



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:54 am BST

PDB ID : 4HNT  
Title : crystal structure of F403A mutant of S. aureus Pyruvate carboxylase  
Authors : Yu, L.P.C.; Tong, L.  
Deposited on : 2012-10-21  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

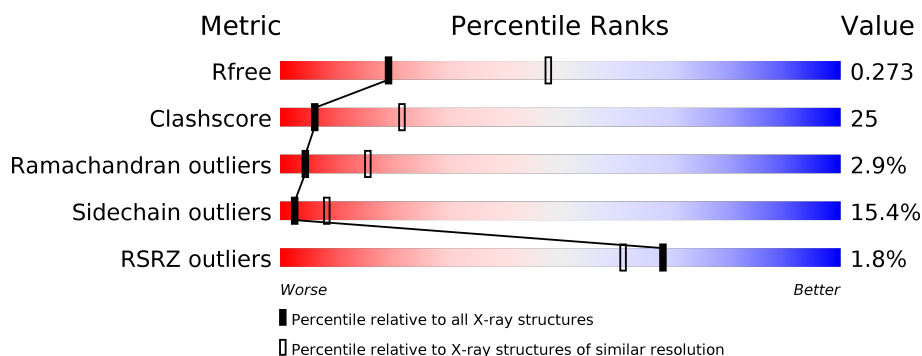
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	1173	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	1173	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>30%</div> <div>6%</div> <div>16%</div> </div> </div>
1	C	1173	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>9%</div> <div>10%</div> </div> </div>
1	D	1173	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>28%</div> <div>8%</div> <div>16%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ATP	C	1202	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8336	5286	1404	1619	27			
1	B	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8373	5307	1412	1626	28			
1	D	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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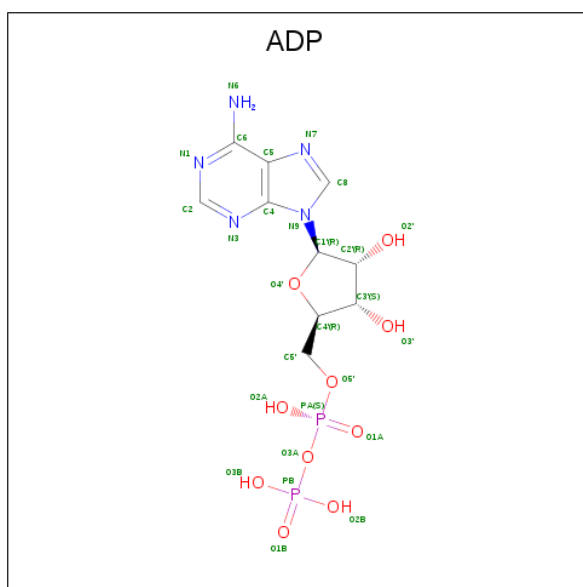
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

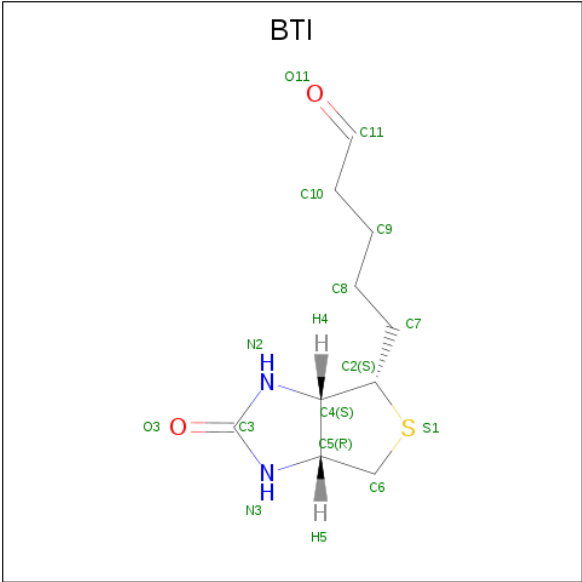


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

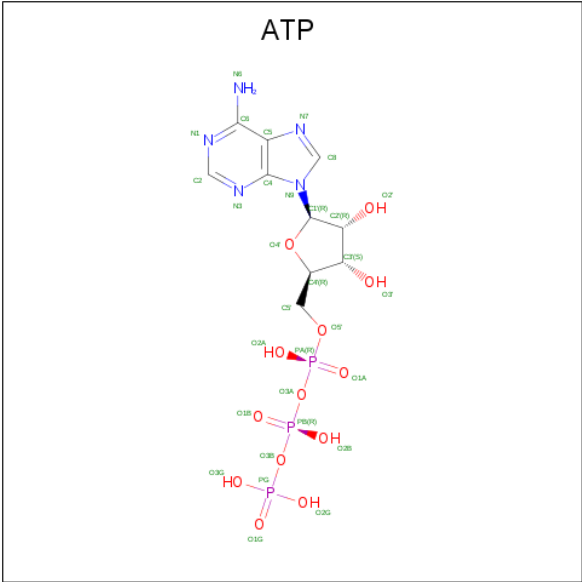
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



