



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:15 PM GMT

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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

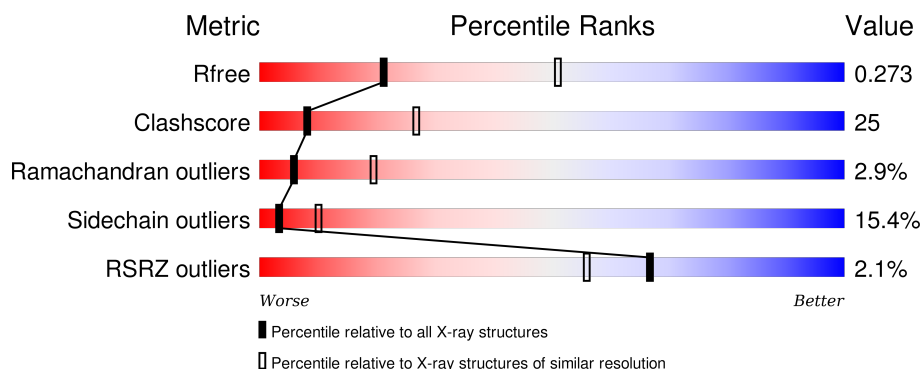
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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
4	BTI	A	1203	-	-	-	X
4	BTI	B	1201	-	-	-	X
4	BTI	D	1201	-	-	-	X
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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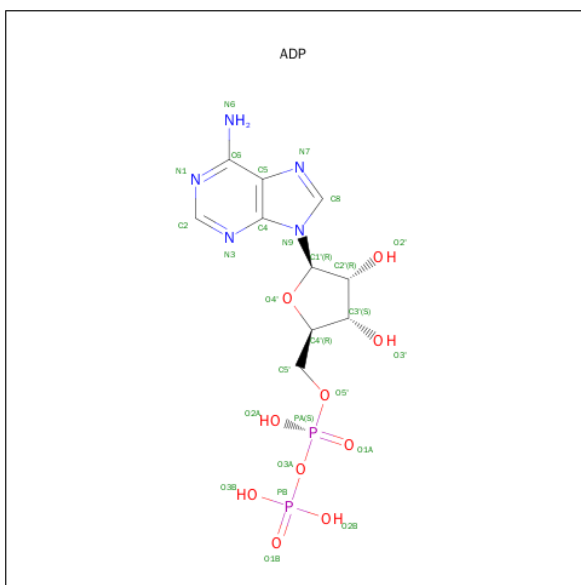
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
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:  $C_{10}H_{15}N_5O_{10}P_2$ ).

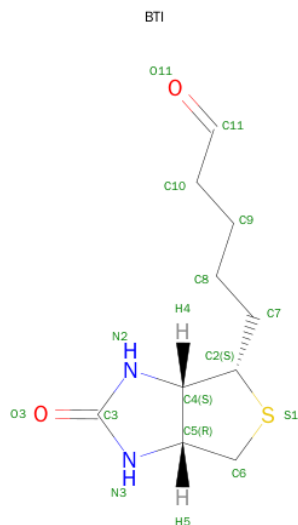


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

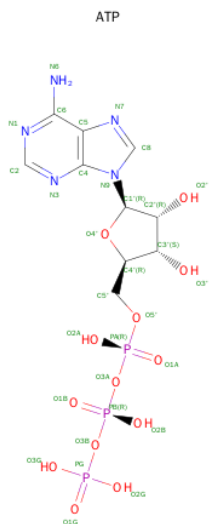
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- 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 15	C 10	N 2	O 2	S 1	0	0
4	B	1	Total 15	C 10	N 2	O 2	S 1	0	0
4	D	1	Total 15	C 10	N 2	O 2	S 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



