



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:54 PM UTC

PDB ID : 3HO8 / pdb_00003ho8
Title : Crystal Structure of S. aureus Pyruvate Carboxylase in complex with Coenzyme A
Authors : Tong, L.; Yu, L.P.C.
Deposited on : 2009-06-01
Resolution : 2.90 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

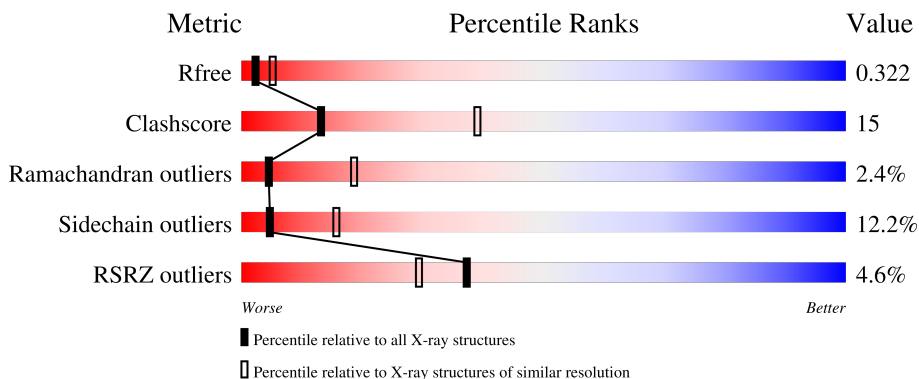
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1150	5% 55% 27% • 14%
1	B	1150	% 50% 29% 6% 14%
1	C	1150	2% 55% 26% 5% 13%
1	D	1150	7% 53% 25% • 19%

2 Entry composition [i](#)

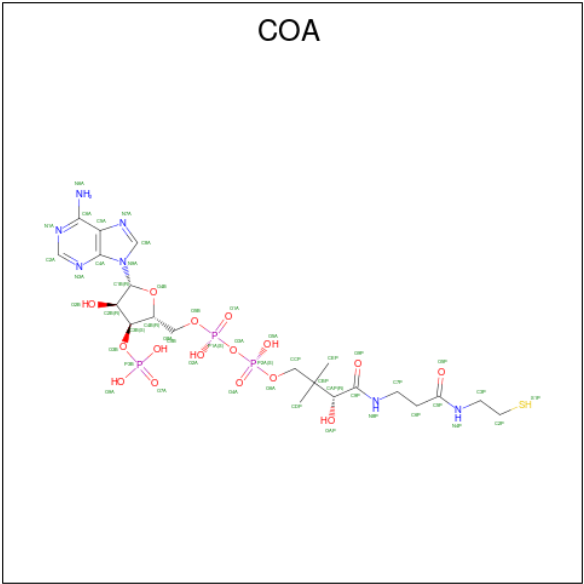
There are 4 unique types of molecules in this entry. The entry contains 31229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	994	Total	C	N	O	S	0	0	0
			7880	5000	1329	1525	26			
1	D	934	Total	C	N	O	S	0	0	0
			7396	4696	1250	1426	24			
1	C	995	Total	C	N	O	S	0	0	0
			7889	5005	1330	1528	26			
1	B	989	Total	C	N	O	S	0	0	0
			7838	4975	1321	1516	26			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	D	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

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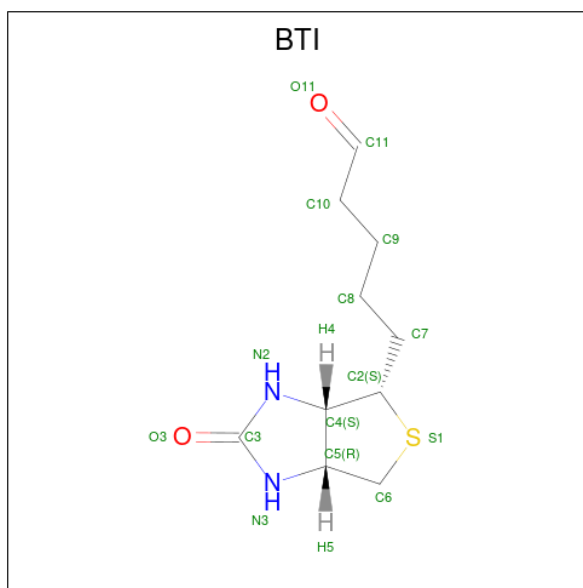
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- 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	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	B	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).

