



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:39 am BST

PDB ID : 2PXZ
Title : E. coli phosphoenolpyruvate carboxykinase (PEPCK) complexed with ATP, Mg²⁺, Mn²⁺, carbon dioxide and oxaloacetate
Authors : Delbaere, L.T.J.; Cotelesage, J.J.H.; Goldie, H.
Deposited on : 2007-05-14
Resolution : 2.23 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

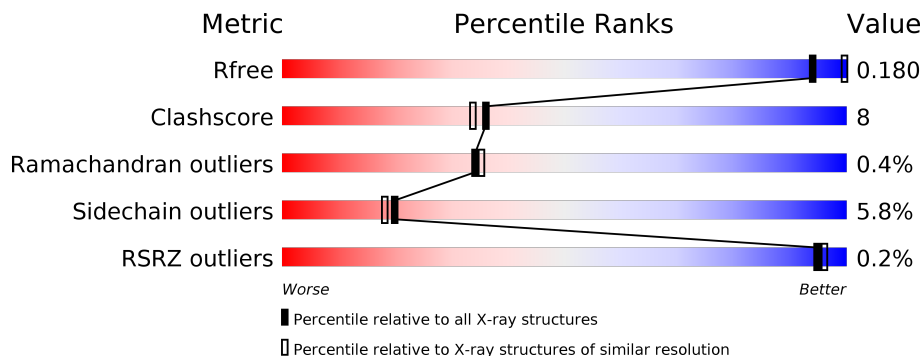
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 $\leq 5\%$. 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	X	540	

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
4	OAA	X	701	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4338 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	526	4007	2554	676	762	15	0	0	0

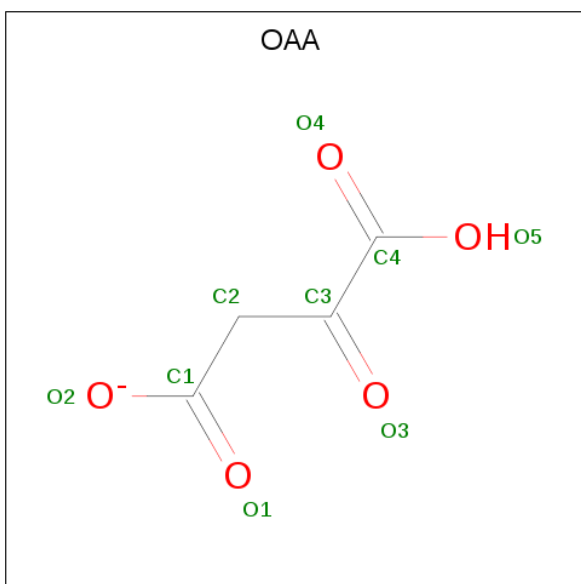
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Mg	0	0
			1	1		

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

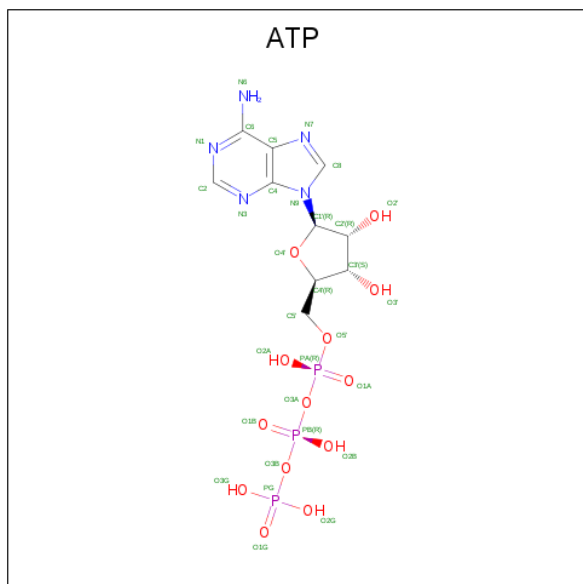
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Mn	0	0
			1	1		

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).



