



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:35 PM UTC

PDB ID : 4HNT / pdb_00004hnt
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

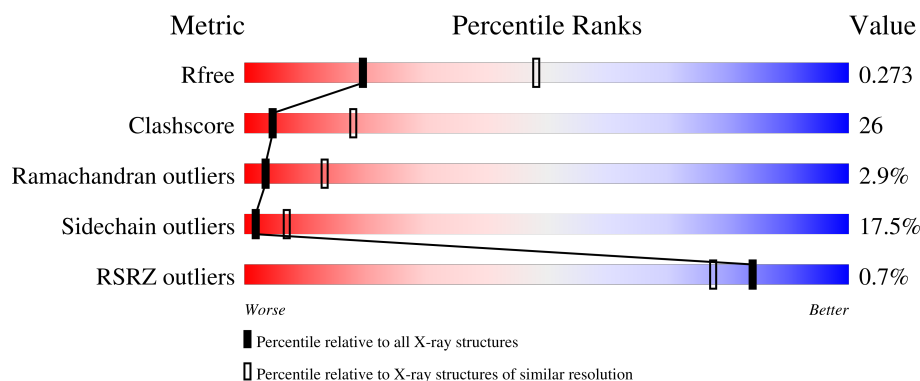
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	47% 33% 9% 10%
1	B	1173	45% 31% 8% 16%
1	C	1173	44% 35% 10% 10%
1	D	1173	46% 29% 9% 16%

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	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

Continued on next page...

Continued from previous page...

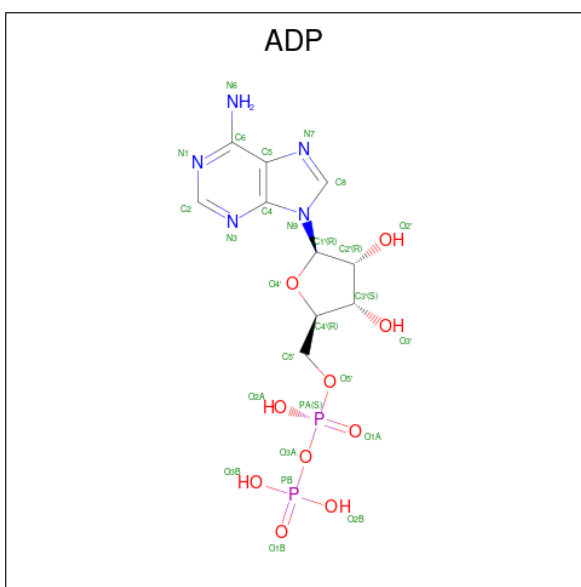
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag	UNP Q99UY8
B	15	HIS	-	expression tag	UNP Q99UY8
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

Continued on next page...

Continued from previous page...

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

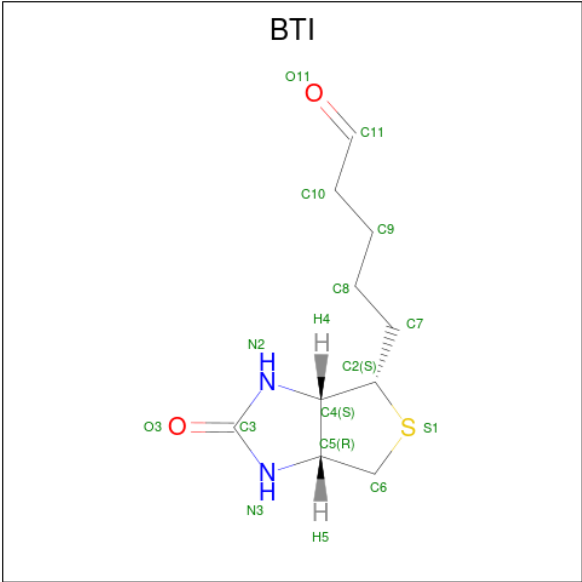


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

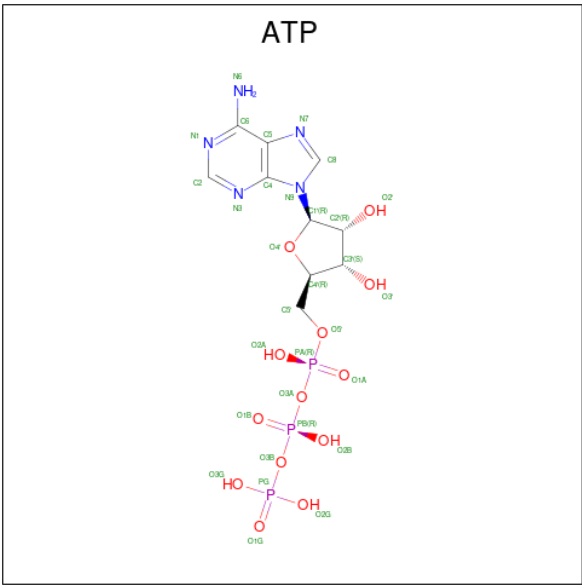
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