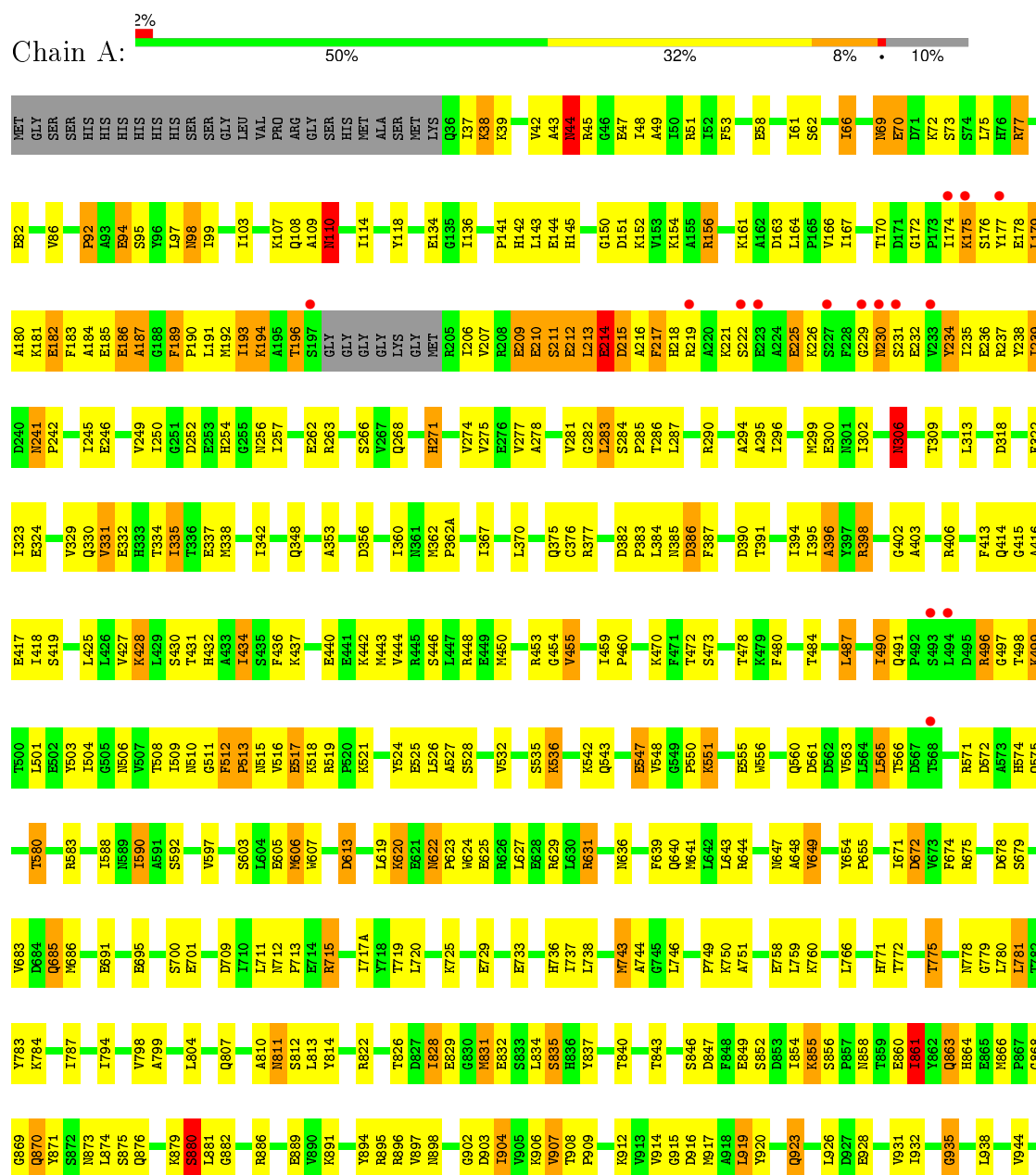


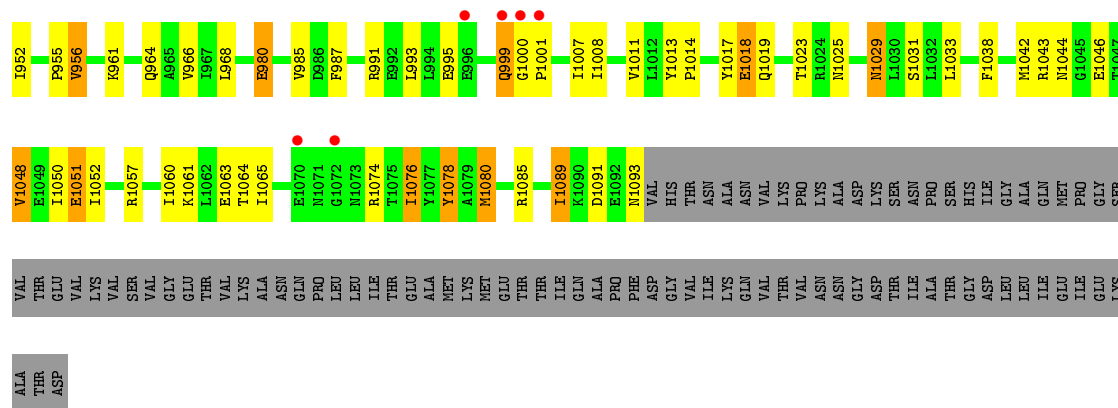
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