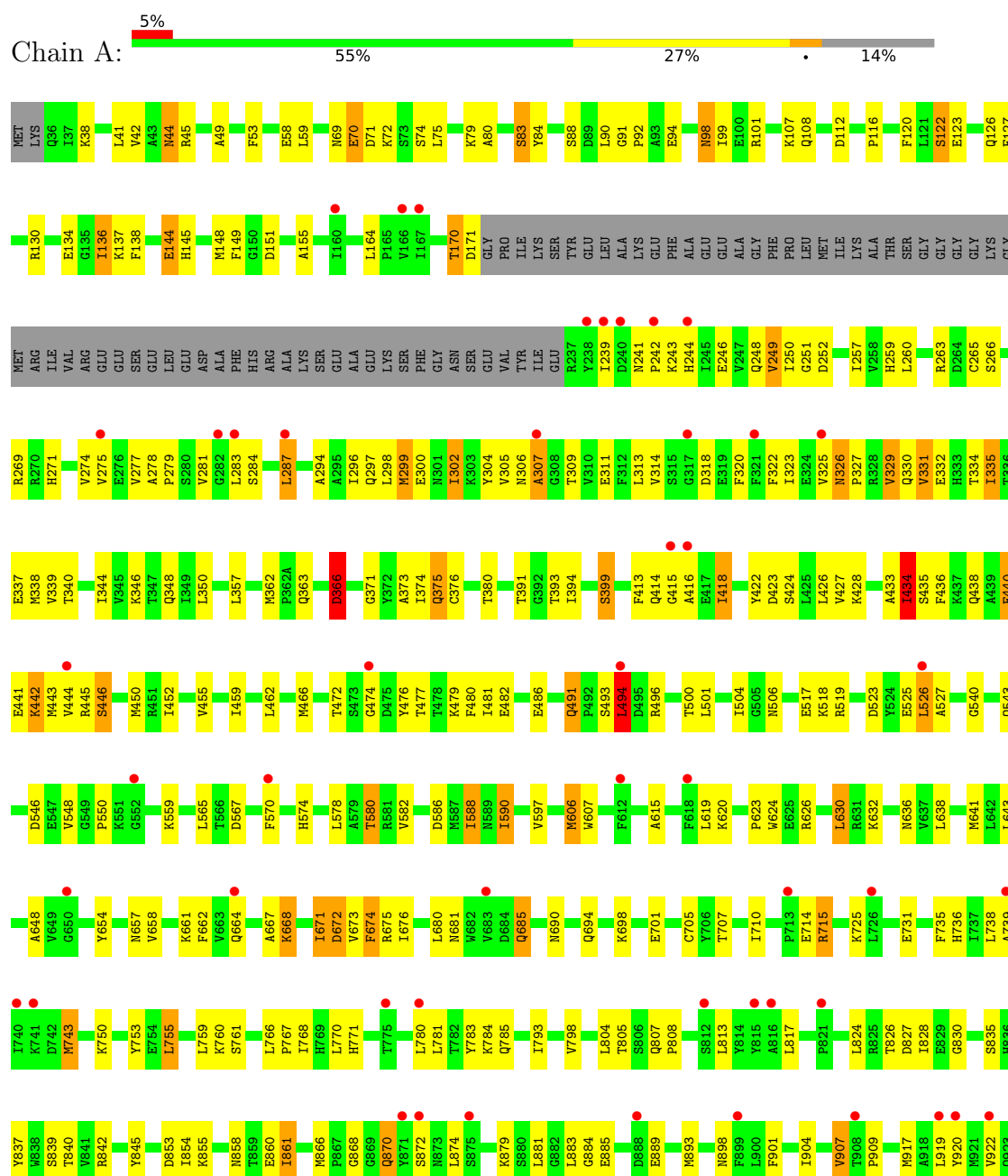


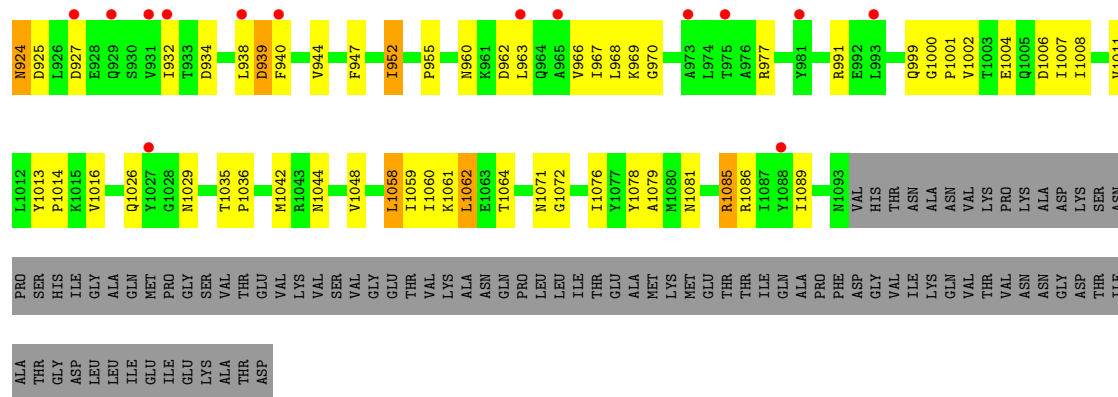
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