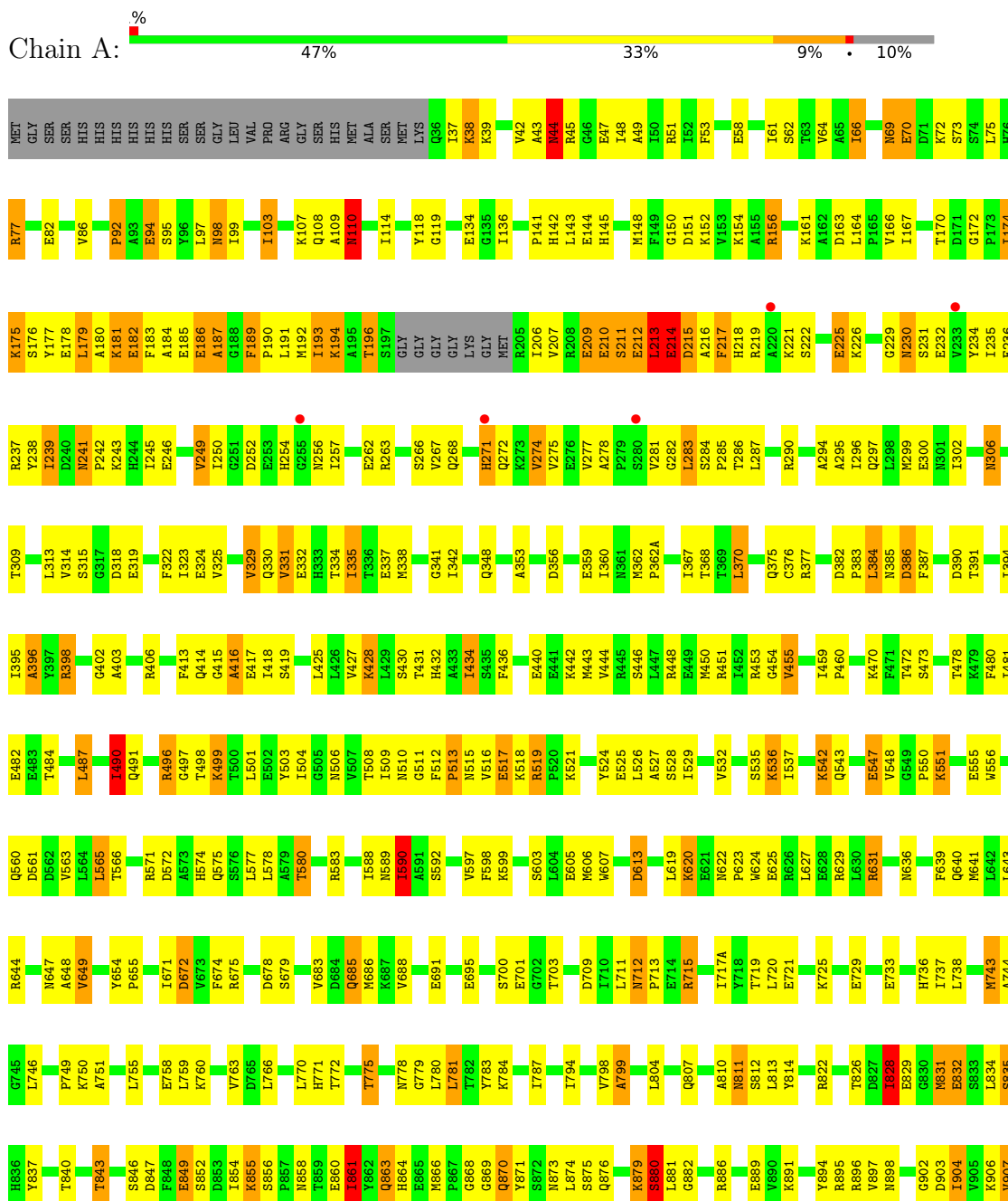


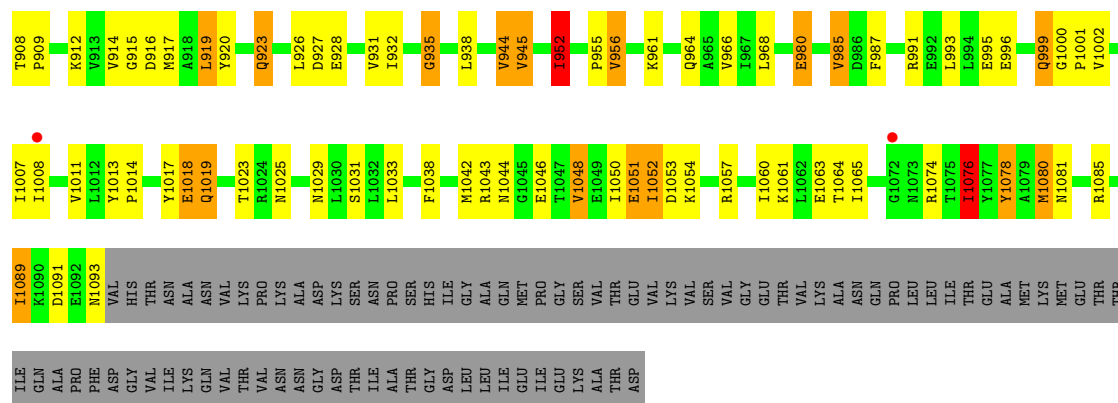
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

