



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 12:27 AM UTC

PDB ID : 4HNV / pdb_00004hnv
Title : Crystal structure of R54E 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

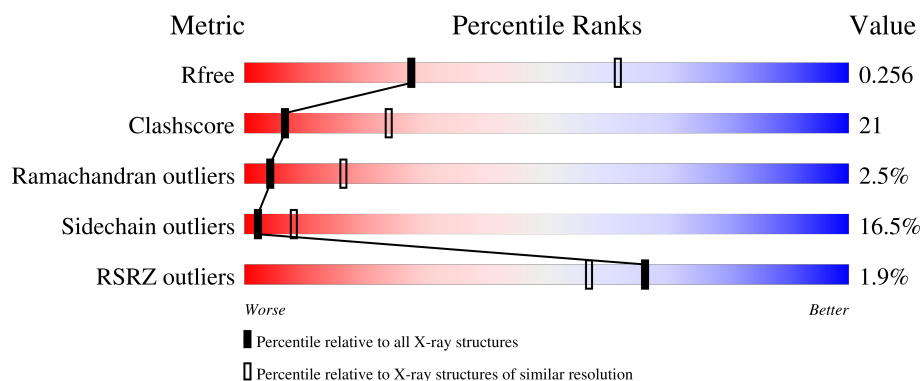
1 Overall quality at a glance

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	% 57% 31% 8% • •
1	B	1173	2% 48% 31% 8% • 12%
1	C	1173	2% 52% 30% 8% • 9%
1	D	1173	% 55% 28% 7% • 9%

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	BTI	B	1201	-	-	X	-
4	BTI	B	1202	-	-	X	-
6	CL	D	1201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34066 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	1133	Total	C	N	O	S	0	0	0
			8938	5663	1502	1743	30			
1	B	1033	Total	C	N	O	S	0	0	0
			8155	5169	1375	1583	28			
1	C	1067	Total	C	N	O	S	0	0	0
			8439	5349	1418	1642	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8411	5333	1413	1636	29			

There are 96 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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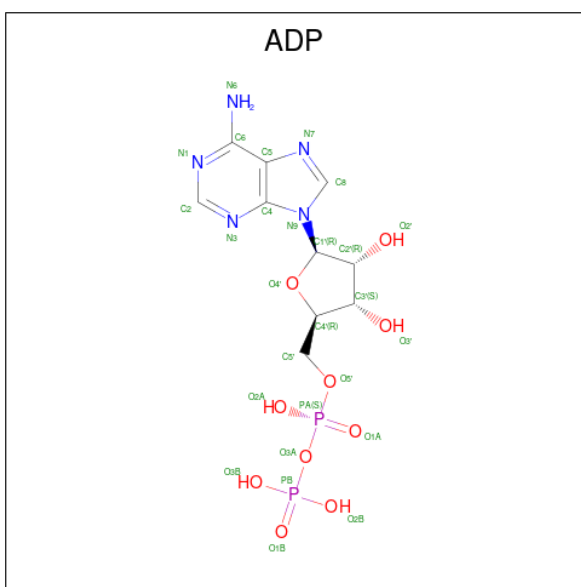
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
A	54	GLU	ARG	engineered mutation	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag	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
B	54	GLU	ARG	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	PRO	-	expression tag	UNP Q99UY8
C	27	ARG	-	expression tag	UNP Q99UY8
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
C	54	GLU	ARG	engineered mutation	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
D	54	GLU	ARG	engineered mutation	UNP Q99UY8

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

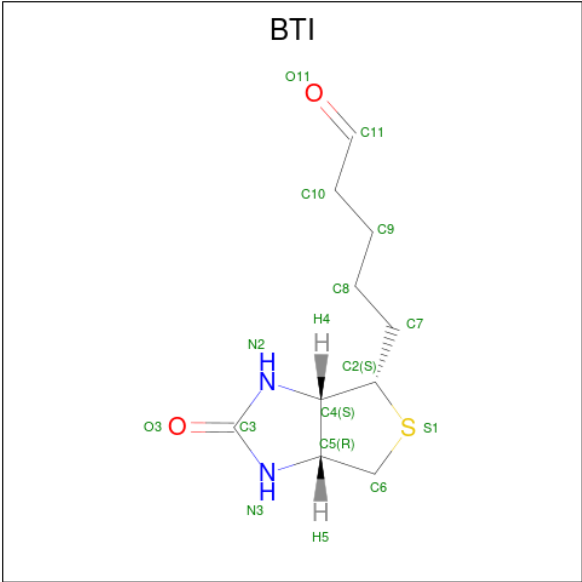


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

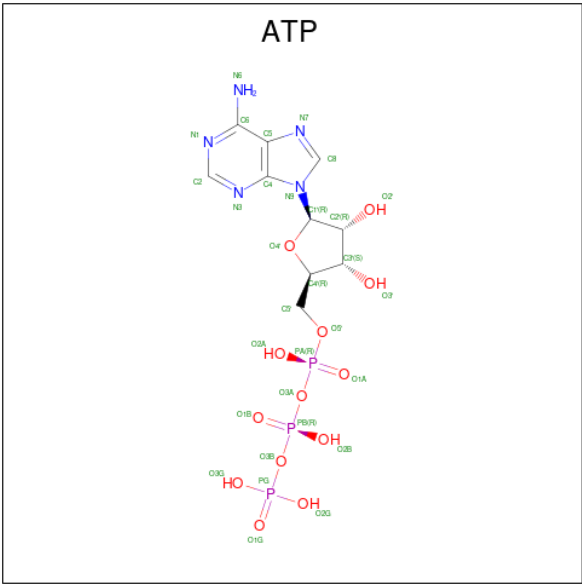
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- 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	B	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	C	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		