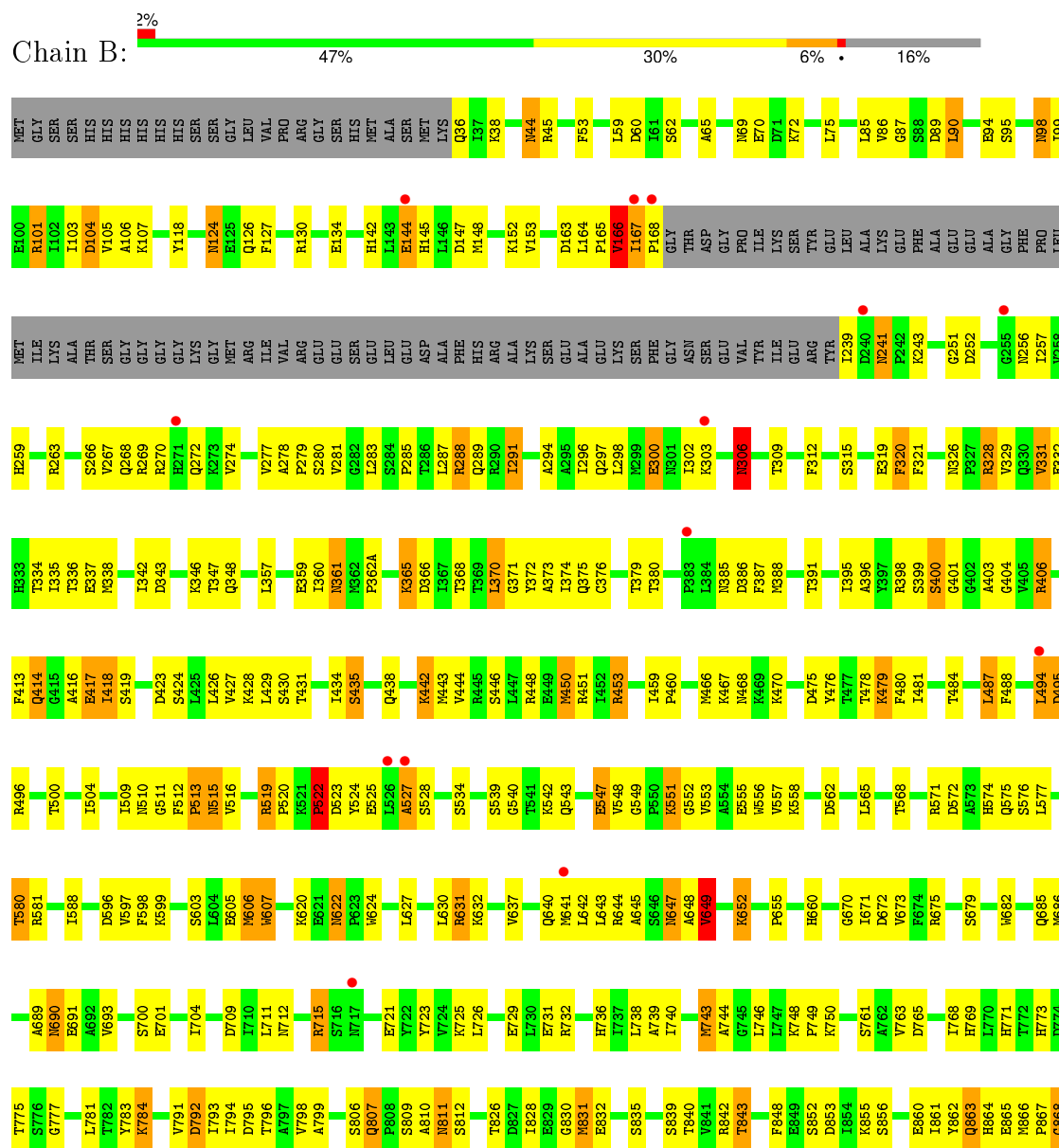
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