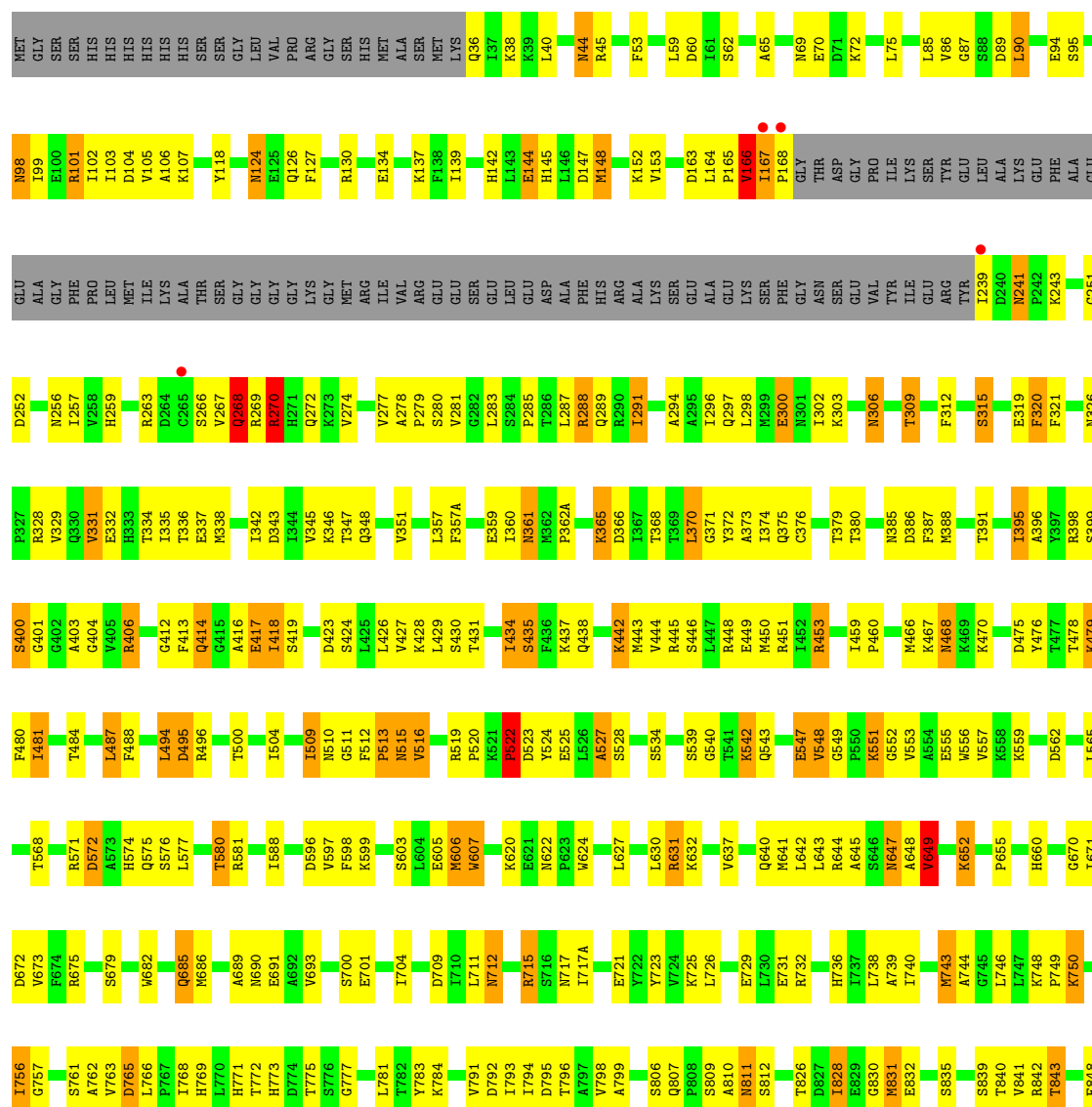
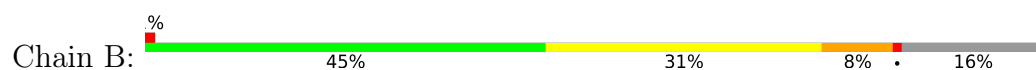
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