3 Residue-property plots [i](#)

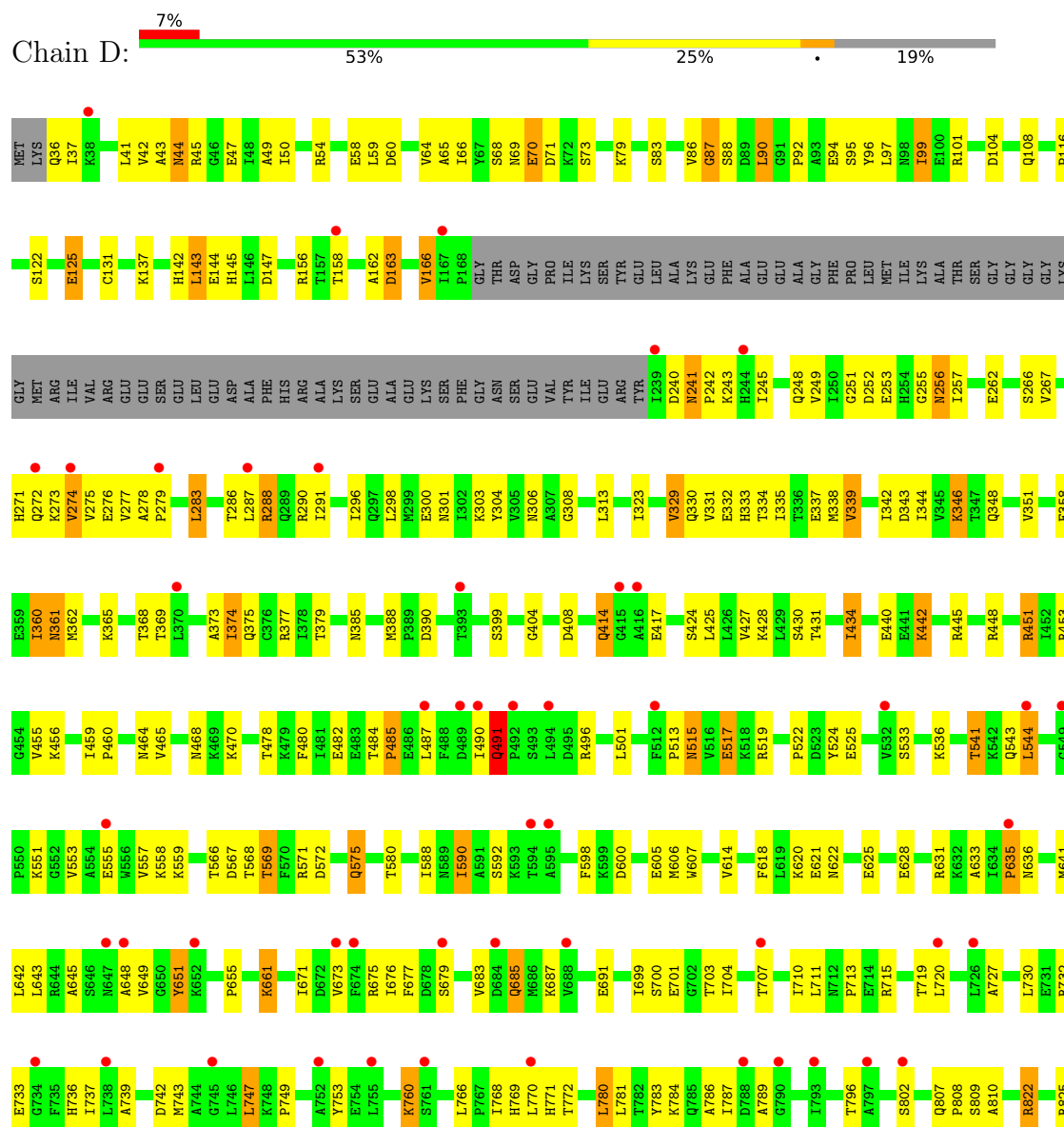
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