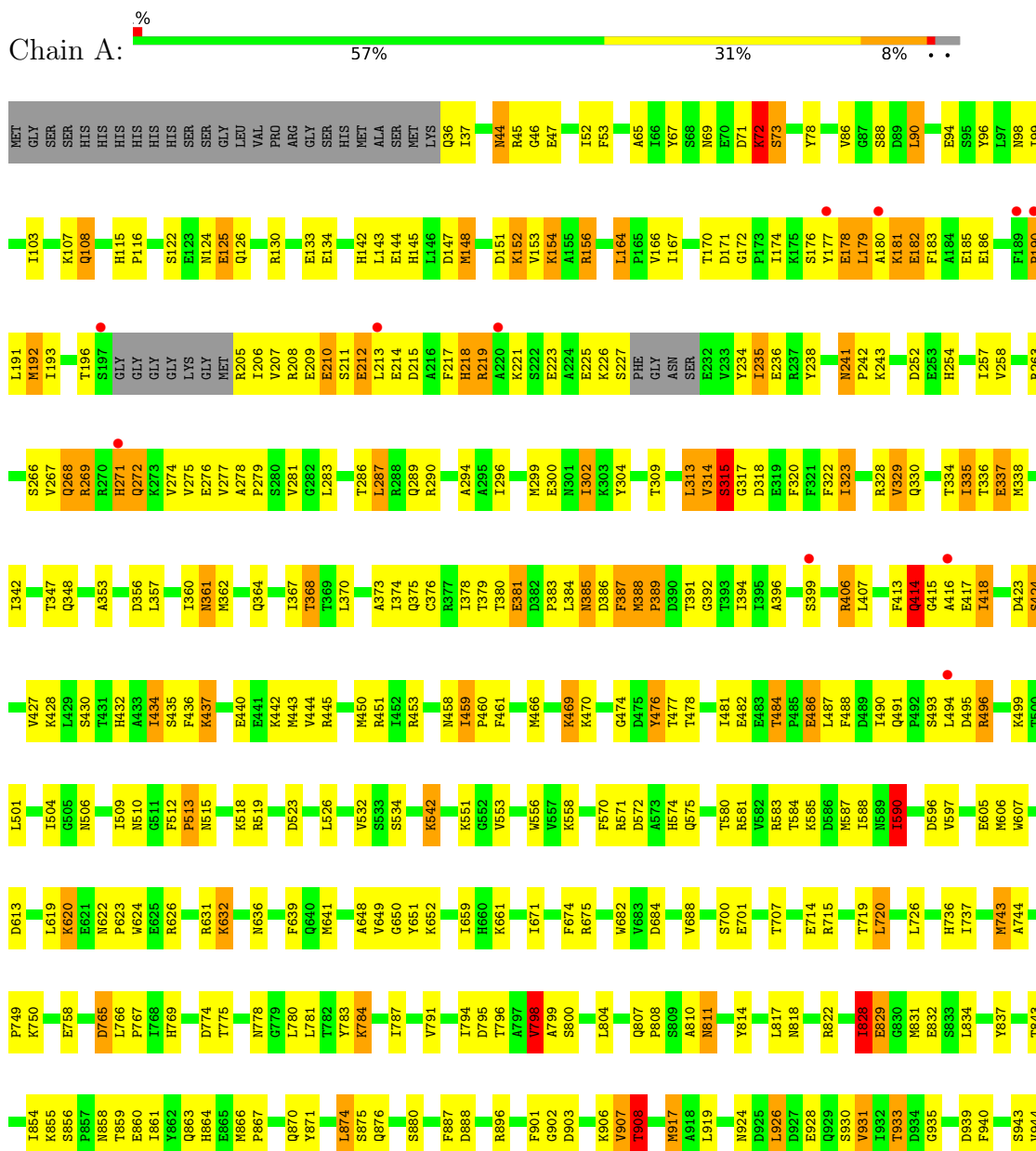
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

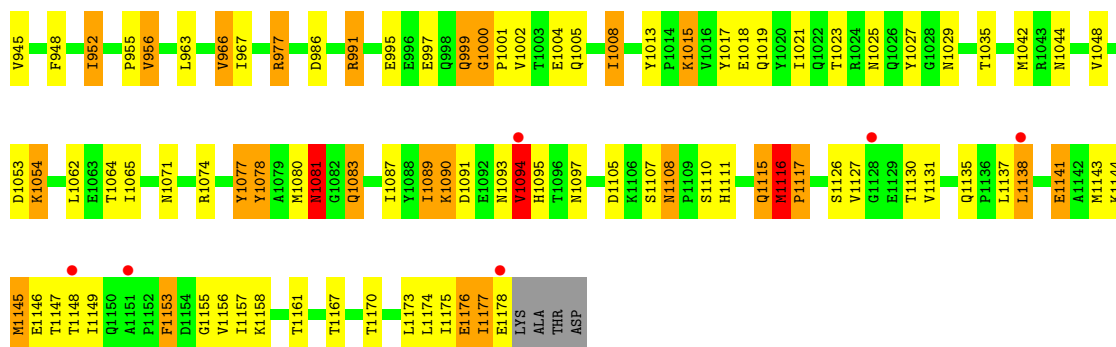
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