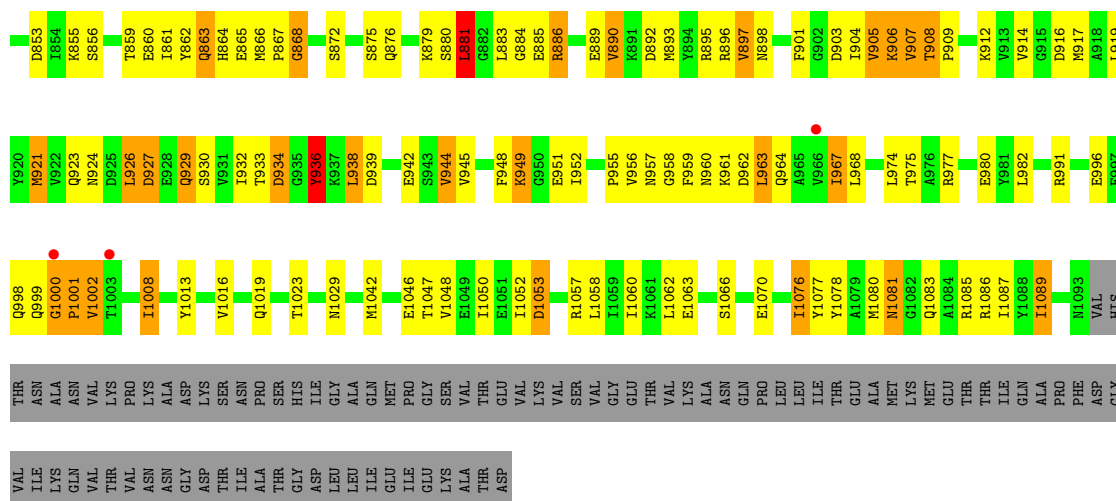
• Molecule 1: Pyruvate carboxylase



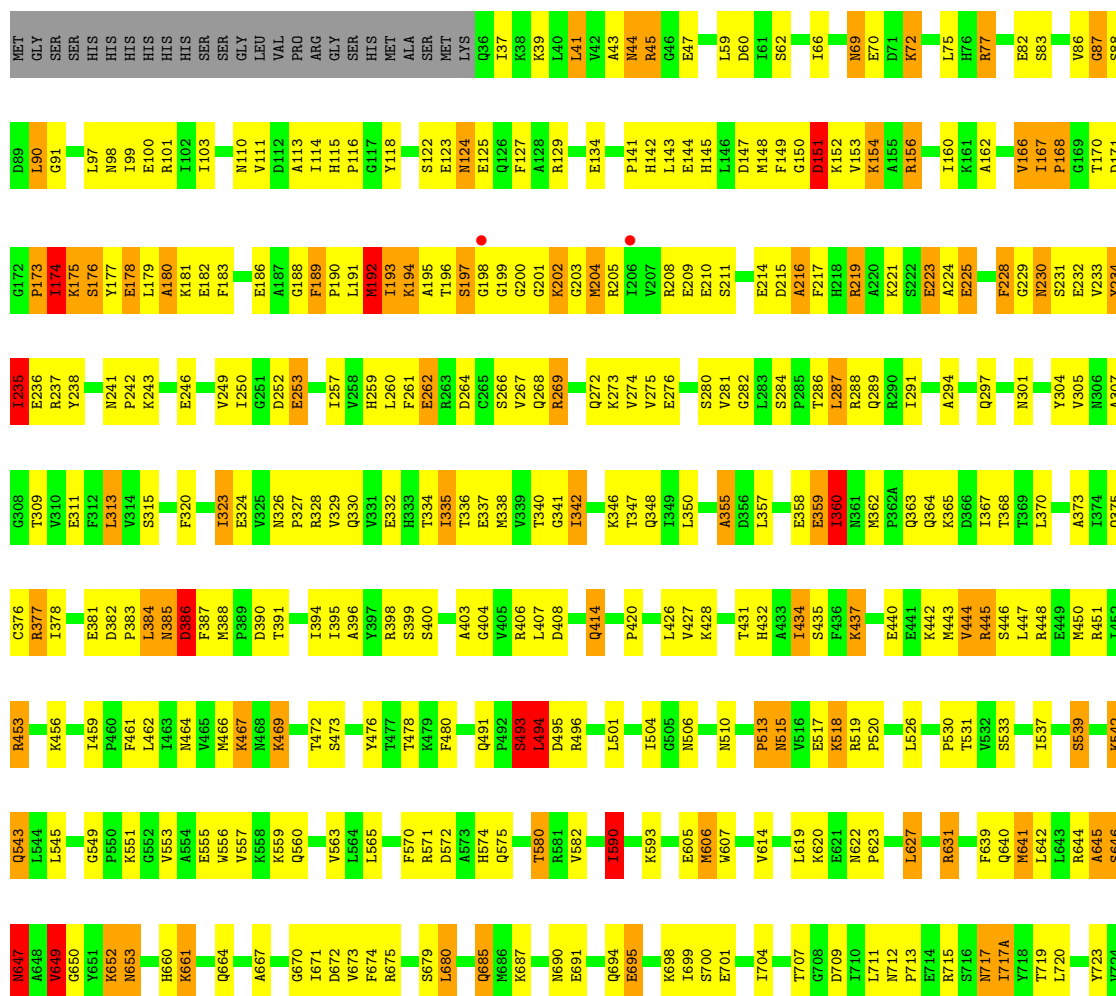


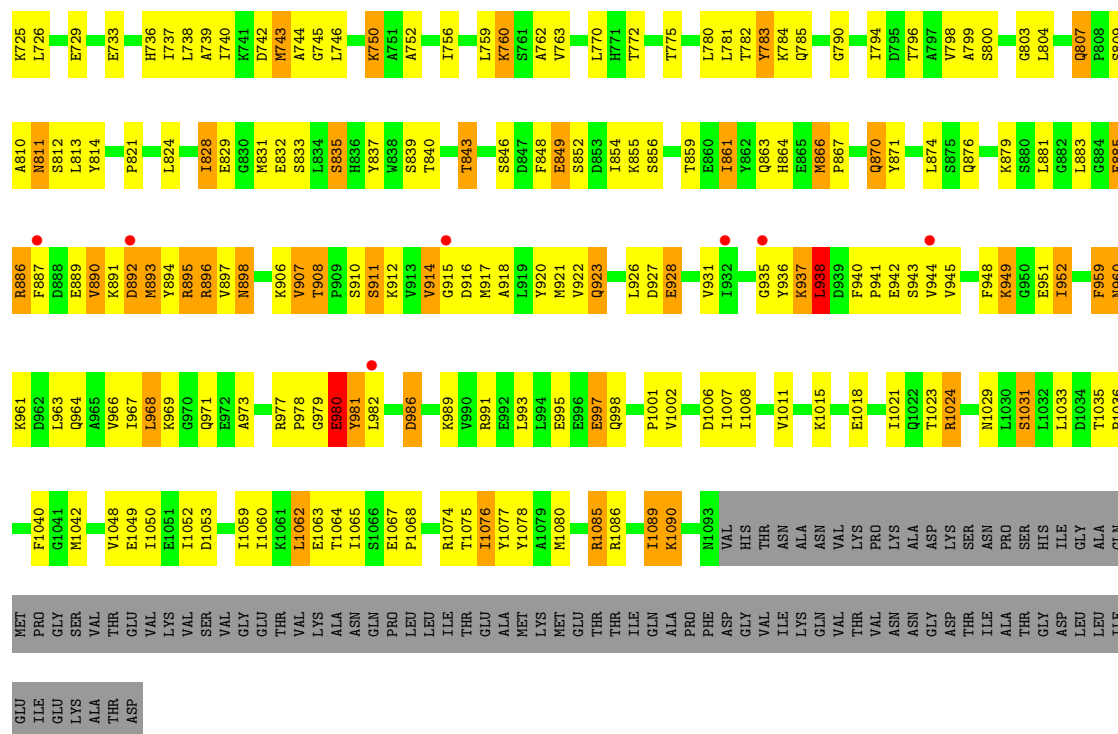
• Molecule 1: Pyruvate carboxylase



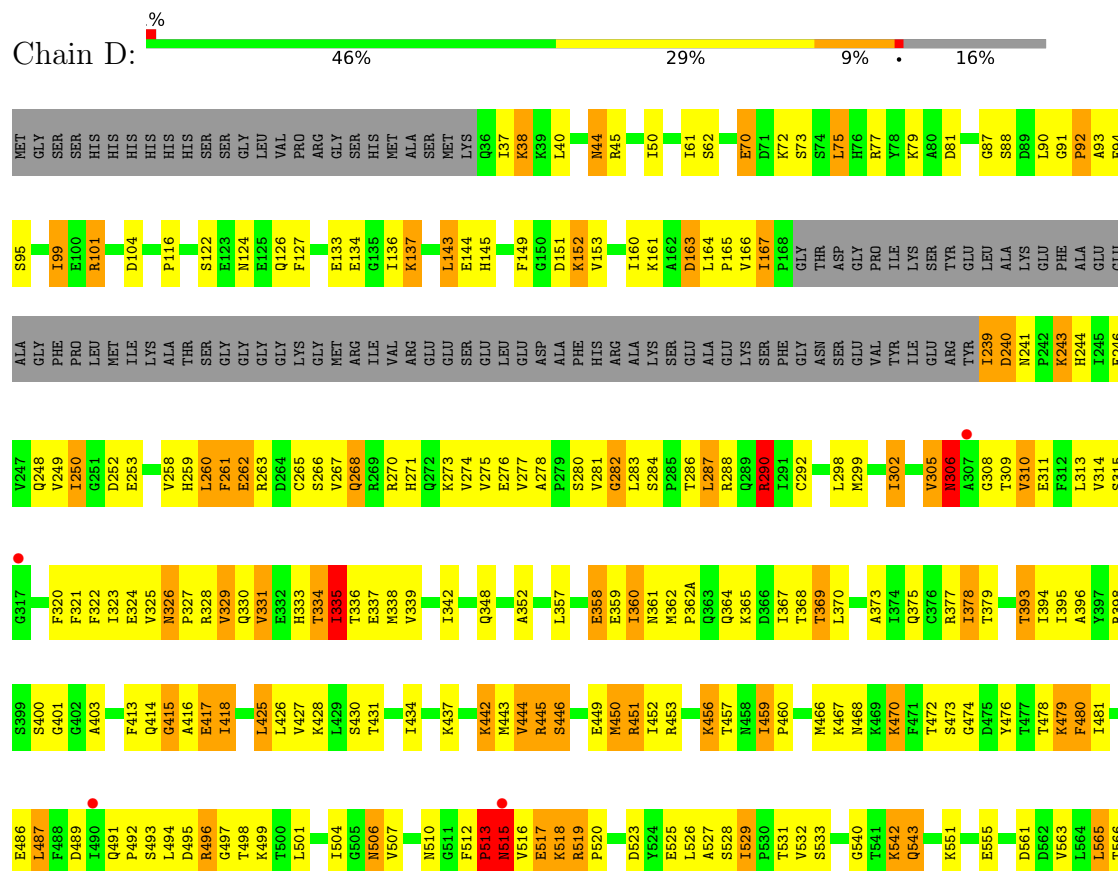


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



ASN	ASN	GLY	ASP	THR	ILE	ALA	THR	ALA	THR	GLY	ASP	LEU	LEU	ALA	GLN	MET	PRO	ILE	GLY	LYS	ALA	THR	ASP																														
LVS	P1014	K1015	V1016	T1023	D1034	T1035	P1036	M1042	R1043	N1044	G1045	E1046	T1047	I1052	D1053	K1054	G1055	K1056	R1057	I1060	K1061	L1062	E1063	T1064	I1065	ALA	ASN	GLN	PRO	LEU	ILE	THR	ALA	THR	GLY	ASP	LEU	LEU	ALA	GLN	MET	PRO	ILE	GLY	LYS	ALA	THR	ASP					
L919	Y920	Y921	N924	D925	L926	D927	E928	Q929	S930	Y931	G935	L938	D939	F940	Y944	Y945	1952	N957	N960	L963	Y966	1967	L974	P978	Y981	L982	E983	D986	F987	E988	R991	E995	E996	G1000	P1001	V1002	T1003	E1004	I1008	Y1009	N1093	VAL	HIS	THR	VAL	ILE	LYS	ALA	ASN	GLN	VAL	THR	VAL
F948	E849	S852	D853	I854	K855	S856	P857	E860	I861	Y862	Q863	H864	E865	M866	G869	Y871	S872	N873	L874	S875	Q876	Q877	A878	K879	S880	L881	G882	L883	G884	E885	R886	F887	D888	K891	D892	M893	R896	V897	N898	F899	L900	F901	G902	D903	I904	V907	T908	P909	S910	S911	M917		
V763	D765	L766	P767	I768	H769	L770	H771	T772	T775	S776	T782	Y783	K784	I699	S700	E701	G702	T703	T707	L711	E714	R715	S716	N717	I717A	L720	K725	L730	F735	H736	I737	L738	A739	I740	K741	D742	M743	A744	G745	L746	K750	A751	A752	I756	G757	E758	L759	Y844	K760				