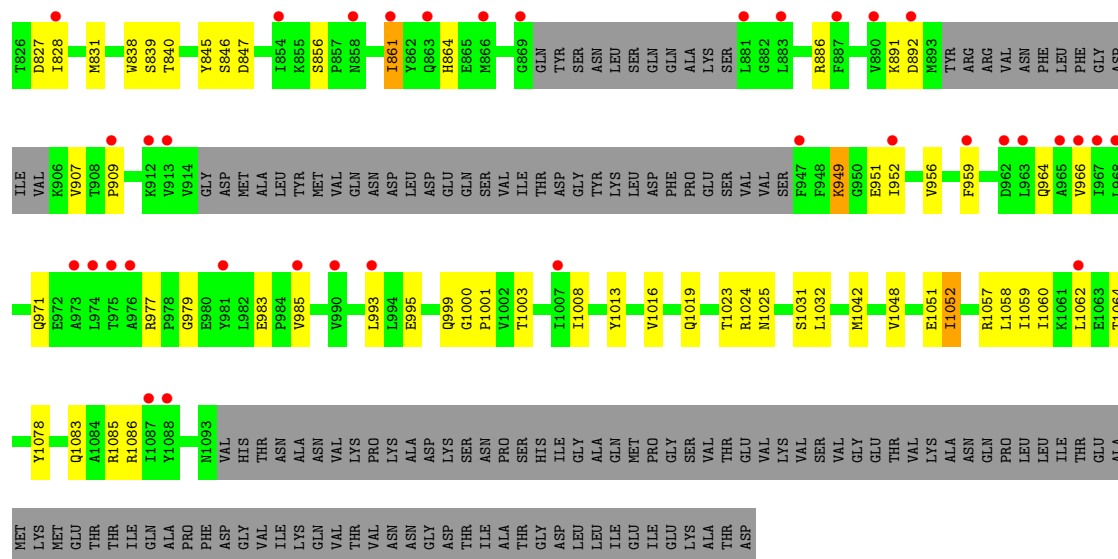
• Molecule 1: Pyruvate carboxylase



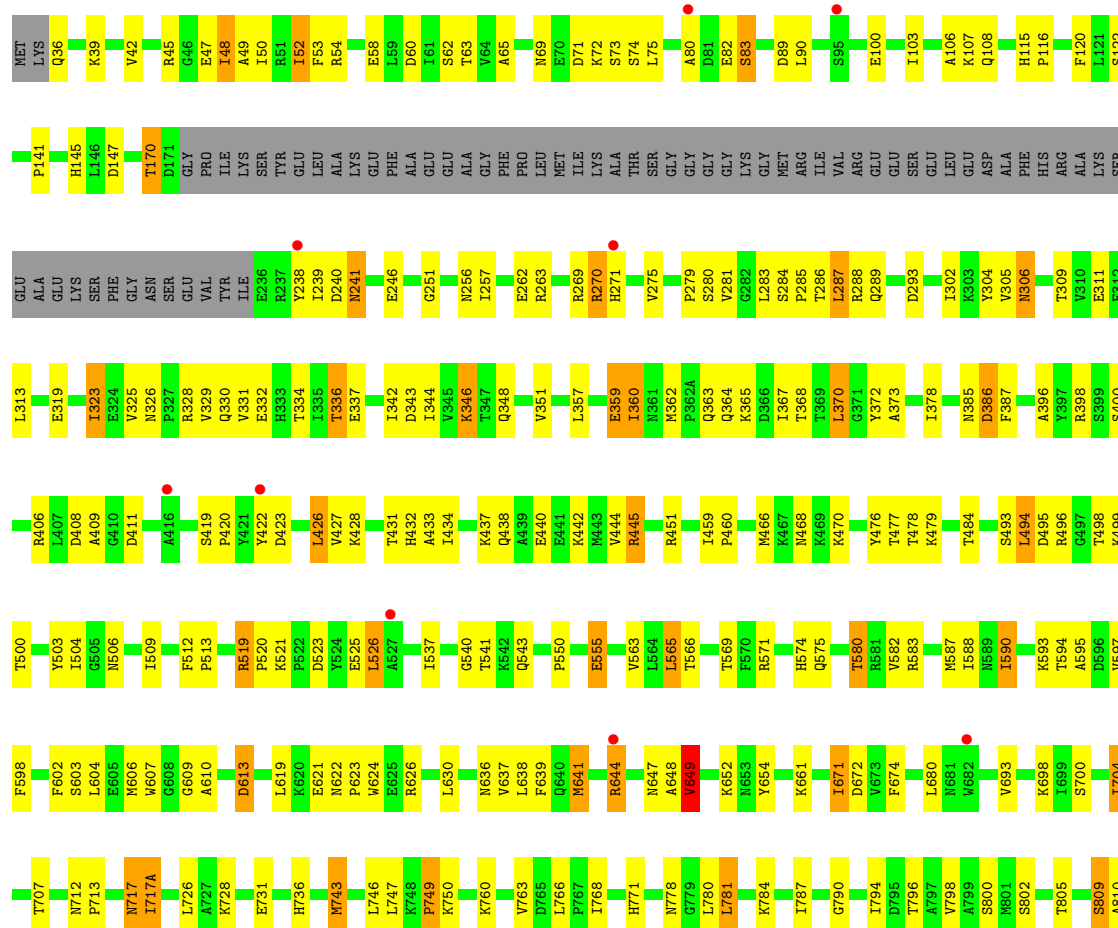


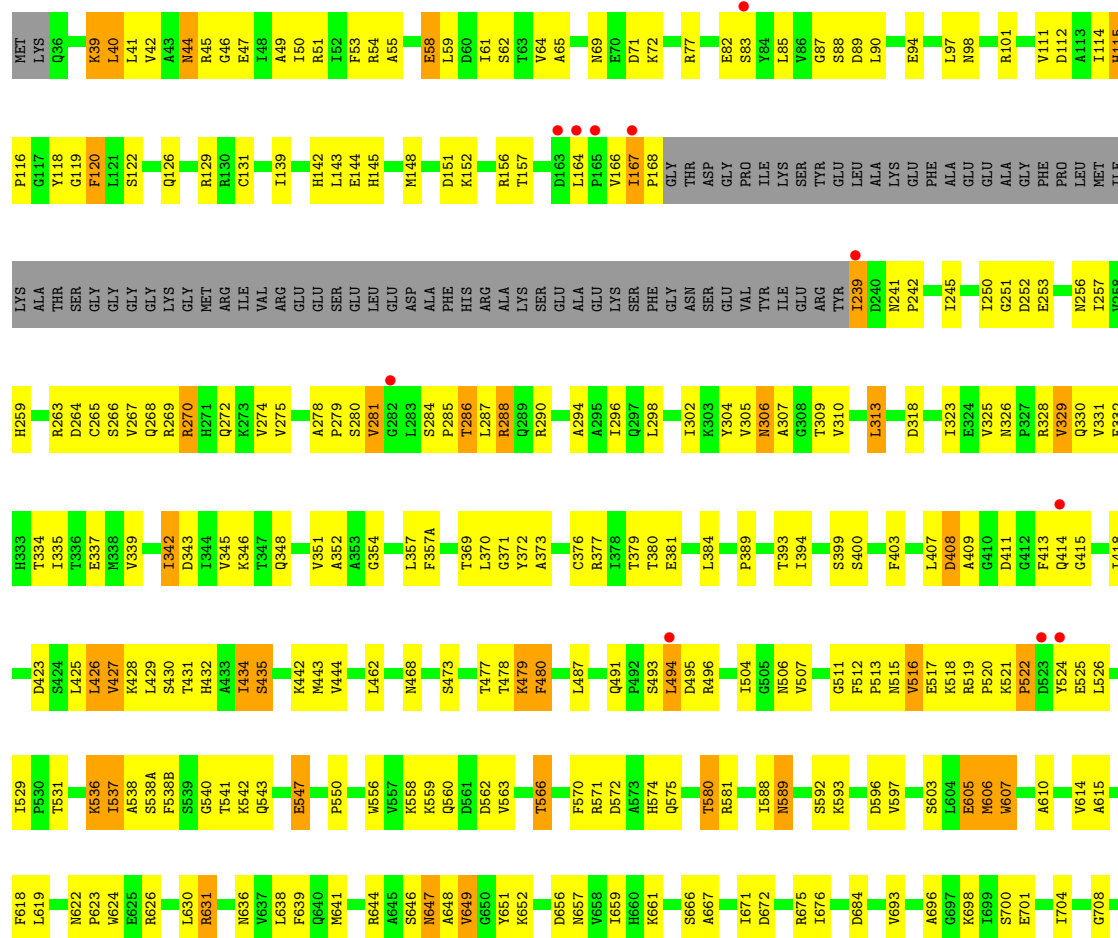
● Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase





GLY	ASP	HIS	S1009	N898	S806	L711
ASP	LEU	ILE	Y1010	F901	S809	R715
LEU	LEU	ALA	V1011	K906	A810	S716
ILE	ILE	GLN	Y1017	N811	N717	I717A
GLU	GLU	MET	E1018	V907	I718	Y718
ILE	ILE	PRO	Q1019	T908	Y814	I719
GLU	GLU	GLY	Q1022	M917	T615	I720
LYS	LYS	SER	A918	A918	A816	E721
ALA	ALA	VAL	N1029	L919	L817	Y722
THR	THR	THR	GLU	Y920	F820	Y723
GLU	GLU	GLU	M821	M821	Y724	Y724
VAL	VAL	VAL	T1035	R825	K725	Y725
LYS	LYS	LYS	P1036	D927	L726	L726
VAL	VAL	VAL	M1042	E928	D827	
SER	SER	SER		Q929	H736	H736
VAL	VAL	VAL	Y1048	S930	E829	I737
GLY	GLY	GLY	E1049	V931	Q830	L738
GLU	GLU	GLU	D1053	I932	M831	A739
THR	THR	THR	LYS	T933	E832	
VAL	VAL	VAL	ALA	D934	S833	M743
LYS	LYS	LYS	I1059	G935		
ALA	ALA	ALA	I1060	H836	L747	L747
ASN	ASN	GLN	L838	S839	A751	A751
GLN	GLN	PRO	E1063	V944	A752	
PRO	PRO	LEU	T1064	V945	D847	
LEU	LEU	LEU	I1065		E758	E758
ILE	ILE	ILE	E1070	I952	I854	L759
THR	THR	THR	N1071	N857	K855	K760
GLU	GLU	ALA	G1072		S856	
ALA	ALA	GLU	I1076	N960	P857	L766
MET	MET	LYS	Y1077	D962	E860	P767