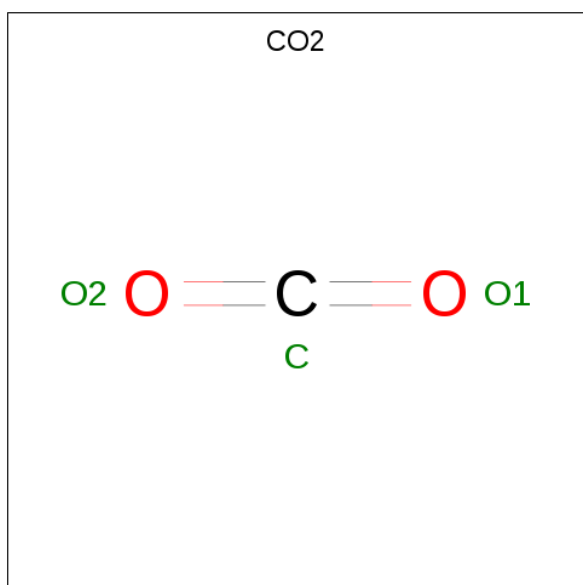
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	C	O	0	0
			9	4	5		

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



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

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO₂) (formula: CO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	X	1	Total	C	O	0	1
			6	2	4		

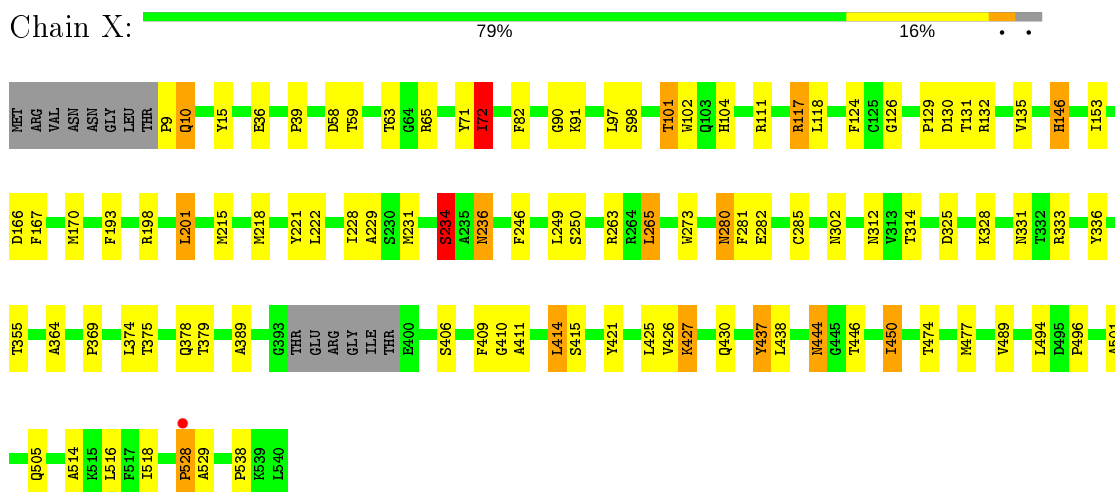
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	X	283	Total	O	0	0
			283	283		

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: Phosphoenolpyruvate carboxykinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.56Å 94.30Å 46.35Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	38.32 – 2.23 38.85 – 1.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.32-2.23) 100.0 (38.85-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.83Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.234 0.176 , 0.180	Depositor DCC
R_{free} test set	4813 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4338	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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: MG, CO2, ATP, OAA, MN

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	X	1.05	10/4103 (0.2%)	1.03	18/5588 (0.3%)

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	X	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	426	VAL	C-N	-9.07	1.13	1.34
1	X	437	TYR	C-N	-7.82	1.16	1.34
1	X	427	LYS	C-N	-6.46	1.19	1.34
1	X	71	TYR	C-N	-6.43	1.19	1.34
1	X	302	ASN	CB-CG	6.07	1.65	1.51
1	X	234	SER	CB-OG	-5.89	1.34	1.42
1	X	379	THR	C-N	-5.49	1.21	1.34
1	X	166	ASP	CB-CG	-5.41	1.40	1.51
1	X	528	PRO	C-O	5.40	1.34	1.23
1	X	409	PHE	CE2-CZ	5.24	1.47	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	437	TYR	O-C-N	-14.81	99.01	122.70
1	X	111	ARG	NE-CZ-NH2	-14.65	112.98	120.30
1	X	117	ARG	NE-CZ-NH1	-12.98	113.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	72	ILE	O-C-N	-11.78	103.86	122.70
1	X	437	TYR	CA-C-N	11.62	142.77	117.20
1	X	72	ILE	CA-C-N	9.21	137.45	117.20
1	X	111	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	X	9	PRO	N-CA-CB	7.07	111.78	103.30
1	X	198	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	X	111	ARG	CG-CD-NE	-6.22	98.73	111.80
1	X	265	LEU	CA-CB-CG	5.96	129.01	115.30
1	X	437	TYR	C-N-CA	5.75	136.07	121.70
1	X	379	THR	O-C-N	-5.63	113.69	122.70
1	X	231	MET	CG-SD-CE	5.57	109.12	100.20
1	X	90	GLY	N-CA-C	5.46	126.74	113.10
1	X	65	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	X	117	ARG	NH1-CZ-NH2	5.25	125.18	119.40
1	X	166	ASP	CB-CG-OD2	-5.05	113.76	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	427	LYS	Mainchain
1	X	437	TYR	Mainchain
1	X	72	ILE	Mainchain