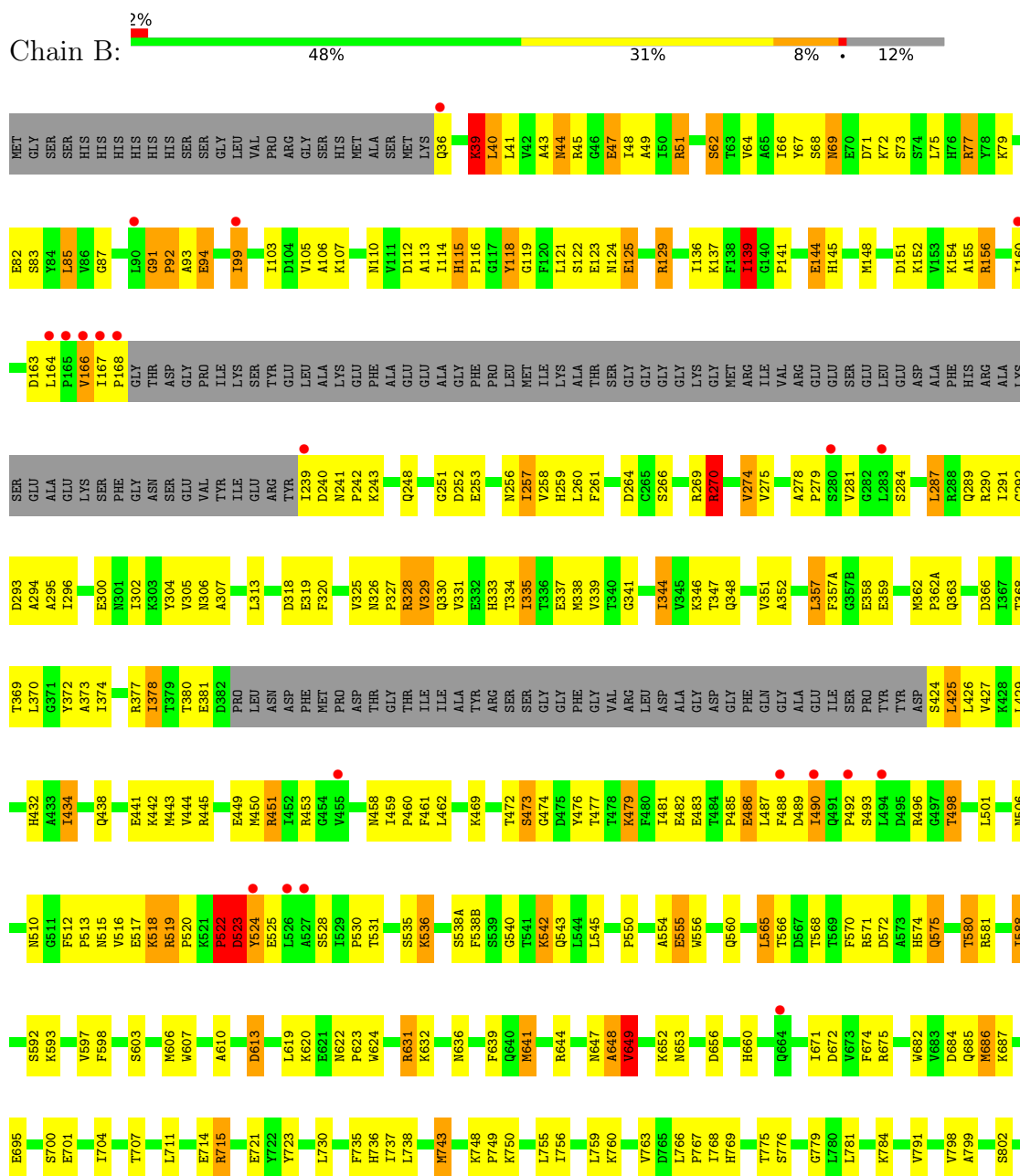
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