D567	F570	R571	D572	H574	Q575	T580	R581	V582	R583	I588	N589	I590	K593	T594	A595	D596	F597	F598	K599	E605	M606	W607	T611	M617	F618	L619	K620	E621	N622	P623	W624	R629	L630	R631	K632	N636	Q640	M641	R644	N647	A648	V649	G650	Y654									

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23Å 256.28Å 126.69Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 90.9 (30.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.80Å)	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	7085 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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: ATP, MN, ADP, BTI

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	0.85	11/8497 (0.1%)	1.02	28/11490 (0.2%)
1	B	0.82	11/7983 (0.1%)	0.96	23/10801 (0.2%)
1	C	0.84	9/8535 (0.1%)	0.98	15/11539 (0.1%)
1	D	0.83	12/7983 (0.2%)	1.01	24/10801 (0.2%)
All	All	0.84	43/32998 (0.1%)	0.99	90/44631 (0.2%)

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 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	20.03	1.80	1.52
1	B	936	TYR	C-N	19.07	1.60	1.33
1	C	513	PRO	C-N	18.08	1.58	1.33
1	B	961	LYS	C-O	15.87	1.42	1.24
1	C	515	ASN	N-CA	13.83	1.67	1.46

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	CA-C-N	13.85	141.87	122.07
1	C	513	PRO	C-N-CA	13.85	141.87	122.07
1	D	515	ASN	CA-CB-CG	10.39	122.99	112.60
1	B	763	VAL	O-C-N	-9.11	113.25	123.00
1	D	938	LEU	N-CA-C	8.95	122.70	111.69

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	455	0
1	B	7832	0	7767	368	0
1	C	8373	0	8287	477	0
1	D	7832	0	7767	400	0
2	A	27	0	12	2	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	1671	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 26.