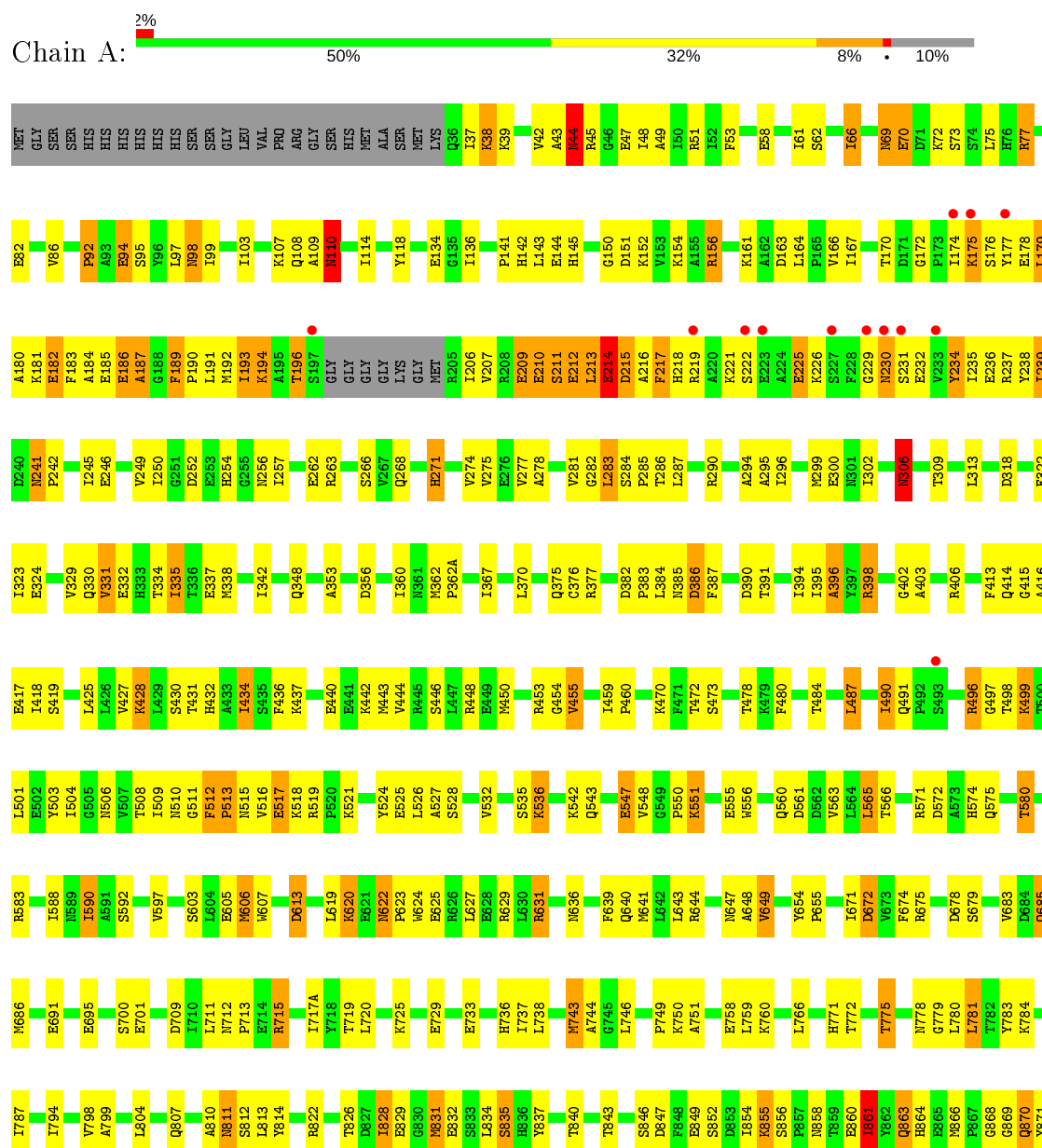


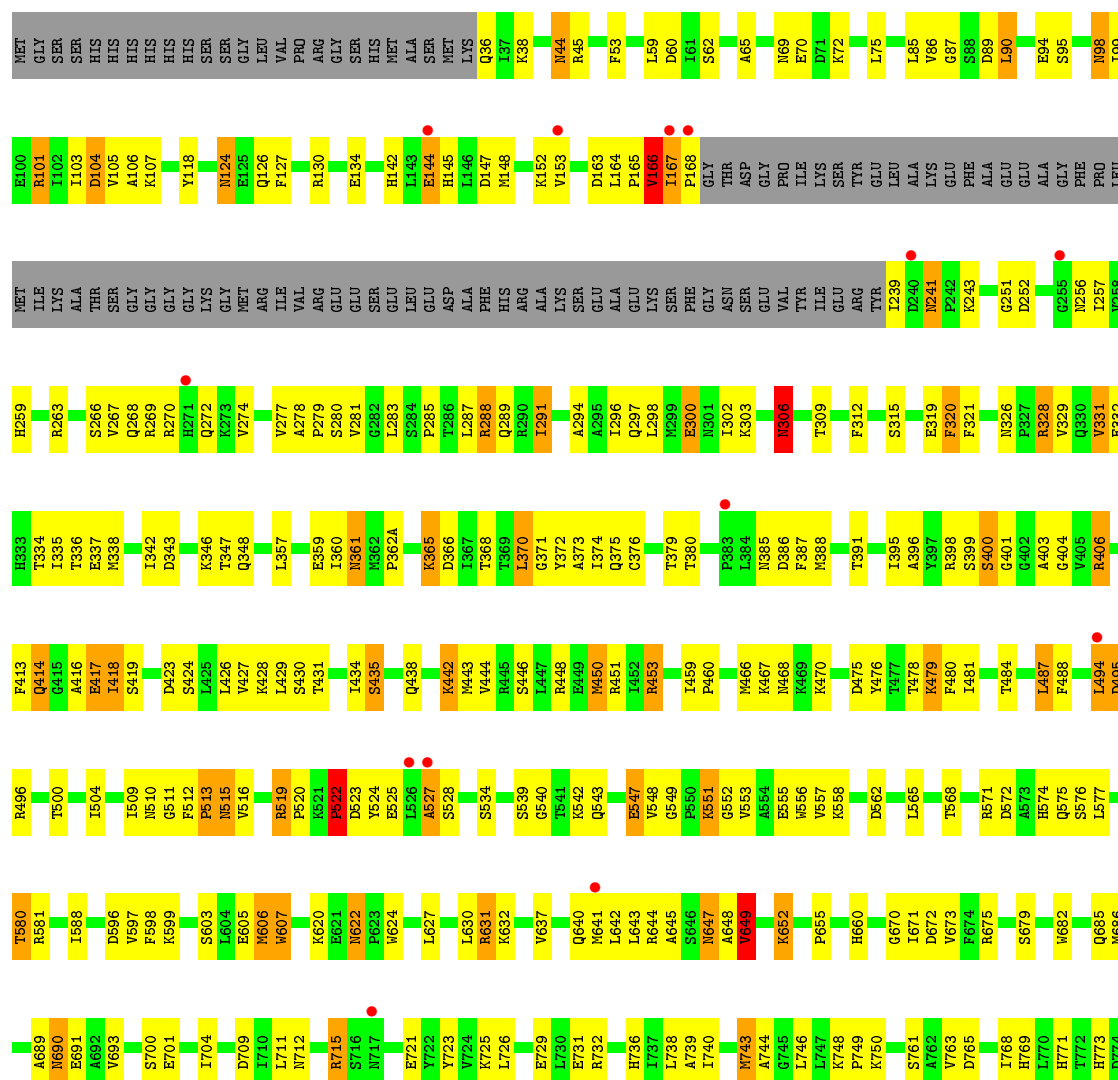
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