LYS	LYS	GLU	M1080	L963	I861	I768
THR	THR	THR	N1081	T975	Q863	H771
ILE	ILE	ILE	I1089	A976	H864	T772
GLN	GLN	ALA		R977	E865	H773
ALA	ALA	PRO	E1092	P978	M866	D774
PRO	PRO	PHE	N1093	K869	P867	T775
ASP	ASP	ASP	VAL	Q868	N778	
GLY	GLY	GLY	HIS	Q869	L781	
VAL	VAL	VAL	THR	V990	I782	
ILE	ILE	ILE	ASN	Y871	Y783	
LYS	LYS	LYS	ALA	S872	K784	
GLN	GLN	GLN	ASN	N873		
VAL	VAL	VAL	ASN	L874	I787	
THR	THR	THR	LYS	E987		
VAL	VAL	VAL	PRO	G1000	K879	I794
ASN	ASN	ASN	LYS	P1001	S880	D795
GLY	GLY	ASN	ALA	V1002	L881	T796
ASP	ASP	GLY	ASP	T1003	G884	A797
LYS	LYS	LYS	LYS	E1004		Y798
THR	THR	THR	SER	Q1005	D888	A799
ILE	ILE	ILE	ASN	D1006		
ALA	ALA	ALA	PRO	I1007	K891	S802
THR	THR	THR	SER	I1008		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.59Å 164.47Å 373.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.90 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.97-2.90) 89.7 (29.97-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.264 , 0.328 0.267 , 0.322	Depositor DCC
R_{free} test set	5969 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31229	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1935e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN, BTI, COA