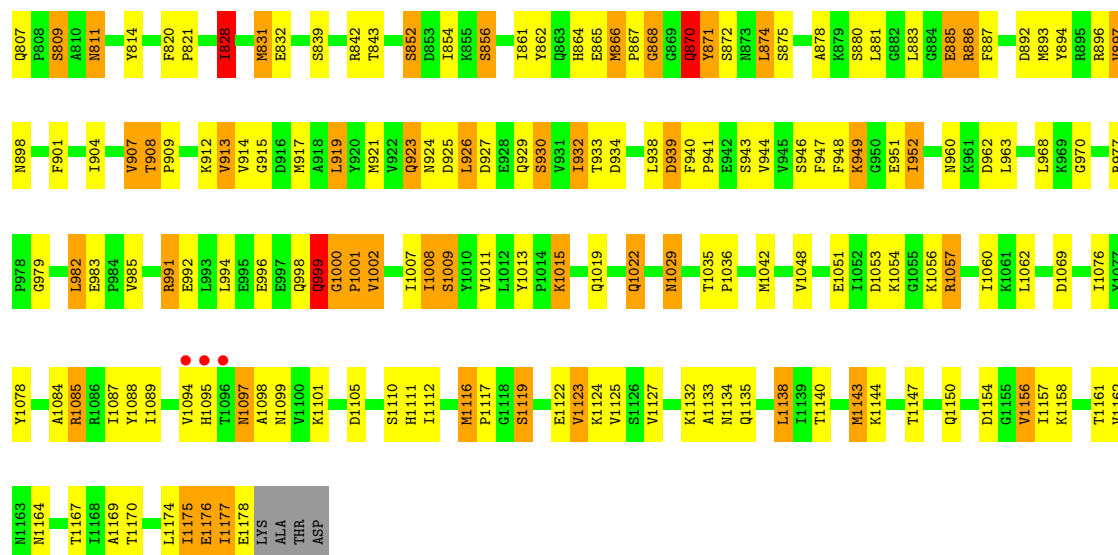
• Molecule 1: Pyruvate carboxylase



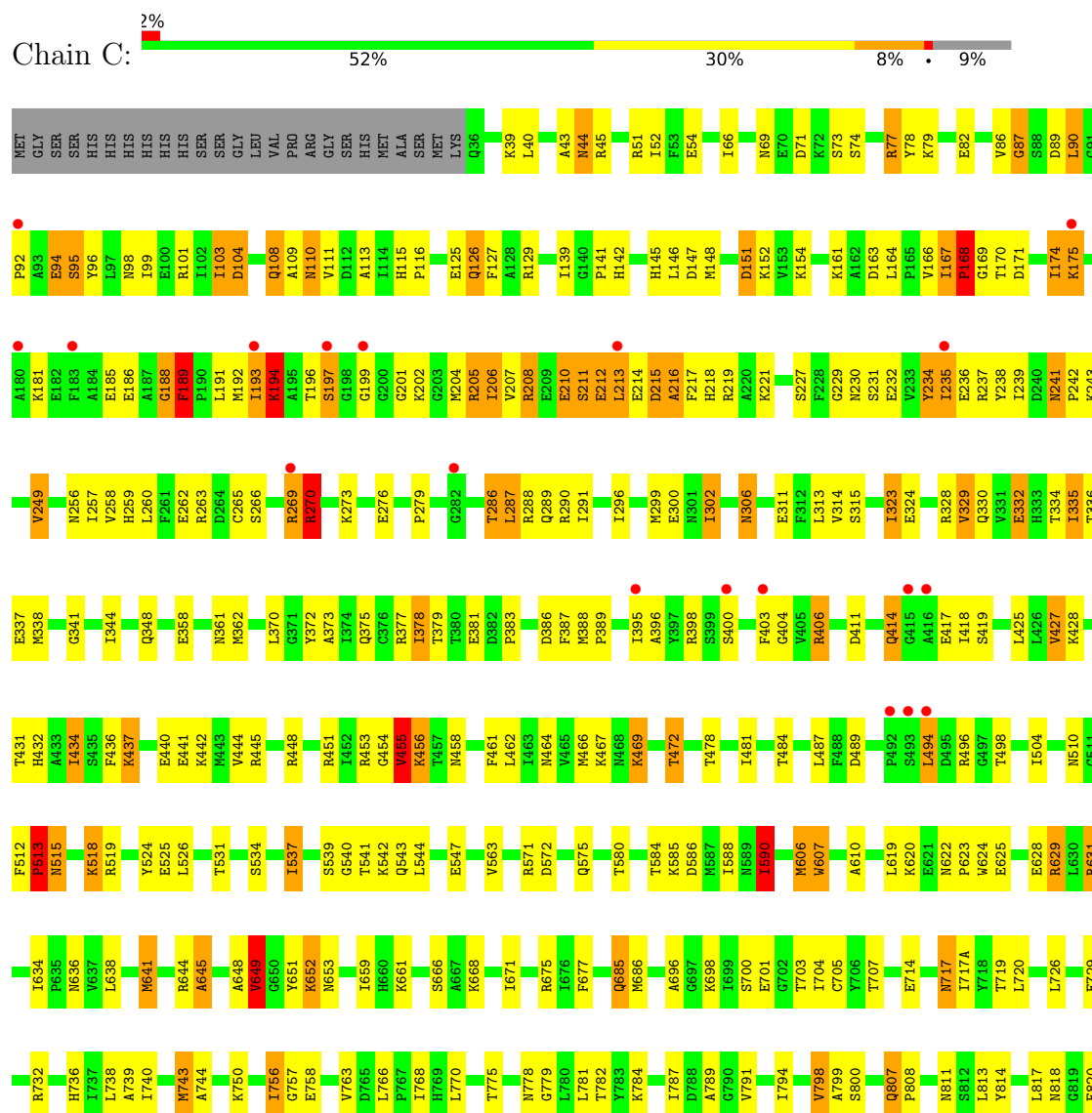


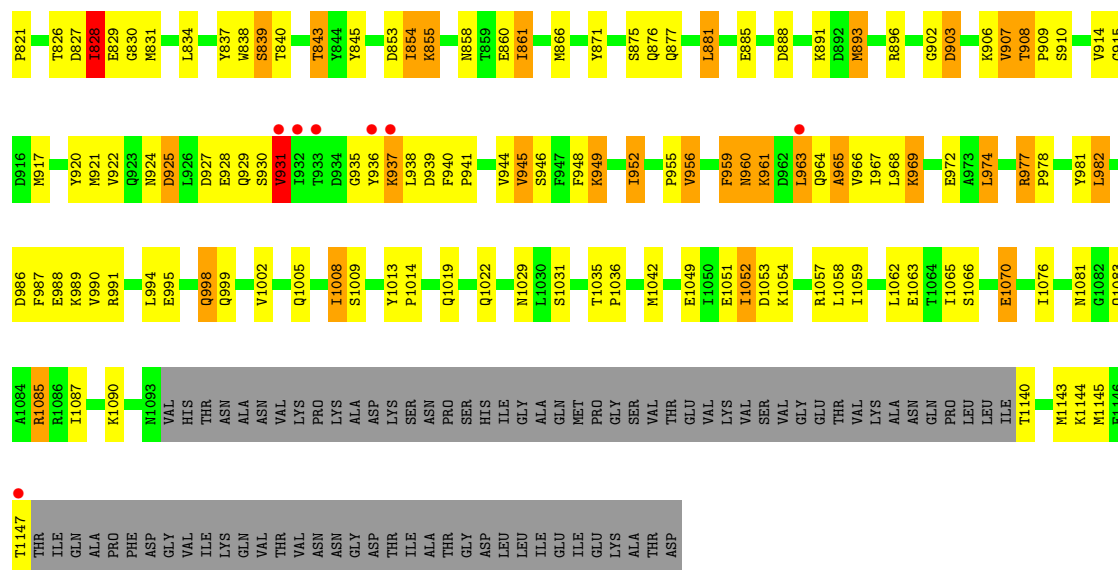
• Molecule 1: Pyruvate carboxylase



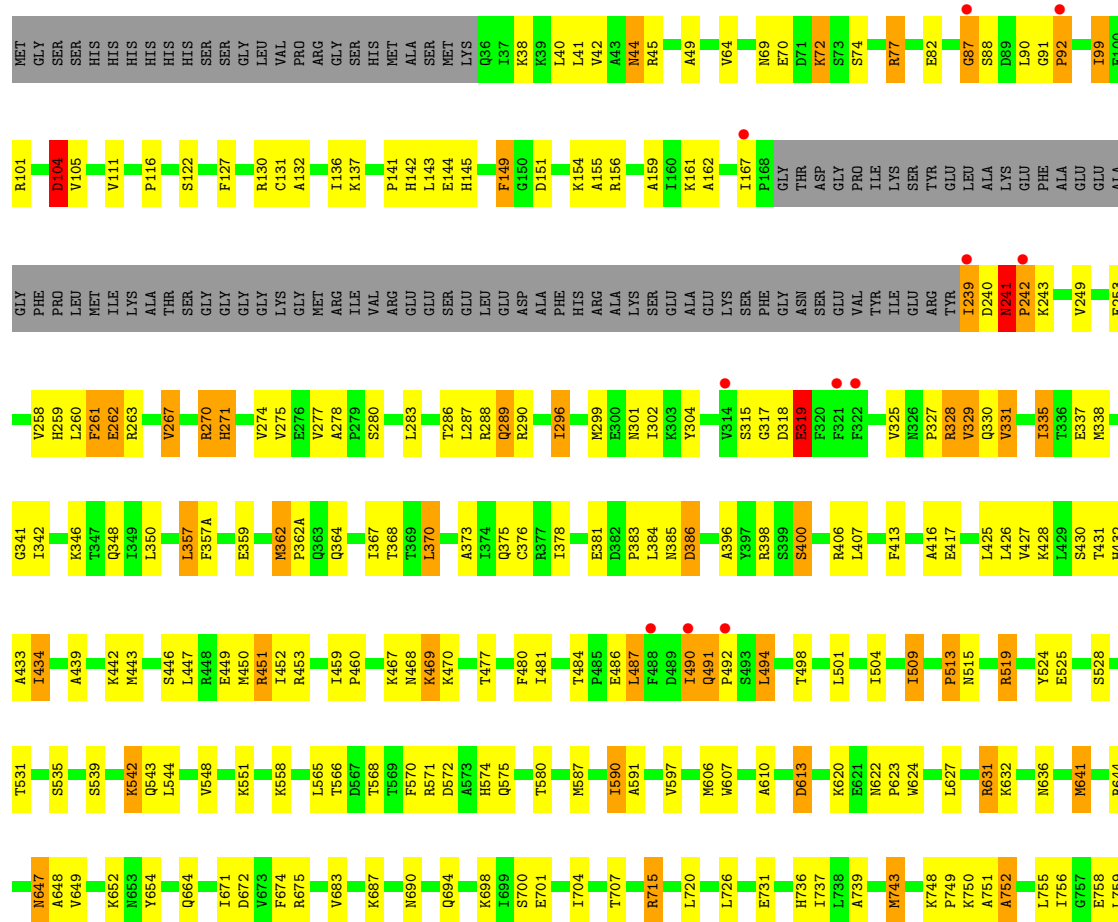


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



K760	S852	I932	K1054	Q1135
D853	D853	G935	G1055	L1138
V763	I854		K1056	
D765	K855	L938	R1057	E1141
P766	S856	D939	I1058	
P767		F940	I1059	K1144
I768	Q863	P941	I1060	
H769	H864		K1061	T1147
L770	E865	V944	L1062	T1148
H771	M866	V945	T1064	I1149
	P867		I1065	Q1150
D774	G868	K949	S1066	A1151
T775	Q869	G950	E1067	P1152
	Q870	E951	P1068	F1153
L780	Y871	I952	D1069	D1154
L781	S872		E1070	G1155
T782	N873	N960	N1071	V1156
Y783	L874	K961		I1157
K784	S875	D962	I1076	I1157
	Q876	L963	Y1077	K1158
V791	Q877	Q964	Y1078	Q1159
	A878	A965	A1079	V1160
D795	K879	V966	M1080	T1161
	S880			V1162
V798	L881	L974	R1085	N1163
A799		P978	I1089	
S800	G884		K1090	T1167
L804	F887	D986		
	M893		N1093	L1173
Q807	Y894	E996	VAL	L1174
M811	R895	E997	HIS	I1175
	R896	Q998	THR	E1176
Y814	V897	Q999	ASN	I1177
	N898	G1000	ALA	E1178
N818		P1001	ASN	LYS
	F901	V1002	VAL	ALA
R823	G902		K1101	THR
	D903	Y1013	P1102	ASP
T826		P1014	P1103	
D827	V907	K1015	A1104	
I828	T908	V1016	D1105	
E829	P909		K1106	
G830		Q1019	S1107	
M831	R912		N1108	
E832	M917	T1023	P1109	
	A918		S1110	
S835	A1042	M1042	H1111	
H836	R1043	N1044	Q1115	
Y837	N1044	G1045	V1123	
W838	G1045	E1046		
S839	T1047	V1048	V1127	
T840		E1049		
	D925	I1050		
T843	L926	E1051	V1131	
	E927	I1052	K1132	
D847			A1133	
F848			N1134	