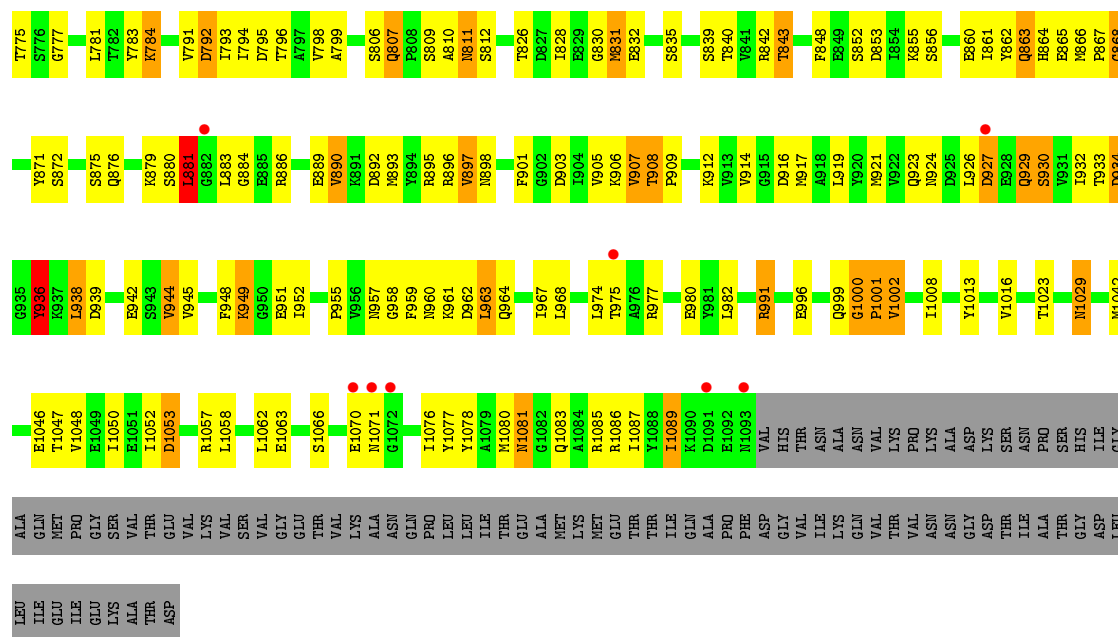
### 3 Residue-property plots

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.