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	0.56	0/8033	0.91	12/10868 (0.1%)
1	B	0.62	1/7990 (0.0%)	0.95	10/10810 (0.1%)
1	C	0.62	1/8042 (0.0%)	0.93	5/10880 (0.0%)
1	D	0.55	0/7537	0.91	4/10192 (0.0%)
All	All	0.59	2/31602 (0.0%)	0.92	31/42750 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	945	VAL	CA-CB	6.92	1.62	1.54
1	C	945	VAL	CA-CB	5.74	1.61	1.54

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	938	LEU	N-CA-C	7.32	119.33	111.36
1	A	91	GLY	CA-C-N	7.31	128.97	119.84
1	A	91	GLY	C-N-CA	7.31	128.97	119.84
1	C	882	GLY	N-CA-C	-7.18	105.92	115.40
1	B	115	HIS	CA-C-N	6.81	126.28	118.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	880	SER	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	7880	0	7807	212	0
1	B	7838	0	7771	303	0
1	C	7889	0	7813	251	0
1	D	7396	0	7347	168	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	2	0
2	D	48	0	32	6	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	15	0	16	0	0
4	C	15	0	16	3	0
All	All	31229	0	30898	923	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 15.

The worst 5 of 923 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:606:MET:HE2	1:C:639:PHE:HB3	1.20	1.15
1:C:704:ILE:HG12	1:C:726:LEU:HD23	1.22	1.12
1:A:304:TYR:HE2	1:A:307:ALA:O	1.35	1.10
1:A:1085:ARG:HG2	1:A:1085:ARG:HH11	1.12	1.06
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.38	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	990/1150 (86%)	862 (87%)	105 (11%)	23 (2%)	5	19
1	B	985/1150 (86%)	875 (89%)	89 (9%)	21 (2%)	5	21
1	C	991/1150 (86%)	887 (90%)	79 (8%)	25 (2%)	4	17
1	D	924/1150 (80%)	777 (84%)	123 (13%)	24 (3%)	4	17
All	All	3890/4600 (85%)	3401 (87%)	396 (10%)	93 (2%)	4	18

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	GLY
1	A	939	ASP
1	D	87	GLY
1	D	163	ASP
1	D	272	GLN

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	860/987 (87%)	761 (88%)	99 (12%)	5	18
1	B	856/987 (87%)	746 (87%)	110 (13%)	4	13
1	C	861/987 (87%)	754 (88%)	107 (12%)	4	15
1	D	806/987 (82%)	709 (88%)	97 (12%)	5	16
All	All	3383/3948 (86%)	2970 (88%)	413 (12%)	5	16

5 of 413 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	427	VAL
1	C	971	GLN
1	B	957	ASN
1	C	494	LEU
1	C	728	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	297	GLN
1	B	811	ASN
1	C	778	ASN
1	B	778	ASN
1	B	960	ASN

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 10 ligands modelled in this entry, 4 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
2	COA	C	2001	-	47,50,50	1.17	4 (8%)	69,75,75	1.61	12 (17%)
2	COA	B	2001	-	47,50,50	1.36	7 (14%)	69,75,75	1.63	12 (17%)
4	BTI	C	2000	-	15,16,16	1.70	2 (13%)	20,21,21	2.23	3 (15%)
2	COA	A	2001	-	47,50,50	1.44	5 (10%)	69,75,75	1.65	13 (18%)
4	BTI	B	2000	-	15,16,16	1.62	2 (13%)	20,21,21	1.95	3 (15%)
2	COA	D	2001	-	47,50,50	1.15	2 (4%)	69,75,75	1.68	11 (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	COA	C	2001	-	-	14/48/64/64	0/3/3/3
2	COA	B	2001	-	-	17/48/64/64	0/3/3/3
4	BTI	C	2000	-	-	5/6/27/27	0/2/2/2
2	COA	A	2001	-	-	16/48/64/64	0/3/3/3
4	BTI	B	2000	-	-	3/6/27/27	0/2/2/2
2	COA	D	2001	-	-	4/48/64/64	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	COA	P2A-O3A	5.00	1.64	1.59
4	C	2000	BTI	O3-C3	4.72	1.33	1.23
4	B	2000	BTI	O3-C3	4.41	1.32	1.23
2	A	2001	COA	P1A-O3A	4.10	1.63	1.59
4	C	2000	BTI	C2-S1	-3.68	1.76	1.82

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2000	BTI	C6-C5-N3	-6.36	104.99	113.18
4	C	2000	BTI	C2-C4-N2	-6.31	106.66	113.34
4	C	2000	BTI	C6-C5-N3	-6.26	105.12	113.18
2	D	2001	COA	C5A-C4A-N3A	-5.61	119.00	126.72
2	A	2001	COA	C5A-C4A-N3A	-5.13	119.66	126.72