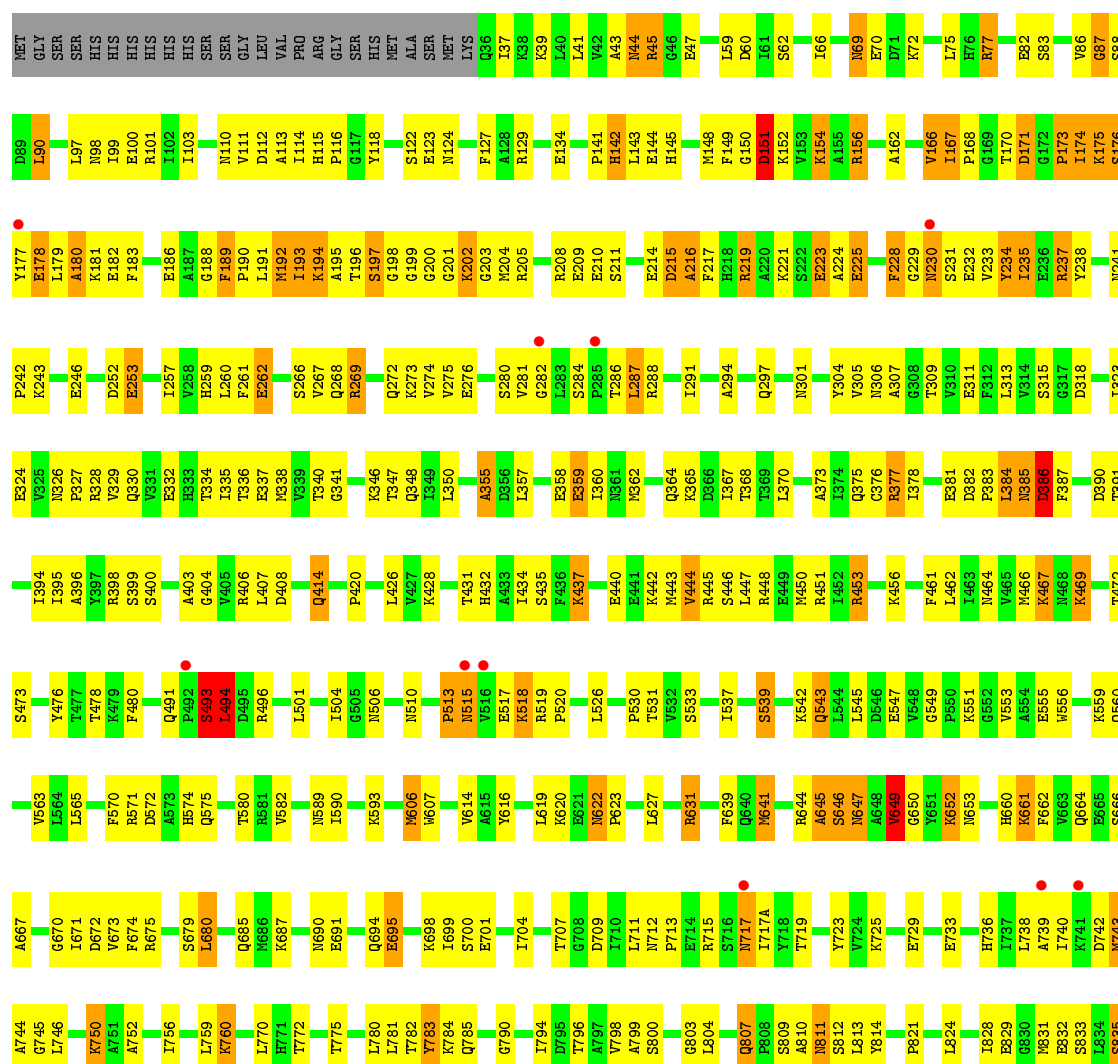
#### • Molecule 1: Pyruvate carboxylase

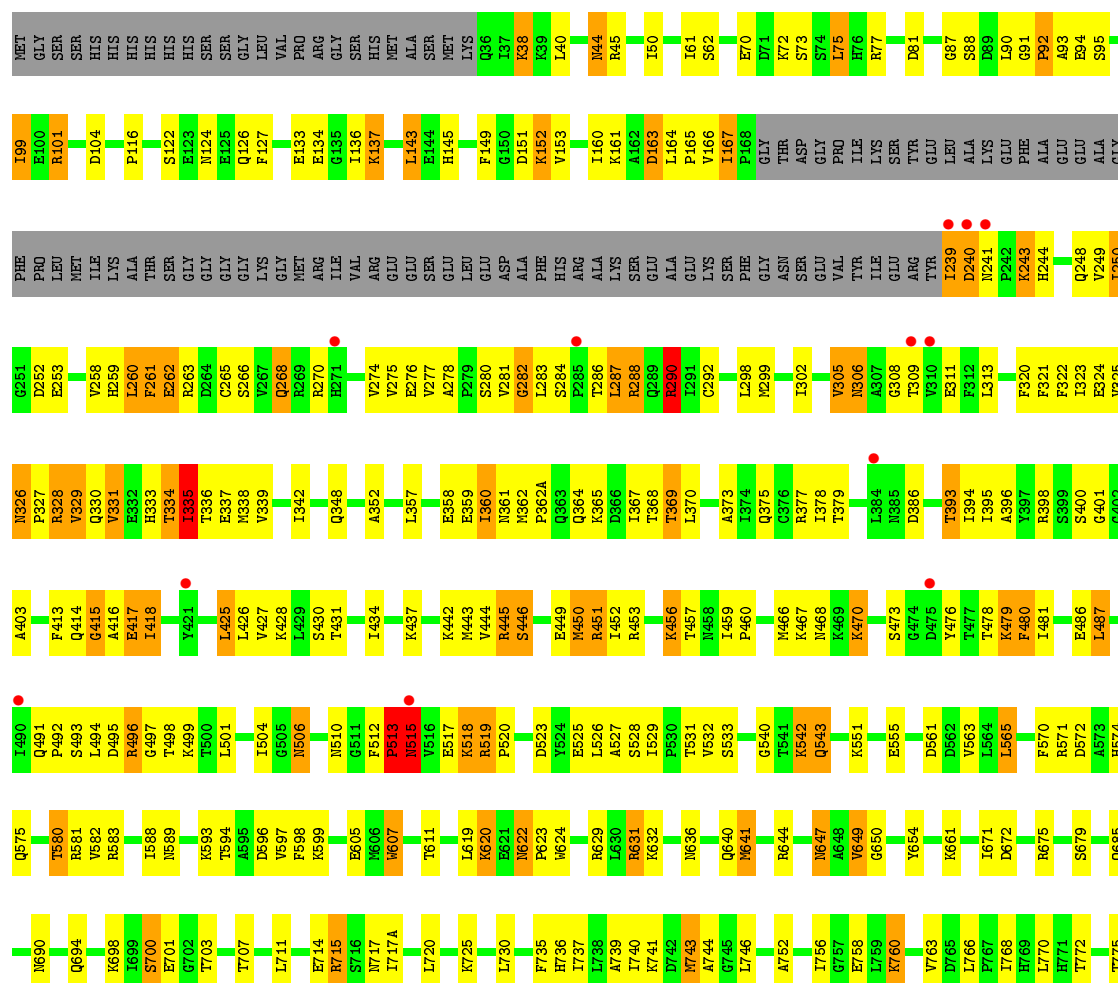




### • Molecule 1: Pyruvate carboxylase







VAL	R1057	D939	H864	S776
GLY	I1060	F940	E865	
GLU	K1061	V944	M866	T782
THR	I1062	V945	G869	Y783
VAL	E1063	I952	Q870	K784
LYS	T1064	N957	Y871	Q785
ALA				A786
ASN	D1069	N974	L874	I787
GLN	E1070	N960	S875	V791
PRO	N1071	L963	A878	T796
LEU	G1072	V966	K879	
ILE	N1073	I967	S880	A799
THR		I974	L881	S800
GLU	Y1078	R977	L883	L804
GLU	A1079	P978	G884	
ALA	M1080	Y981	E885	Q807
MET	Q1083	D886	R886	A810
MET	A1084	F887	D888	N811
GLU	R1085	E988		
THR	R1086	R991	R896	Y814
THR	I1087	E995	V897	Y815