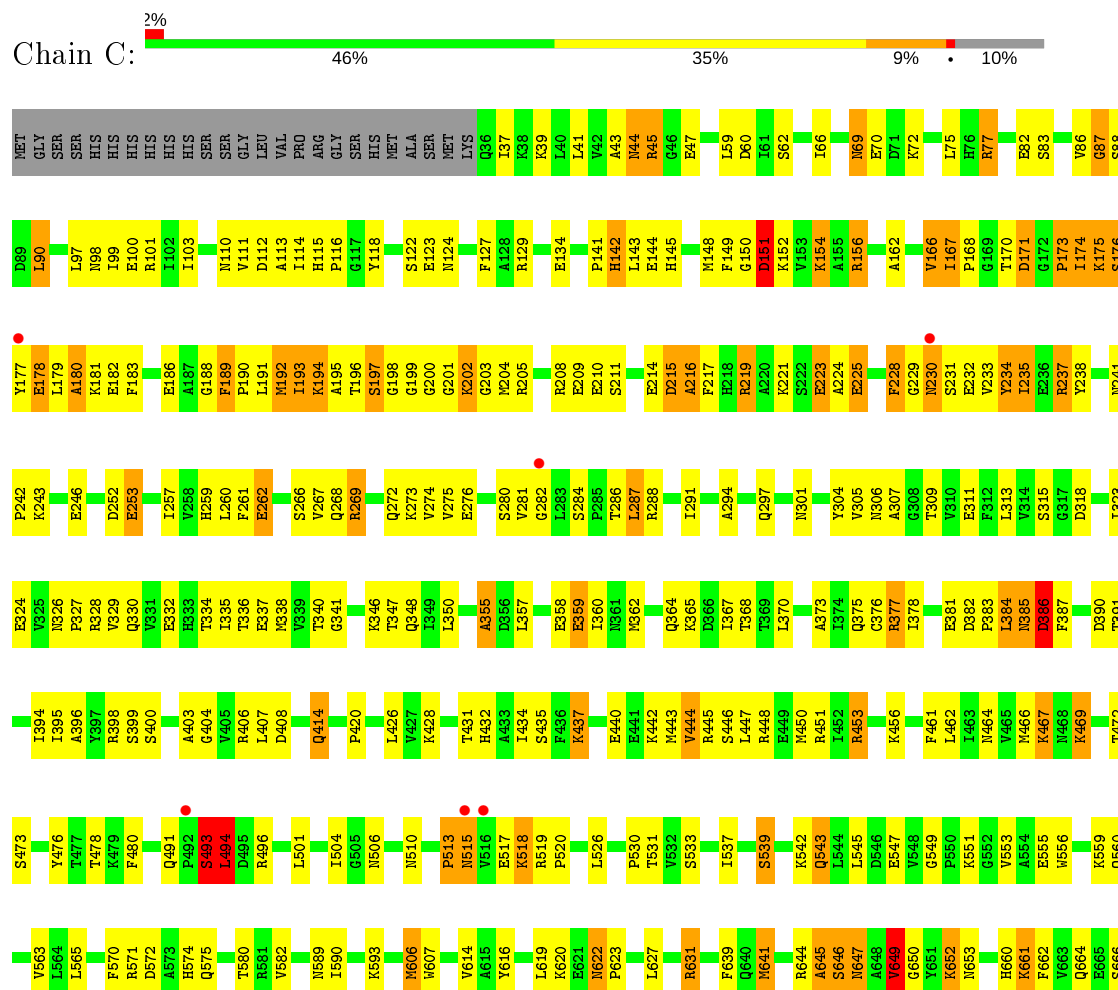
#### • Molecule 1: Pyruvate carboxylase







• Molecule 1: Pyruvate carboxylase





VAL	R1057	D939	H864	S776	M690	Q575	I490
GLY		F940	E865		M690		Q491
GLU	I1060		M866	T782		T580	P492
THR	K1061	V944		Y783	Q694	R581	S493
VAL	L1062	V945	G869	T784		V582	L494
LYS	E1063		Q870	Q785	K698	R583	D495
ALA	T1064	I952	Y871	A786	L699		R496
ASN				I787	S700	I588	Q497
GLN	D1069	N957	L874	V791	E701	N589	T498
PRO	E1070	N960	S875		T703	K593	K499
LEU	N1071						
LEU	G1072		A878	T796	T707	T594	L501
ILE	N1073	I963	K879			A595	
THR			S880	A799		D596	I504
GLU	Y1078	V966	L881	S800	L711	D597	G505
ALA	A1079	I967	G882			F598	N506
MET	M1080		L883	L804	E714	K599	
LYS		L974	G884	Q807	R715		N510
MET	Q1083		E885		S716	E605	G511
GLU	A1084	R977	R886		S717	R606	F512
THR	R1085	F978	F887	A810	I717	W607	P513
THR	R1086		D888	N811	I717A		R515
ILE	I1087	Y981			L720	T611	V516
GLN	Y1088		K891	Y814			E517
ALA	I1089	D886	D892	Y815	K725	L619	K518
PRO		F987	M893	A816		K620	R519
PHE	N1093	E988		L817	L730	E621	P520
ASP	VAL		R896				
GLY	HIS	R991	R897	F820	F735	P623	D523
THR	THR		N898	P821	H736	W624	Y524
ILE	ASN	E995	F899	R822	I737		E525
LYS	ALA	E996	L900		L738	R629	L526
GLN	ASN	E1004	F901	I828	A739	L630	A527
VAL	VAL		I904	E829	I740	R631	S528
THR	LYS	I1008		G830	K741	K632	I529
VAL	PRO			M831	D742		P530
ASN	LYS		V907	E832	M743	N636	T531
ASN	ALA	Y1013	T908		A744		V532
GLY	ASP	P1014	P909	H836	G745	Q640	S533
ASP	LYS	K1015	S910		L746	M641	
THR	SER	V1016	S911	S839			
ILE	ASN			T840	A752	R644	G540
ALA	PRO	T1023	M917				T541
THR	SER		A818	T843	I756	M647	K542
GLY	HIS	D1034	L919	Y844	G757	A645	Q543
ASP	ILE	T1035	Y920	Y845	E758	V649	
LEU	GLY	P1036	M921		L759	G650	K551
LEU	ALA			F848	K760		E555
ILE	GLN	M1042	N924	E849		Y654	
GLU	MET	R1043	D925	S852	V763		D561
ILE	PRO	N1044	L926	D853	D765	K661	D562
GLU	GLY	G1045	D927	I854	L766		V563
LYS	SER	E1046	E928	K855	P767	I671	L564
ALA	VAL	T1047	Q929	S856	I768	D672	L565
THR	THR		S930	P857	H769		
ASP	GLU	I1052	V931		L770	R675	F570
	VAL	D1053		E860	H771		R571
	LYS	K1054	G935	I861	I772	S679	D572
	VAL	G1055		Y862			A573
	SER	K1056	L938	Q863	T775	Q685	H574