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

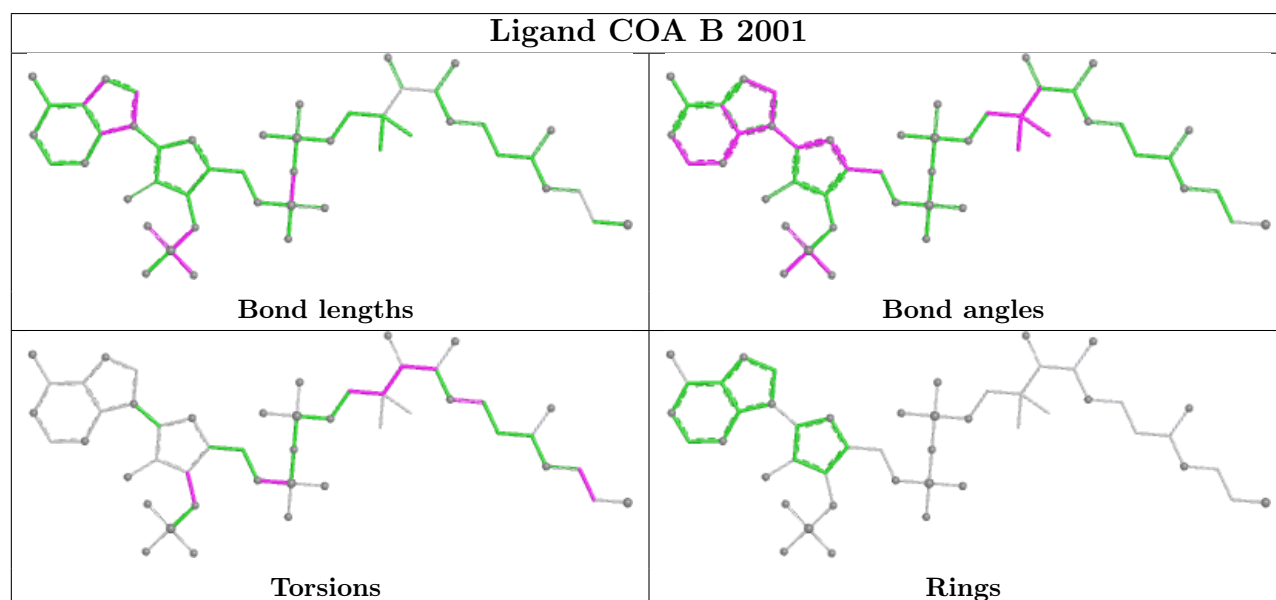
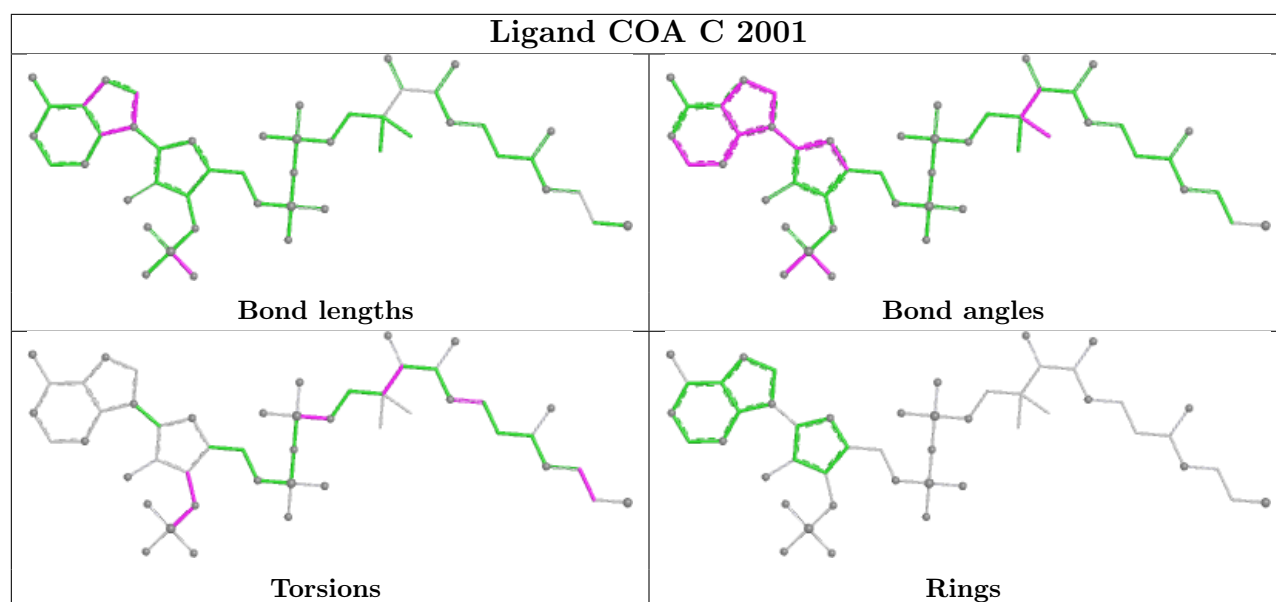
Mol	Chain	Res	Type	Atoms
2	A	2001	COA	CCP-O6A-P2A-O3A
2	A	2001	COA	CCP-O6A-P2A-O4A
2	A	2001	COA	CCP-O6A-P2A-O5A
2	A	2001	COA	C9P-CAP-CBP-CCP
2	D	2001	COA	S1P-C2P-C3P-N4P