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	X	4007	0	3834	62	0
2	X	1	0	0	0	0
3	X	1	0	0	0	0
4	X	9	0	2	4	0
5	X	31	0	12	0	0
6	X	6	0	0	0	0
7	X	283	0	0	8	1
All	All	4338	0	3848	63	1

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 8.

All (63) 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:X:117:ARG:HG2	1:X:117:ARG:HH11	0.96	1.07
1:X:117:ARG:NH1	1:X:117:ARG:HG2	1.67	1.05
1:X:117:ARG:HH11	1:X:117:ARG:CG	1.74	0.99
4:X:701:OAA:O5	7:X:801:HOH:O	1.95	0.85
1:X:250:SER:H	4:X:701:OAA:H21	1.43	0.82
1:X:528:PRO:O	1:X:529:ALA:HB3	1.87	0.74
1:X:98:SER:OG	1:X:101:THR:HG23	1.89	0.73
1:X:331:ASN:HD21	1:X:333:ARG:HE	1.37	0.71
1:X:36:GLU:OE1	1:X:146:HIS:HD2	1.75	0.69
1:X:411:ALA:HA	1:X:414:LEU:HD22	1.77	0.67
1:X:15:TYR:HB3	1:X:170:MET:CE	2.26	0.66
1:X:117:ARG:NH1	1:X:117:ARG:CG	2.38	0.65
1:X:236:ASN:ND2	1:X:263:ARG:HE	1.95	0.64
1:X:331:ASN:ND2	1:X:333:ARG:HE	1.97	0.62
1:X:218:MET:O	1:X:222:LEU:HD13	1.99	0.62
1:X:450:ILE:CG2	7:X:918:HOH:O	2.48	0.60
1:X:450:ILE:HG23	7:X:918:HOH:O	2.02	0.59
1:X:221:TYR:HD2	1:X:222:LEU:HD12	1.67	0.59
1:X:10:GLN:H	1:X:10:GLN:HE21	1.50	0.58
1:X:102:TRP:CZ3	1:X:201:LEU:HD22	2.39	0.57
1:X:59:THR:H	1:X:312:ASN:HD21	1.49	0.57
1:X:528:PRO:O	1:X:529:ALA:CB	2.51	0.57
1:X:36:GLU:OE1	1:X:146:HIS:CD2	2.58	0.56
1:X:221:TYR:HB2	1:X:415:SER:CB	2.37	0.55
1:X:234:SER:HB2	1:X:246:PHE:HB2	1.89	0.55
1:X:364:ALA:H	1:X:389:ALA:HB3	1.73	0.53
1:X:518:ILE:HD11	1:X:538:PRO:O	2.09	0.52
1:X:249:LEU:HD21	1:X:406:SER:HB3	1.92	0.52
1:X:280:ASN:ND2	1:X:282:GLU:H	2.08	0.52
1:X:285:CYS:HB2	1:X:336:TYR:CE1	2.45	0.51
1:X:314:THR:HG21	1:X:325:ASP:OD1	2.10	0.51
1:X:501:ALA:H	1:X:505:GLN:NE2	2.09	0.51
1:X:10:GLN:N	1:X:10:GLN:HE21	2.09	0.51
1:X:58:ASP:OD1	1:X:328:LYS:NZ	2.44	0.50
1:X:414:LEU:HG	1:X:421:TYR:CE2	2.49	0.48
1:X:474:THR:OG1	7:X:857:HOH:O	2.15	0.48
1:X:131:THR:HG21	1:X:228:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:514:ALA:O	1:X:518:ILE:HG12	2.14	0.47
1:X:15:TYR:HB3	1:X:170:MET:HE1	1.95	0.47
1:X:15:TYR:HB3	1:X:170:MET:HE3	1.95	0.47
1:X:444:ASN:HB3	1:X:446:THR:H	1.80	0.46
1:X:236:ASN:C	1:X:236:ASN:HD22	2.18	0.46
1:X:104:HIS:HB3	7:X:727:HOH:O	2.16	0.46
1:X:229:ALA:HB3	1:X:273:TRP:HB3	1.96	0.46
1:X:489:VAL:HG11	1:X:494:LEU:HD21	1.98	0.46
1:X:129:PRO:HA	1:X:132:ARG:NE	2.31	0.46
1:X:135:VAL:HG22	1:X:215:MET:HE1	1.98	0.45
1:X:72:ILE:HD13	1:X:193:PHE:HB2	1.99	0.45
1:X:450:ILE:HG21	7:X:918:HOH:O	2.14	0.44
1:X:72:ILE:CD1	1:X:193:PHE:HB2	2.48	0.44
1:X:249:LEU:HB3	4:X:701:OAA:H21	2.00	0.44
1:X:375:THR:H	1:X:378:GLN:HE21	1.65	0.43
1:X:102:TRP:CH2	1:X:201:LEU:HD22	2.54	0.43
1:X:124:PHE:HB2	1:X:153:ILE:HB	2.00	0.43
1:X:117:ARG:HD2	7:X:786:HOH:O	2.20	0.41
1:X:59:THR:H	1:X:312:ASN:ND2	2.15	0.41
1:X:250:SER:HB3	4:X:701:OAA:H22	2.01	0.41
1:X:221:TYR:CD2	1:X:222:LEU:HD12	2.52	0.41
1:X:126:GLY:HA2	1:X:281:PHE:HA	2.02	0.41
1:X:98:SER:OG	1:X:101:THR:CG2	2.64	0.41
1:X:39:PRO:HD3	7:X:712:HOH:O	2.21	0.40
1:X:280:ASN:HD22	1:X:281:PHE:N	2.20	0.40
1:X:369:PRO:HB3	1:X:496:PRO:HD3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:712:HOH:O	7:X:712:HOH:O 2_656	1.47	0.73