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.23 Å   256.28 Å   126.69 Å 90.00°   109.86°   90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 91.0 (29.79-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, $R_{free}$	0.209   ,   0.279 0.207   ,   0.273	Depositor DCC
$R_{free}$ test set	6458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31   ,   48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN, BTI, ATP, ADP

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	0.68	1/8497 (0.0%)	0.73	1/11490 (0.0%)
1	B	0.63	4/7983 (0.1%)	0.66	3/10801 (0.0%)
1	C	0.65	4/8535 (0.0%)	0.68	4/11539 (0.0%)
1	D	0.66	5/7983 (0.1%)	0.70	2/10801 (0.0%)
All	All	0.65	14/32998 (0.0%)	0.69	10/44631 (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	6
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	18

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	14.00	1.80	1.52
1	B	936	TYR	C-N	11.65	1.60	1.34
1	C	513	PRO	C-N	10.85	1.58	1.34
1	C	515	ASN	N-CA	10.62	1.67	1.46
1	B	961	LYS	C-O	10.00	1.42	1.23

The worst 5 of 10 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	C-N-CA	8.07	141.87	121.70
1	D	513	PRO	CA-C-N	7.87	134.51	117.20
1	C	513	PRO	CA-C-N	7.83	134.42	117.20
1	B	763	VAL	CA-C-N	7.35	133.38	117.20
1	C	513	PRO	N-CA-CB	-6.11	95.88	102.60

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	GLY	Peptide
1	A	196	THR	Peptide
1	A	271	HIS	Peptide
1	A	415	GLY	Peptide
1	A	490	ILE	Peptide

## 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	8336	0	8249	430	0
1	B	7832	0	7767	352	0
1	C	8373	0	8287	456	0
1	D	7832	0	7767	376	0
2	A	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	16	4	0
4	B	15	0	16	4	0
4	D	15	0	16	3	0
5	C	31	0	12	10	0
All	All	32480	0	32142	1586	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 25.

The worst 5 of 1586 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:C:515:ASN:N	1:C:515:ASN:CA	1.67	1.56
1:C:513:PRO:CA	1:C:513:PRO:C	1.80	1.47
1:D:607:TRP:HE3	1:D:641:MET:CE	1.51	1.23
1:C:918:ALA:O	1:C:922:VAL:HG23	1.39	1.22
1:B:403:ALA:O	1:B:442:LYS:HE2	1.42	1.18

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	1048/1173 (89%)	916 (87%)	102 (10%)	30 (3%)	4	15
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	6	20
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	3	11
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	5	17
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	4	15

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	211	SER
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE

### 5.3.2 Protein sidechains ⓘ

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	907/1005 (90%)	778 (86%)	129 (14%)	3	10
1	B	855/1005 (85%)	726 (85%)	129 (15%)	3	9
1	C	909/1005 (90%)	751 (83%)	158 (17%)	2	6
1	D	855/1005 (85%)	727 (85%)	128 (15%)	3	9
All	All	3526/4020 (88%)	2982 (85%)	544 (15%)	2	8

5 of 544 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	944	VAL
1	C	269	ARG
1	D	714	GLU
1	B	1057	ARG
1	C	154	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	998	GLN
1	C	330	GLN
1	D	778	ASN
1	B	1025	ASN
1	C	98	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
2	ADP	A	1201	-	24,29,29	1.04	2 (8%)	29,45,45	1.46	6 (20%)
4	BTI	D	1201	-	16,16,16	1.64	2 (12%)	21,21,21	2.05	5 (23%)
5	ATP	C	1202	-	26,33,33	0.99	2 (7%)	31,52,52	1.37	4 (12%)
4	BTI	A	1203	-	16,16,16	1.69	2 (12%)	21,21,21	1.98	5 (23%)
4	BTI	B	1201	-	16,16,16	1.62	2 (12%)	21,21,21	2.49	5 (23%)

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
2	ADP	A	1201	-	-	6/12/32/32	0/3/3/3
4	BTI	D	1201	-	-	1/5/27/27	0/2/2/2
5	ATP	C	1202	-	-	3/18/38/38	0/3/3/3
4	BTI	A	1203	-	-	4/5/27/27	0/2/2/2
4	BTI	B	1201	-	-	3/5/27/27	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	O3-C3	5.10	1.34	1.23
4	B	1201	BTI	O3-C3	5.08	1.34	1.23
4	D	1201	BTI	O3-C3	4.88	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	C2-S1	-3.60	1.76	1.82
4	D	1201	BTI	C2-S1	-3.32	1.77	1.82

