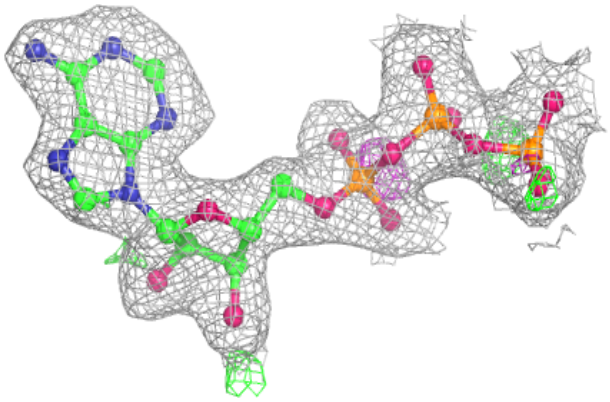
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

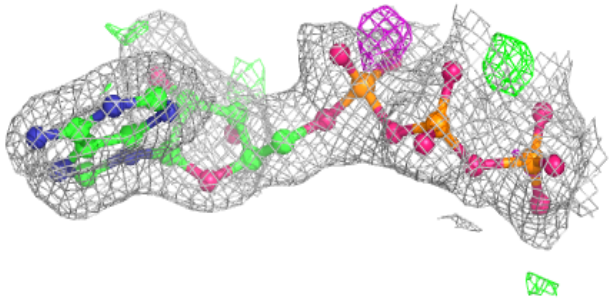
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OXD	B	1543	6/6	0.95	0.14	18,19,20,20	0
5	OXD	A	543	6/6	0.96	0.11	19,21,24,27	0
3	MN	B	1999	1/1	0.97	0.18	26,26,26,26	0
4	ATP	A	541	31/31	0.97	0.12	19,24,26,28	0
4	ATP	B	1541	31/31	0.98	0.12	19,24,26,28	0
3	MN	A	999	1/1	0.99	0.17	22,22,22,22	0
2	MG	B	1998	1/1	0.99	0.29	13,13,13,13	0
2	MG	A	998	1/1	1.00	0.28	10,10,10,10	0

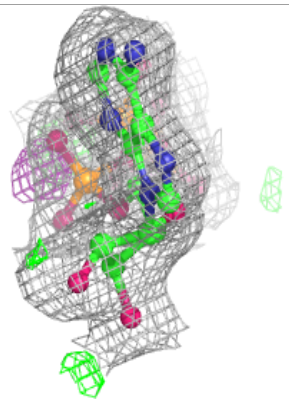
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 541:

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

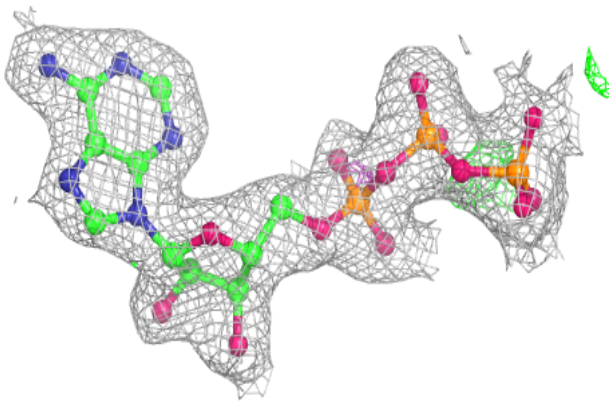


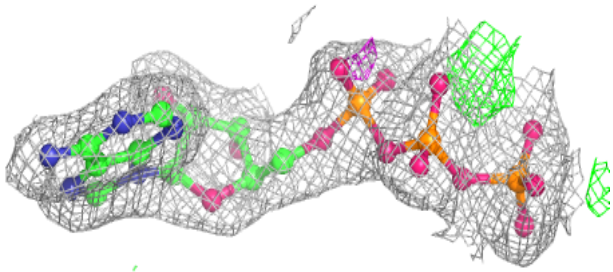


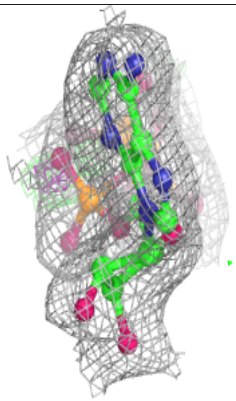


Electron density around ATP B 1541:

$2mF_o$-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.