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	X	522/540 (97%)	508 (97%)	12 (2%)	2 (0%)	34 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	91	LYS
1	X	410	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	X	412/448 (92%)	388 (94%)	24 (6%)	20 18

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	10	GLN
1	X	63	THR
1	X	82	PHE
1	X	97	LEU
1	X	101	THR
1	X	118	LEU
1	X	130	ASP
1	X	146	HIS
1	X	167	PHE
1	X	201	LEU
1	X	234	SER
1	X	236	ASN
1	X	265	LEU
1	X	280	ASN
1	X	355	THR
1	X	374	LEU
1	X	414	LEU

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Mol	Chain	Res	Type
1	X	425	LEU
1	X	430	GLN
1	X	438	LEU
1	X	444	ASN
1	X	450	ILE
1	X	477	MET
1	X	516	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	10	GLN
1	X	21	HIS
1	X	94	ASN
1	X	128	ASN
1	X	144	GLN
1	X	146	HIS
1	X	200	GLN
1	X	236	ASN
1	X	280	ASN
1	X	312	ASN
1	X	331	ASN
1	X	378	GLN
1	X	444	ASN
1	X	505	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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
5	ATP	X	541	-	26,33,33	1.13	2 (7%)	31,52,52	1.22	3 (9%)
6	CO2	X	656[A]	-	2,2,2	1.38	0	1,1,1	0.78	0
6	CO2	X	656[B]	-	2,2,2	1.62	0	1,1,1	0.31	0
4	OAA	X	701	-	2,8,8	4.09	1 (50%)	2,10,10	1.11	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
5	ATP	X	541	-	-	7/18/38/38	0/3/3/3
4	OAA	X	701	-	-	0/2/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	701	OAA	O3-C3	5.72	1.31	1.22
5	X	541	ATP	O4'-C1'	2.97	1.45	1.41
5	X	541	ATP	C5-C4	2.74	1.48	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	541	ATP	N3-C2-N1	-2.68	124.48	128.68
5	X	541	ATP	O4'-C1'-C2'	-2.54	103.22	106.93
5	X	541	ATP	C4-C5-N7	-2.46	106.83	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