E849	V931	D1053		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.43Å 256.74Å 127.05Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.80) 93.0 (30.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.256	Depositor DCC
R_{free} test set	7149 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34066	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: CL, ATP, BTI, MN, 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	0.72	2/9106 (0.0%)	0.96	28/12319 (0.2%)
1	B	0.63	4/8305 (0.0%)	0.90	9/11239 (0.1%)
1	C	0.69	6/8601 (0.1%)	0.92	16/11625 (0.1%)
1	D	0.71	5/8569 (0.1%)	0.94	17/11596 (0.1%)
All	All	0.69	17/34581 (0.0%)	0.93	70/46779 (0.1%)

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	4
1	B	0	3
1	D	0	2
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	11.64	1.69	1.52
1	D	513	PRO	CA-C	9.25	1.63	1.52
1	C	763	VAL	N-CA	9.23	1.56	1.46
1	D	849	GLU	N-CA	7.16	1.55	1.45
1	C	515	ASN	N-CA	6.59	1.56	1.46

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	THR	CA-C-N	-7.38	110.86	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	THR	C-N-CA	-7.38	110.86	119.05
1	A	314	VAL	O-C-N	-7.17	115.33	123.07
1	A	828	ILE	CB-CA-C	-7.05	102.49	112.22
1	C	828	ILE	CB-CA-C	-6.87	103.00	111.87

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	1080	MET	Peptide
1	A	271	HIS	Peptide
1	A	494	LEU	Peptide
1	B	92	PRO	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	8938	0	8865	393	0
1	B	8155	0	8127	373	0
1	C	8439	0	8345	389	0
1	D	8411	0	8357	337	0
2	A	27	0	12	3	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	B	30	0	32	17	0
4	C	15	0	16	1	0
4	D	15	0	16	5	0
5	C	31	0	12	6	0
6	D	1	0	0	3	0
All	All	34066	0	33782	1457	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 21.