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	BTI	C2-C4-N2	-8.60	105.42	113.13
4	D	1201	BTI	C2-C4-N2	-5.95	107.80	113.13
4	A	1203	BTI	C5-C6-S1	4.96	110.56	106.31
4	B	1201	BTI	C6-C5-N3	-4.91	106.80	113.03
4	A	1203	BTI	C6-C5-N3	-4.90	106.80	113.03

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O1A
2	A	1201	ADP	C5'-O5'-PA-O2A
2	A	1201	ADP	C5'-O5'-PA-O3A
5	C	1202	ATP	O4'-C4'-C5'-O5'
5	C	1202	ATP	C3'-C4'-C5'-O5'

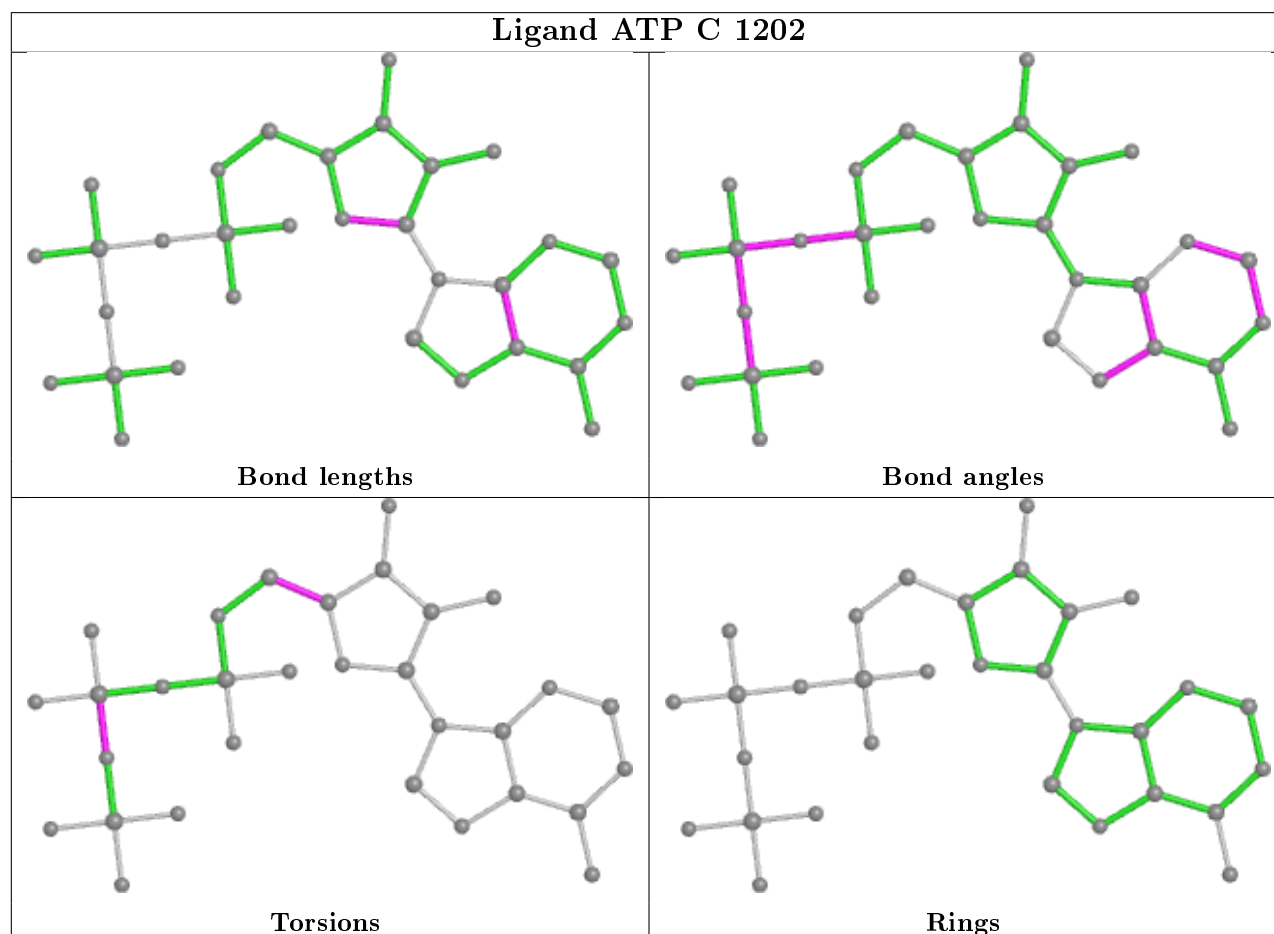
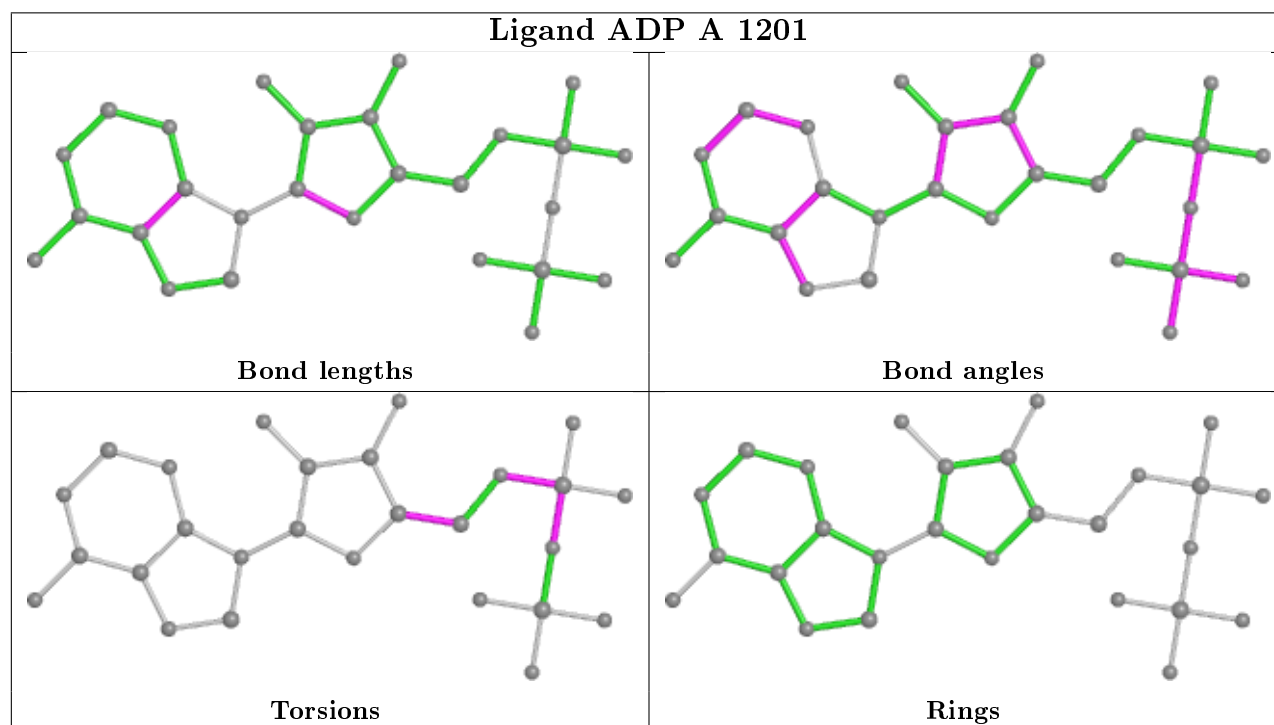
There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ADP	1	0
4	D	1201	BTI	3	0
5	C	1202	ATP	10	0
4	A	1203	BTI	4	0
4	B	1201	BTI	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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	936:TYR	C	937:LYS	N	1.60