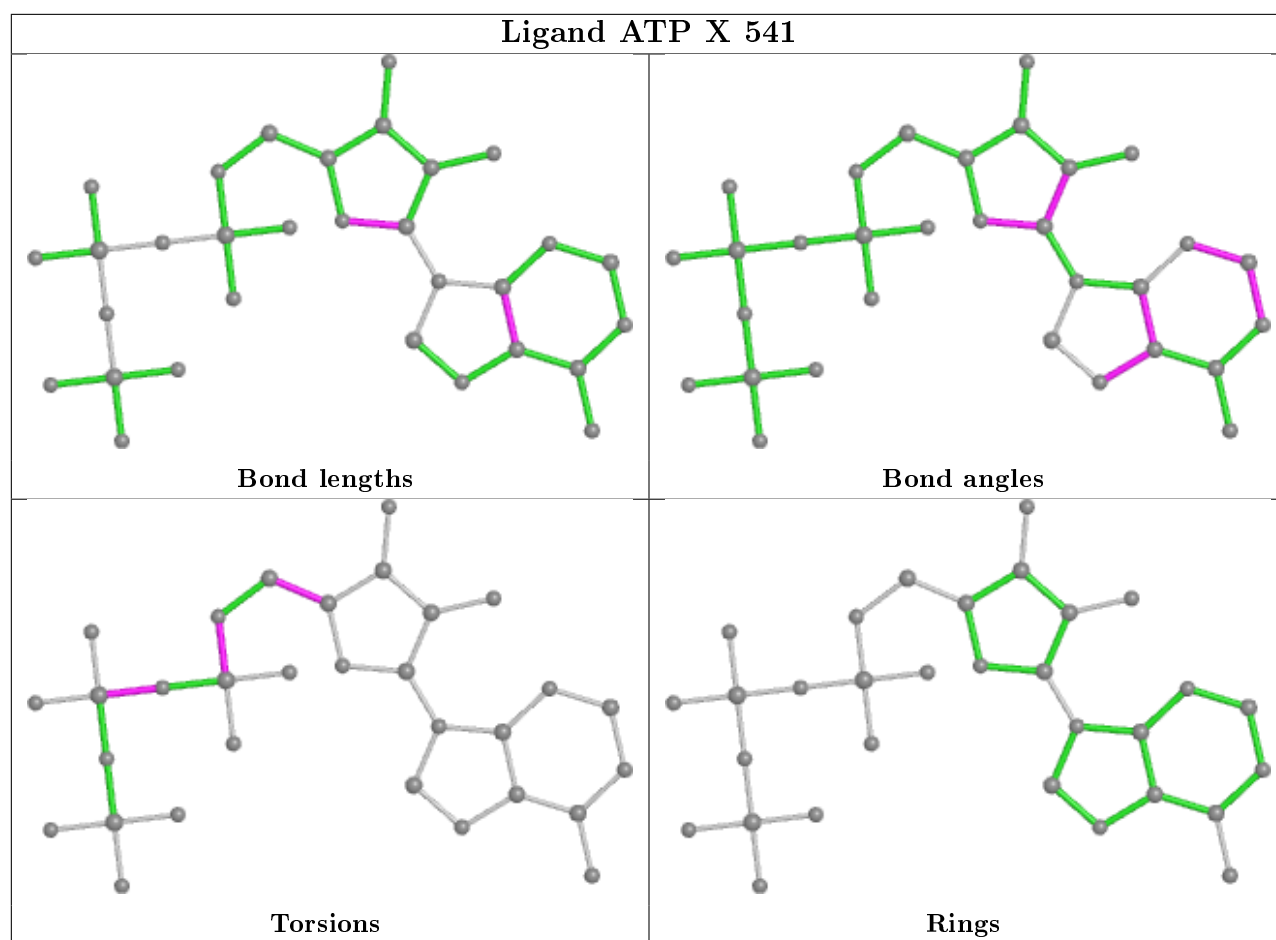
Mol	Chain	Res	Type	Atoms
5	X	541	ATP	C5'-O5'-PA-O1A
5	X	541	ATP	C5'-O5'-PA-O3A
5	X	541	ATP	C5'-O5'-PA-O2A
5	X	541	ATP	PA-O3A-PB-O2B
5	X	541	ATP	O4'-C4'-C5'-O5'
5	X	541	ATP	PA-O3A-PB-O1B
5	X	541	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	701	OAA	4	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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	71:TYR	C	72:ILE	N	1.19
1	X	427:LYS	C	428:ARG	N	1.19
1	X	437:TYR	C	438:LEU	N	1.16
1	X	426:VAL	C	427:LYS	N	1.13