The worst 5 of 1457 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:1144:LYS:NZ	4:D:1202:BTI:H11	1.21	1.52
1:B:1144:LYS:NZ	4:B:1202:BTI:C11	1.74	1.46
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.66	1.29
1:C:1144:LYS:NZ	4:D:1202:BTI:C11	1.91	1.29
1:C:1144:LYS:HZ1	4:D:1202:BTI:C11	1.44	1.29

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	1127/1173 (96%)	1022 (91%)	81 (7%)	24 (2%)	5	20
1	B	1027/1173 (88%)	906 (88%)	92 (9%)	29 (3%)	4	14
1	C	1063/1173 (91%)	926 (87%)	105 (10%)	32 (3%)	3	12
1	D	1061/1173 (90%)	947 (89%)	90 (8%)	24 (2%)	5	18
All	All	4278/4692 (91%)	3801 (89%)	368 (9%)	109 (2%)	4	16

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	181	LYS
1	A	211	SER
1	A	956	VAL
1	A	1094	VAL

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	977/1006 (97%)	826 (84%)	151 (16%)	2	9
1	B	897/1006 (89%)	736 (82%)	161 (18%)	2	6
1	C	917/1006 (91%)	754 (82%)	163 (18%)	2	6
1	D	922/1006 (92%)	783 (85%)	139 (15%)	3	10
All	All	3713/4024 (92%)	3099 (84%)	614 (16%)	2	8

5 of 614 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1052	ILE
1	D	925	ASP
1	D	44	ASN
1	C	1022	GLN
1	D	469	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	289	GLN
1	D	1073	ASN
1	D	364	GLN
1	D	818	ASN
1	B	543	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	C	1203	-	15,16,16	1.71	2 (13%)	20,21,21	2.13	3 (15%)
4	BTI	B	1202	-	15,16,16	1.77	2 (13%)	20,21,21	2.11	4 (20%)
2	ADP	A	1201	-	28,29,29	1.42	4 (14%)	43,45,45	1.78	10 (23%)
5	ATP	C	1202	-	32,33,33	1.41	5 (15%)	48,52,52	1.71	9 (18%)
4	BTI	B	1201	-	15,16,16	1.74	2 (13%)	20,21,21	2.38	4 (20%)
4	BTI	D	1202	-	15,16,16	1.79	2 (13%)	20,21,21	1.92	3 (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
4	BTI	C	1203	-	-	4/6/27/27	0/2/2/2
4	BTI	B	1202	-	-	3/6/27/27	0/2/2/2
2	ADP	A	1201	-	-	4/16/32/32	0/3/3/3
5	ATP	C	1202	-	-	5/22/38/38	0/3/3/3
4	BTI	B	1201	-	-	2/6/27/27	0/2/2/2
4	BTI	D	1202	-	-	4/6/27/27	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1201	BTI	O3-C3	5.46	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ADP	C5-C4	4.70	1.47	1.39
5	C	1202	ATP	C5-C4	4.70	1.47	1.39
4	B	1202	BTI	O3-C3	4.67	1.33	1.23
4	C	1203	BTI	O3-C3	4.61	1.33	1.23

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	-8.11	104.75	113.34
4	D	1202	BTI	C2-C4-N2	-6.38	106.59	113.34
4	C	1203	BTI	C2-C4-N2	-5.93	107.07	113.34
4	C	1203	BTI	C6-C5-N3	-5.87	105.61	113.18
2	A	1201	ADP	C5-C4-N3	-5.70	118.86	126.72

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O2A
4	B	1202	BTI	S1-C2-C7-C8
4	B	1202	BTI	C4-C2-C7-C8
4	C	1203	BTI	C9-C10-C11-O11
4	C	1203	BTI	S1-C2-C7-C8

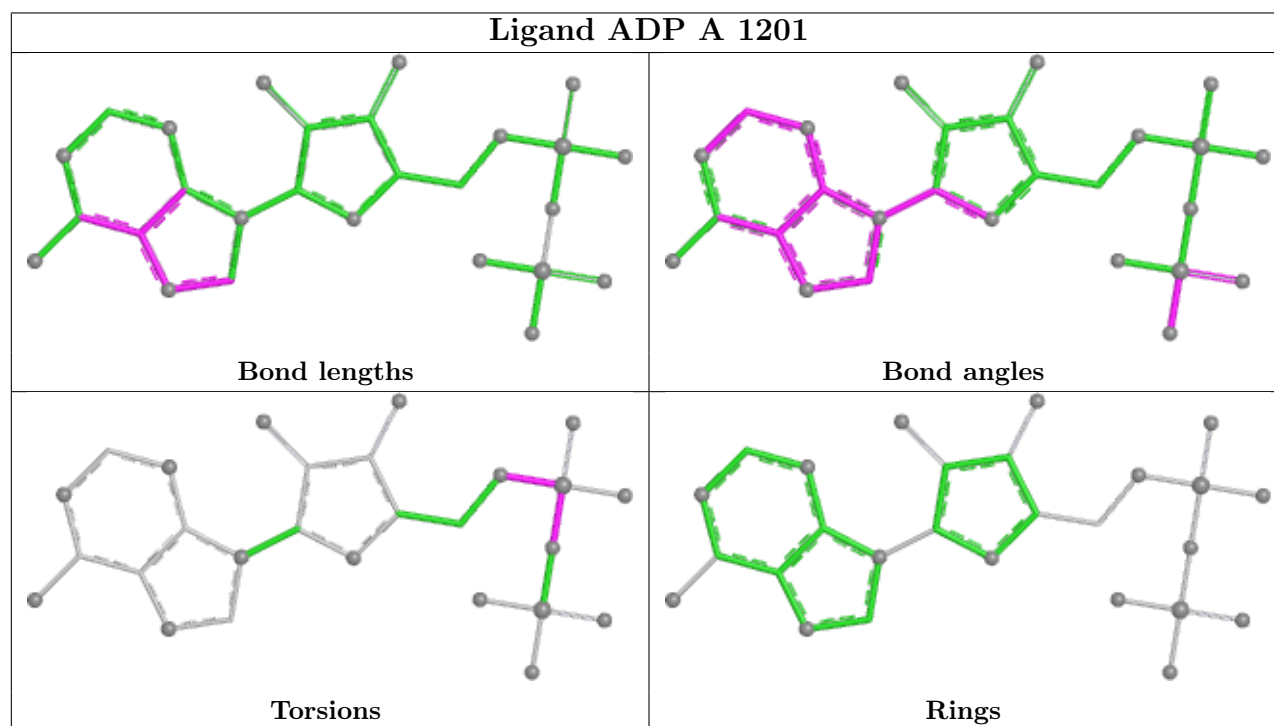
There are no ring outliers.