ILE	Y1088	E996	N898	A816
GLN	I1089	E1004	F899	L817
ALA		I1008	L900	
PRO	N1093	Y1013	F901	
ASP	VAL	P1014	I904	
GLY	HIS	R1015	V907	
THR	THR	LYS	T908	H836
ILE	ASN	THR	P909	
LYS	ALA	ASN	S910	S839
GLN	ASN	SER	S911	T840
VAL	VAL	ASN		
THR	PRO	PRO	M917	
VAL	LYS	LYS	A918	T843
ASN	ALA	ALA	L919	T844
ASN	ASP	ASP	Y920	Y845
GLY	LYS	THR	M921	
ASP	THR	ILE		F848
THR	ILE	ALA	N924	E849
ALA	PRO	GLN	D925	S852
THR	SER	MET	L926	D853
GLY	HIS	PRO	N927	K854
ASP	ILE	ILE	E928	K855
LEU	GLY	GLY	Q929	S856
LEU	LEU	SER	S930	P857
ILE	ALA	VAL	Y931	
GLU	GLN	THR		E860
ILE	MET	THR		L861
ILE	PRO	THR		Y862
GLU	GLY	THR		Q863
LYS	GLY	THR		
LYS	VAL	THR		
ALA	VAL	THR		
THR	VAL	THR		
ASP	SER	THR		