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	526/540 (97%)	-0.57	1 (0%) 95 96	10, 19, 34, 43	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	528	PRO	2.8

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](#)

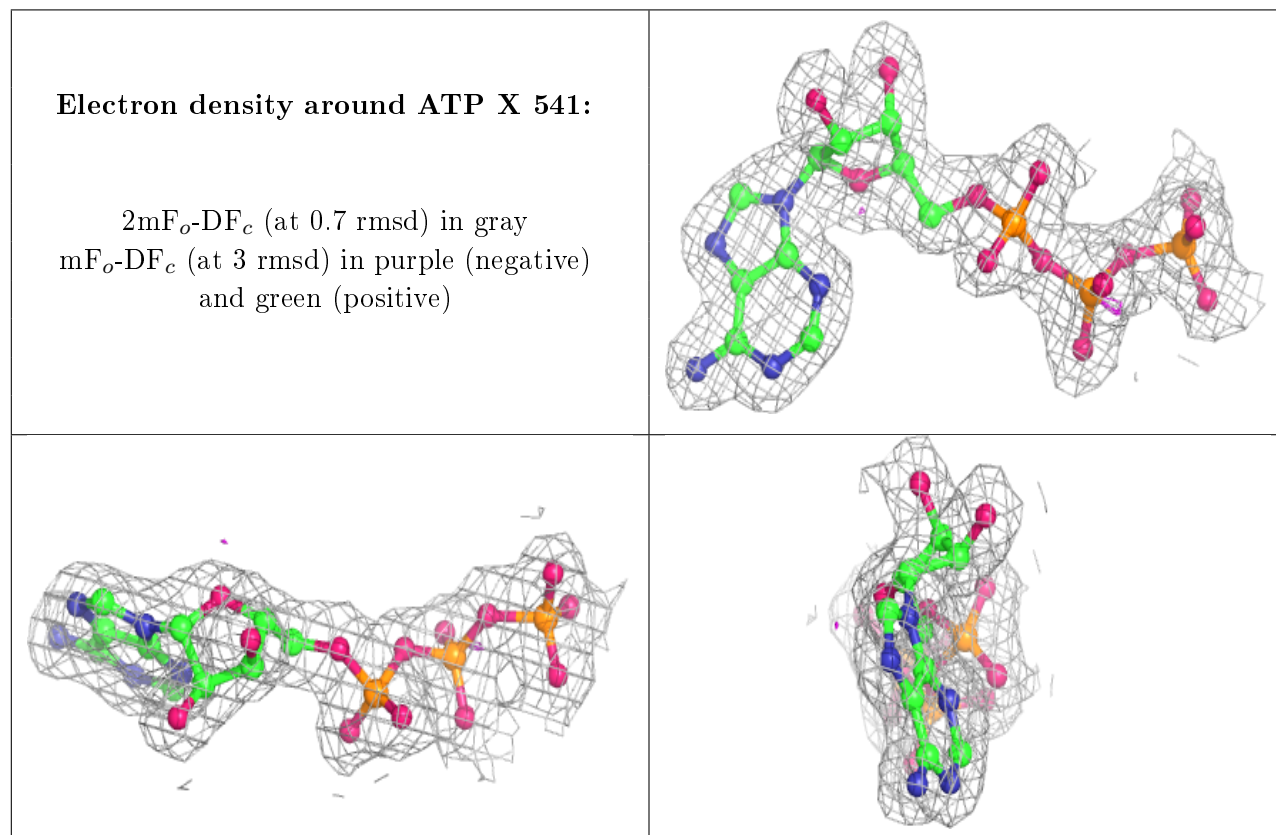
There are no carbohydrates in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OAA	X	701	9/9	0.76	0.33	17,28,33,38	9
6	CO2	X	656[B]	3/3	0.96	0.32	13,13,14,17	3
6	CO2	X	656[A]	3/3	0.96	0.32	6,6,6,8	3
5	ATP	X	541	31/31	0.98	0.08	13,19,22,23	0
2	MG	X	543	1/1	0.98	0.08	18,18,18,18	0
3	MN	X	700	1/1	1.00	0.08	27,27,27,27	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.