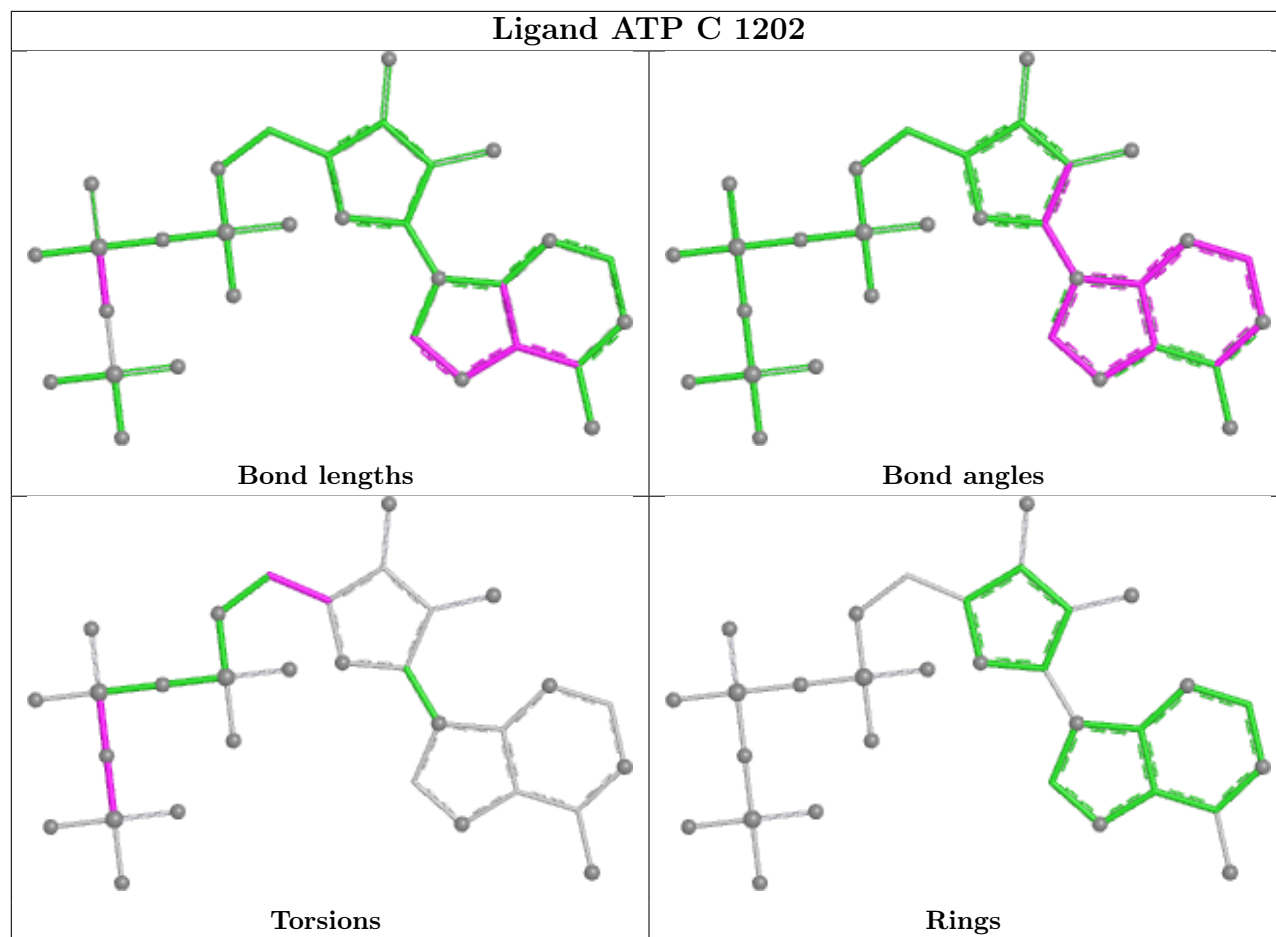
6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	BTI	1	0
4	B	1202	BTI	9	0
2	A	1201	ADP	3	0
5	C	1202	ATP	6	0
4	B	1201	BTI	8	0
4	D	1202	BTI	5	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](#)

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, 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	1133/1173 (96%)	-0.38	17 (1%) 72 63	23, 51, 104, 136	0
1	B	1033/1173 (88%)	-0.17	24 (2%) 61 51	31, 65, 130, 216	0
1	C	1067/1173 (90%)	-0.19	26 (2%) 59 49	36, 62, 108, 133	0
1	D	1067/1173 (90%)	-0.36	15 (1%) 73 64	21, 57, 115, 174	0
All	All	4300/4692 (91%)	-0.28	82 (1%) 66 57	21, 59, 114, 216	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	ILE	4.9
1	D	92	PRO	4.3
1	C	933	THR	4.1
1	A	271	HIS	4.0
1	B	1095	HIS	3.9