## 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	Depositor
R, $R_{free}$	0.209   ,   0.279 0.207   ,   0.273	Depositor DCC
$R_{free}$ test set	7085 reflections (5.81%)	DCC
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   ,   48.9	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 128487 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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%)	6	19
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	7	25
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	4	14
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	6	21
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	6	19

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%)	4	12
1	B	855/1005 (85%)	726 (85%)	129 (15%)	3	10
1	C	909/1005 (90%)	751 (83%)	158 (17%)	2	7
1	D	855/1005 (85%)	727 (85%)	128 (15%)	3	11
All	All	3526/4020 (88%)	2982 (85%)	544 (15%)	3	10

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	-	22,29,29	1.07	2 (9%)	27,45,45	2.10	5 (18%)
4	BTI	A	1203	-	14,16,16	1.89	2 (14%)	13,21,21	1.51	3 (23%)
4	BTI	B	1201	-	14,16,16	1.82	3 (21%)	13,21,21	1.42	2 (15%)
5	ATP	C	1202	-	24,33,33	1.06	2 (8%)	31,52,52	2.14	5 (16%)
4	BTI	D	1201	-	14,16,16	1.83	2 (14%)	13,21,21	1.50	2 (15%)

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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	C2-S1	-3.61	1.76	1.82
4	D	1201	BTI	C2-S1	-3.32	1.77	1.82
4	B	1201	BTI	C2-S1	-2.97	1.77	1.82
4	B	1201	BTI	C3-N2	-2.08	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ADP	O4'-C1'	2.46	1.44	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	N3-C2-N1	-7.22	123.36	128.89
5	C	1202	ATP	C2'-C1'-N9	-6.70	104.06	114.29
5	C	1202	ATP	N3-C2-N1	-6.24	124.12	128.89
5	C	1202	ATP	PA-O3A-PB	-4.64	119.71	132.73
2	A	1201	ADP	C2'-C1'-N9	-4.27	107.77	114.29

There are no chirality outliers.

There are no torsion outliers.

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	A	1203	BTI	4	0
4	B	1201	BTI	4	0
5	C	1202	ATP	10	0
4	D	1201	BTI	3	0

## 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 [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%)	-0.25	21 (1%) 68 58	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.16	25 (2%) 61 48	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.11	26 (2%) 61 48	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.22	13 (1%) 79 71	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.18	85 (2%) 67 56	47, 80, 125, 178	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	SER	5.2
1	A	229	GLY	4.7
1	A	233	VAL	4.6
1	D	490	ILE	4.6
1	D	240	ASP	4.3

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BTI	A	1203	15/15	0.93	0.30	3.03	92,99,104,105	0
4	BTI	B	1201	15/15	0.91	0.33	2.30	105,109,114,115	0
4	BTI	D	1201	15/15	0.92	0.29	2.30	105,109,113,116	0
3	MN	C	1201	1/1	0.98	0.27	0.04	76,76,76,76	0
3	MN	D	1202	1/1	0.99	0.19	-0.14	74,74,74,74	0
3	MN	B	1202	1/1	0.97	0.19	-0.33	82,82,82,82	0
2	ADP	A	1201	27/27	0.89	0.18	-0.36	86,91,110,110	0
3	MN	A	1202	1/1	0.99	0.20	-0.42	74,74,74,74	0
5	ATP	C	1202	31/31	0.94	0.16	-0.65	102,108,115,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.