The worst 5 of 1671 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:C	1:C:513:PRO:CA	1.80	1.52
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%)	3	13
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	4	17
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	2	10
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	4	15
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	3	13

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 [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	907/1005 (90%)	760 (84%)	147 (16%)	2	8
1	B	855/1005 (85%)	714 (84%)	141 (16%)	2	8
1	C	909/1005 (90%)	725 (80%)	184 (20%)	1	4
1	D	855/1005 (85%)	711 (83%)	144 (17%)	2	8
All	All	3526/4020 (88%)	2910 (82%)	616 (18%)	2	7

5 of 616 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1031	SER
1	D	766	LEU
1	D	72	LYS
1	C	1024	ARG
1	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	145	HIS
1	D	1005	GLN
1	D	330	GLN
1	D	589	ASN
1	B	575	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 oligosaccharides 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$
4	BTI	D	1201	-	15,16,16	1.67	2 (13%)	20,21,21	1.89	4 (20%)
4	BTI	B	1201	-	15,16,16	1.65	2 (13%)	20,21,21	2.28	4 (20%)
4	BTI	A	1203	-	15,16,16	1.73	2 (13%)	20,21,21	1.75	3 (15%)
5	ATP	C	1202	-	32,33,33	1.55	6 (18%)	48,52,52	1.75	10 (20%)
2	ADP	A	1201	-	28,29,29	1.62	5 (17%)	43,45,45	1.88	12 (27%)

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	BTI	D	1201	-	-	2/6/27/27	0/2/2/2
4	BTI	B	1201	-	-	4/6/27/27	0/2/2/2
4	BTI	A	1203	-	-	4/6/27/27	0/2/2/2
5	ATP	C	1202	-	-	3/22/38/38	0/3/3/3
2	ADP	A	1201	-	-	7/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	O3-C3	5.05	1.34	1.23
4	B	1201	BTI	O3-C3	5.02	1.34	1.23
5	C	1202	ATP	C5-C4	4.90	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1201	BTI	O3-C3	4.83	1.33	1.23
2	A	1201	ADP	C5-C4	4.67	1.47	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	BTI	C2-C4-N2	-7.48	105.42	113.34
2	A	1201	ADP	C5-C4-N3	-5.93	118.55	126.72
5	C	1202	ATP	C5-C4-N3	-5.64	118.95	126.72
4	D	1201	BTI	C2-C4-N2	-5.24	107.80	113.34
4	B	1201	BTI	C6-C5-N3	-4.96	106.80	113.18

There are no chirality outliers.

5 of 20 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
4	A	1203	BTI	C11-C10-C9-C8
4	A	1203	BTI	S1-C2-C7-C8
4	A	1203	BTI	C4-C2-C7-C8