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1052/1173 (89%)	-0.29	18 (1%) 70 63	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.19	21 (2%) 63 54	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.15	22 (2%) 63 54	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.25	11 (1%) 80 75	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.22	72 (1%) 68 61	47, 80, 125, 178	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	SER	4.8
1	A	233	VAL	4.4
1	D	490	ILE	4.3
1	A	229	GLY	4.3
1	A	177	TYR	4.1

### 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.

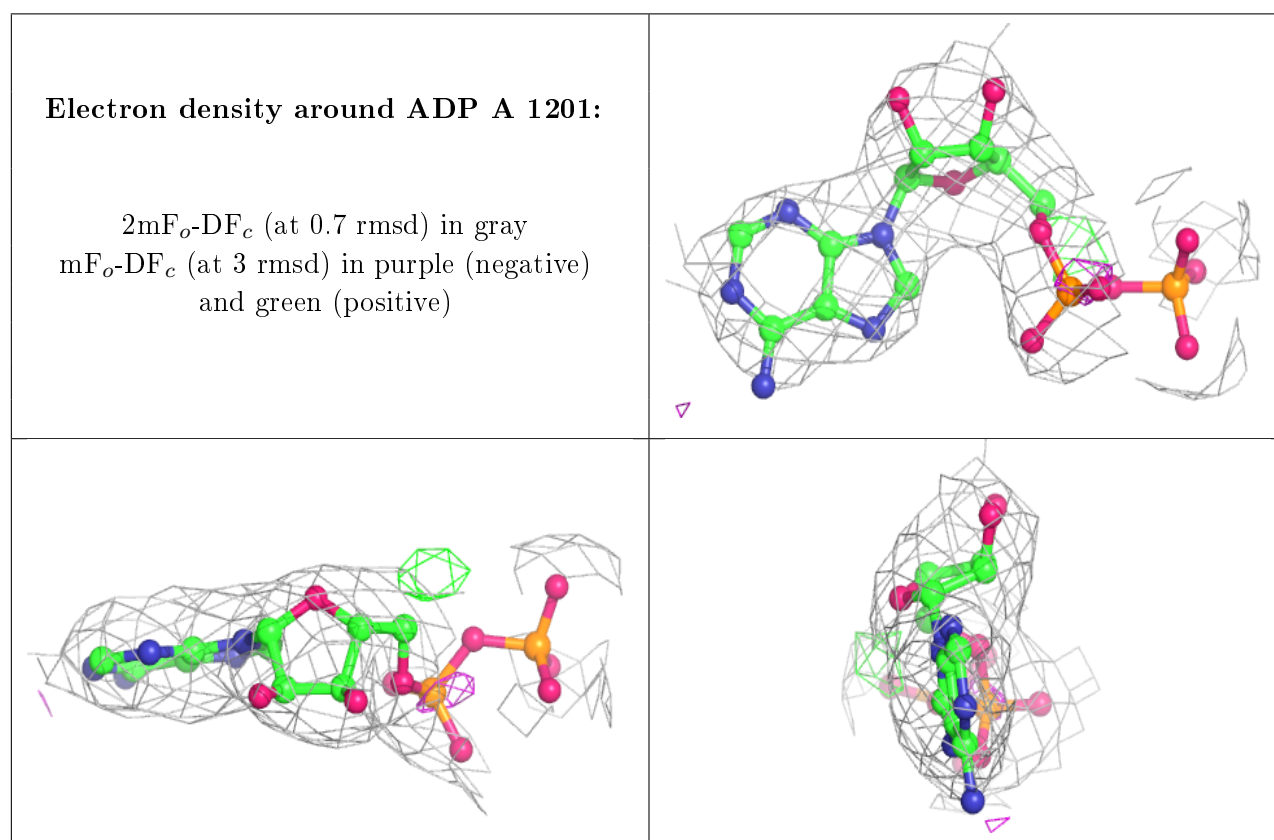
### 6.4 Ligands [i](#)