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](#)

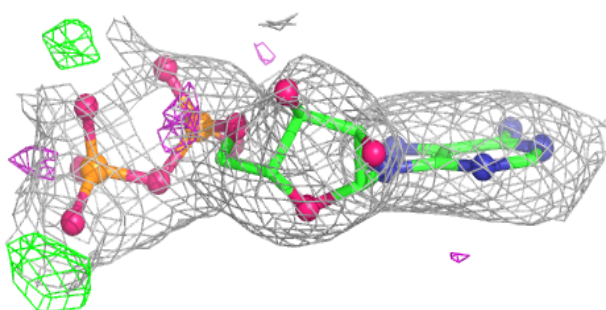
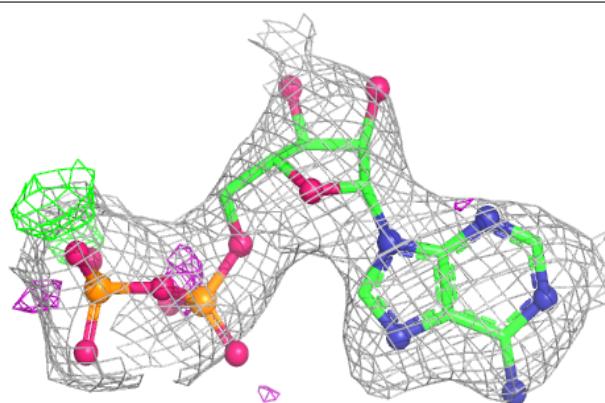
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

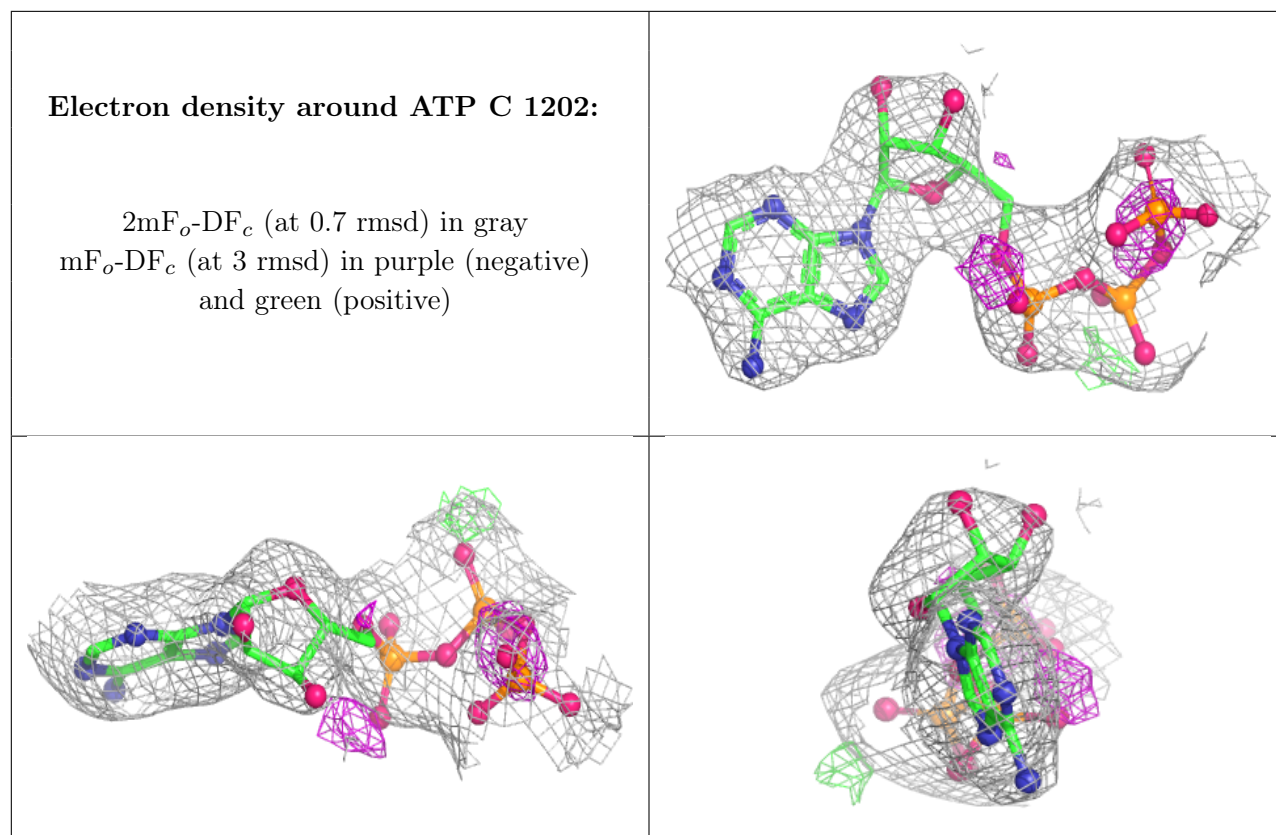
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1201	27/27	0.87	0.10	75,82,96,97	0
5	ATP	C	1202	31/31	0.91	0.09	69,72,104,105	0
3	MN	D	1203	1/1	0.96	0.05	85,85,85,85	0
4	BTI	B	1201	15/15	0.96	0.09	56,59,61,64	0
4	BTI	C	1203	15/15	0.96	0.07	55,59,61,63	0
3	MN	A	1202	1/1	0.96	0.06	94,94,94,94	0
4	BTI	D	1202	15/15	0.97	0.07	46,50,51,52	0
3	MN	B	1203	1/1	0.98	0.03	83,83,83,83	0
3	MN	C	1201	1/1	0.98	0.10	55,55,55,55	0
4	BTI	B	1202	15/15	0.98	0.05	31,40,44,50	0
6	CL	D	1201	1/1	0.98	0.06	45,45,45,45	0

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

Electron density around ADP A 1201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.