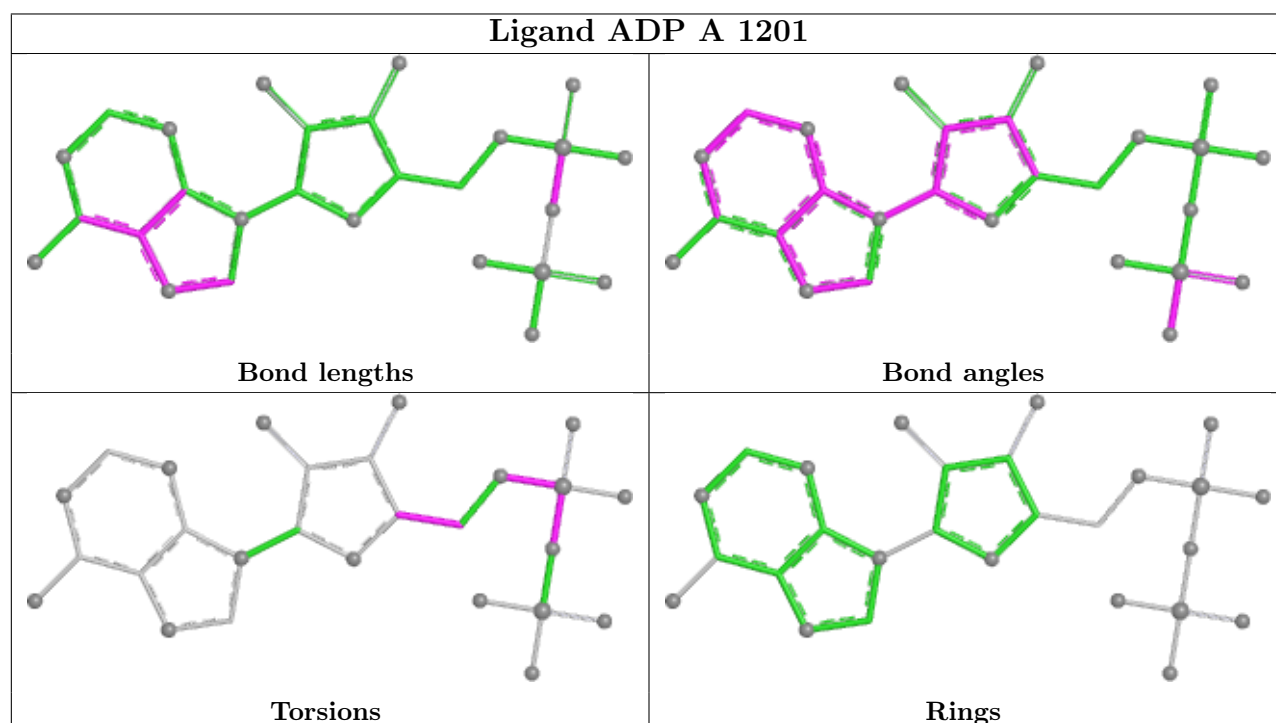
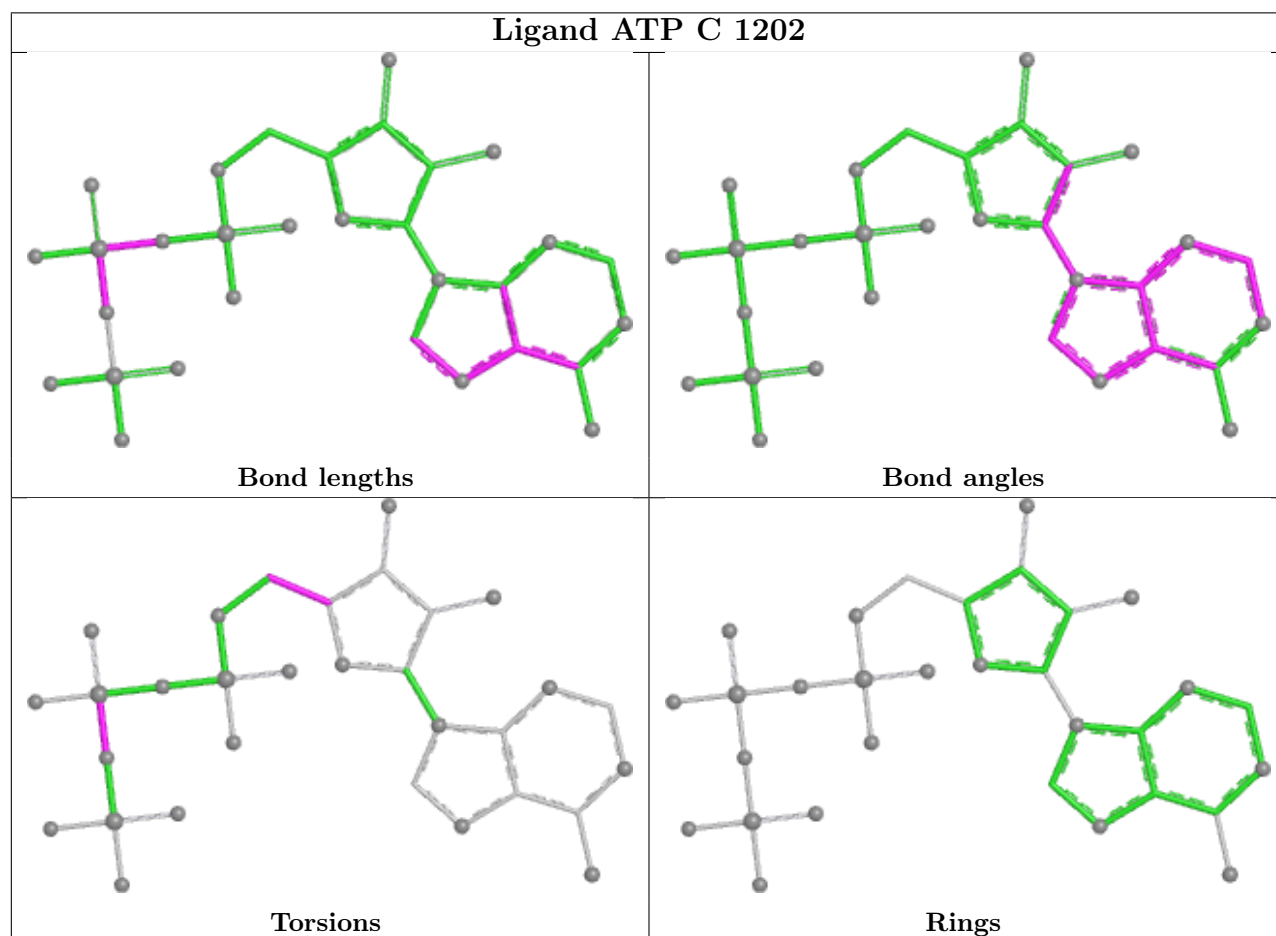
There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1201	BTI	3	0
4	B	1201	BTI	4	0
4	A	1203	BTI	4	0
5	C	1202	ATP	10	0
2	A	1201	ADP	2	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, 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	A	1052/1173 (89%)	-0.25	7 (0%) 84 77	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.19	7 (0%) 84 77	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.14	9 (0%) 82 75	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.24	6 (0%) 85 80	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.21	29 (0%) 84 77	47, 80, 125, 178	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	915	GLY	5.5
1	A	233	VAL	4.4
1	C	935	GLY	4.1
1	C	198	GLY	3.6
1	B	167	ILE	3.6

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](#)

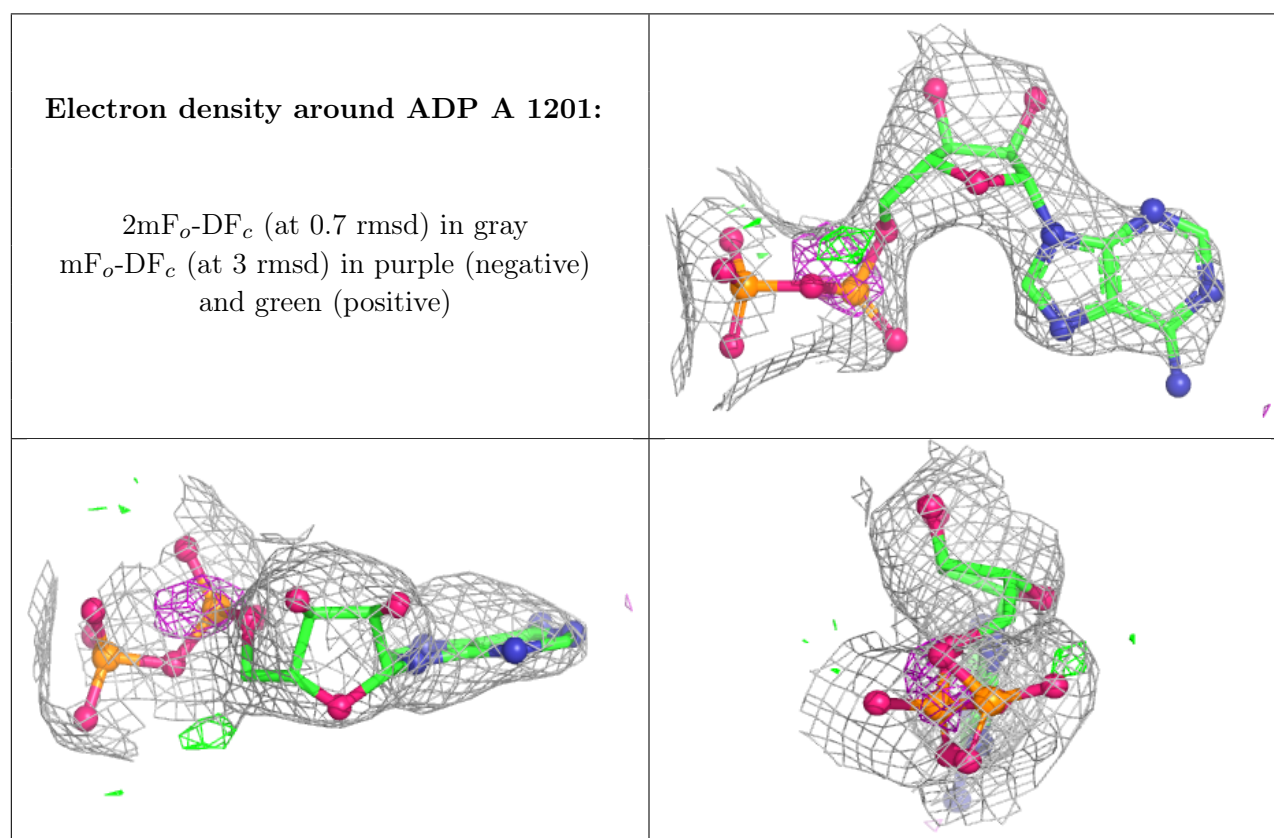
There are no oligosaccharides in this entry.