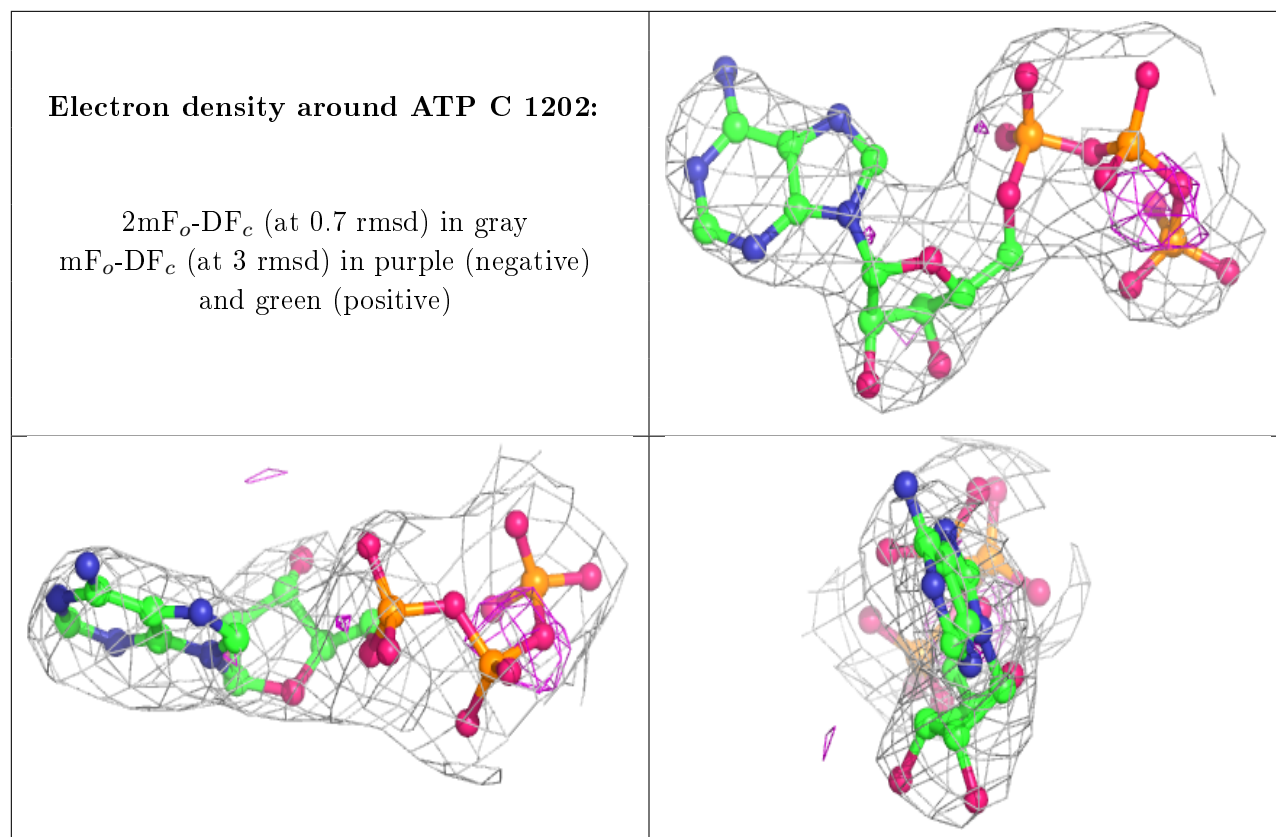
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
2	ADP	A	1201	27/27	0.89	0.18	86,91,110,110	0
4	BTI	B	1201	15/15	0.91	0.34	105,109,114,115	0
4	BTI	D	1201	15/15	0.92	0.30	105,109,113,116	0
4	BTI	A	1203	15/15	0.93	0.29	92,99,104,105	0
5	ATP	C	1202	31/31	0.94	0.14	102,108,115,115	0
3	MN	B	1202	1/1	0.97	0.18	82,82,82,82	0
3	MN	C	1201	1/1	0.98	0.26	76,76,76,76	0
3	MN	A	1202	1/1	0.99	0.19	74,74,74,74	0
3	MN	D	1202	1/1	0.99	0.19	74,74,74,74	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.