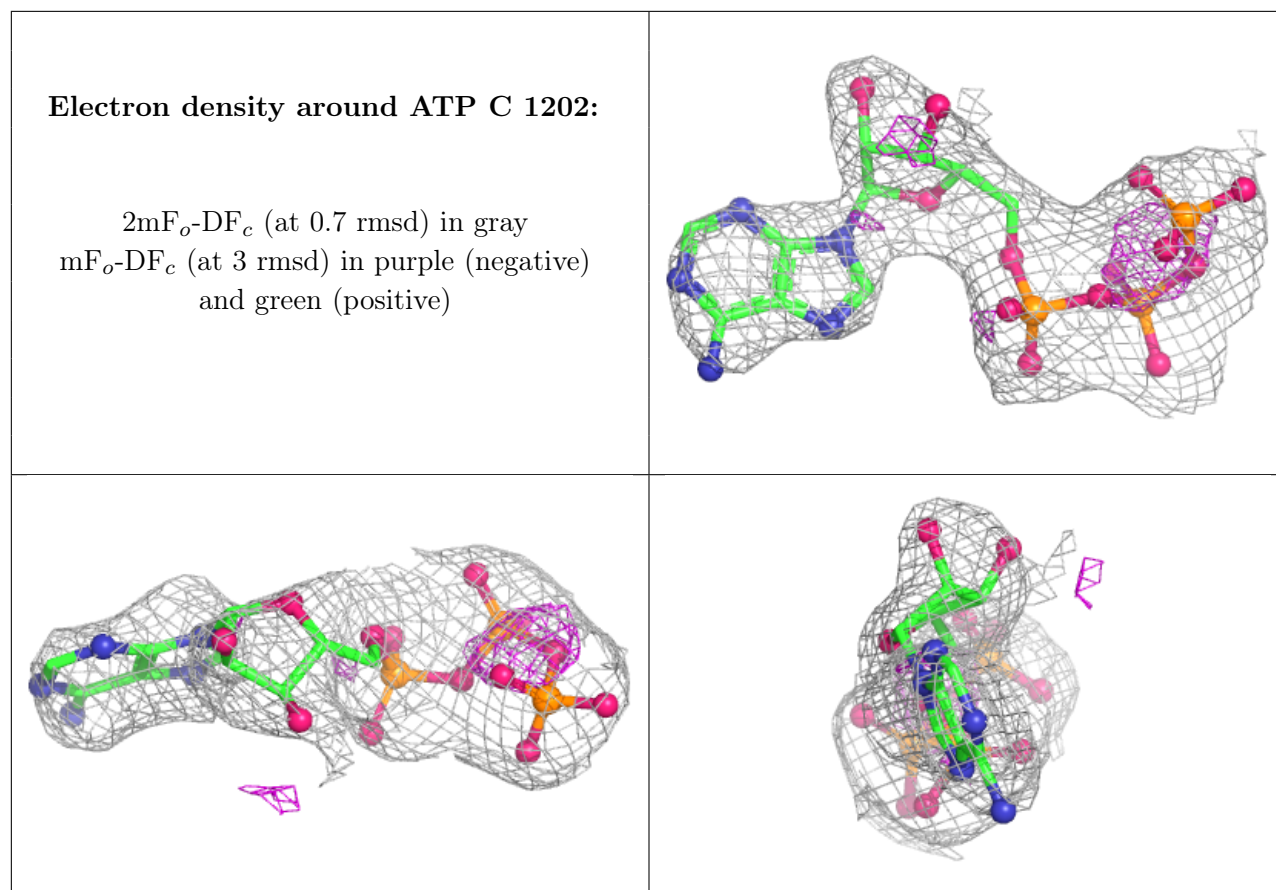
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	ADP	A	1201	27/27	0.85	0.10	86,91,110,110	0
4	BTI	B	1201	15/15	0.88	0.12	105,109,114,115	0
4	BTI	A	1203	15/15	0.89	0.12	92,99,104,105	0
4	BTI	D	1201	15/15	0.90	0.11	105,109,113,116	0
5	ATP	C	1202	31/31	0.90	0.09	102,108,115,115	0
3	MN	B	1202	1/1	0.96	0.05	82,82,82,82	0
3	MN	C	1201	1/1	0.98	0.08	76,76,76,76	0
3	MN	D	1202	1/1	0.98	0.04	74,74,74,74	0
3	MN	A	1202	1/1	0.98	0.04	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 ⓘ

There are no such residues in this entry.