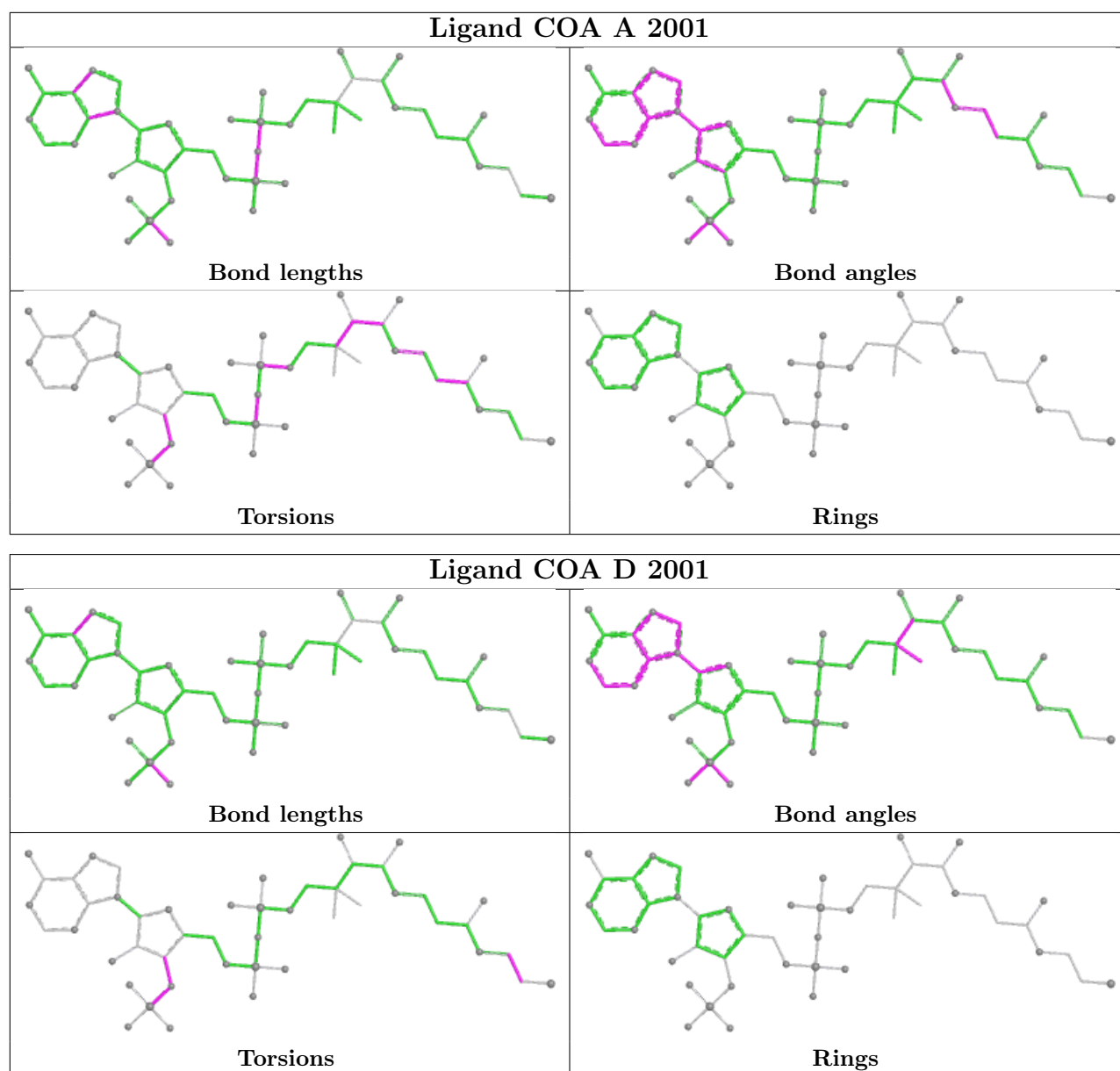
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	COA	2	0
2	B	2001	COA	1	0
4	C	2000	BTI	3	0
2	D	2001	COA	6	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	994/1150 (86%)	0.70	63 (6%) 26 20	39, 76, 117, 151	0
1	B	989/1150 (86%)	0.20	11 (1%) 78 71	26, 52, 83, 102	0
1	C	995/1150 (86%)	0.22	18 (1%) 67 59	29, 52, 83, 107	0
1	D	934/1150 (81%)	0.93	86 (9%) 14 12	41, 83, 128, 173	0
All	All	3912/4600 (85%)	0.50	178 (4%) 37 29	26, 64, 111, 173	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	GLN	5.5
1	D	239	ILE	5.4
1	D	890	VAL	5.2
1	B	163	ASP	5.0
1	D	981	TYR	4.6

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](#)

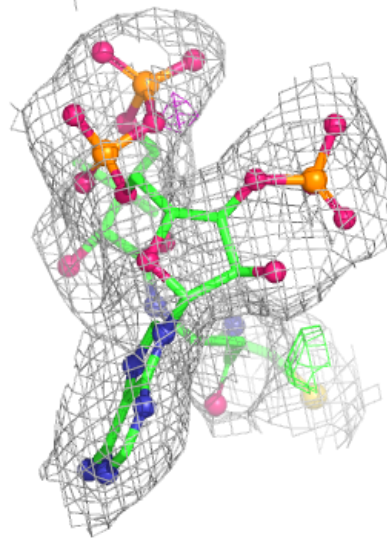
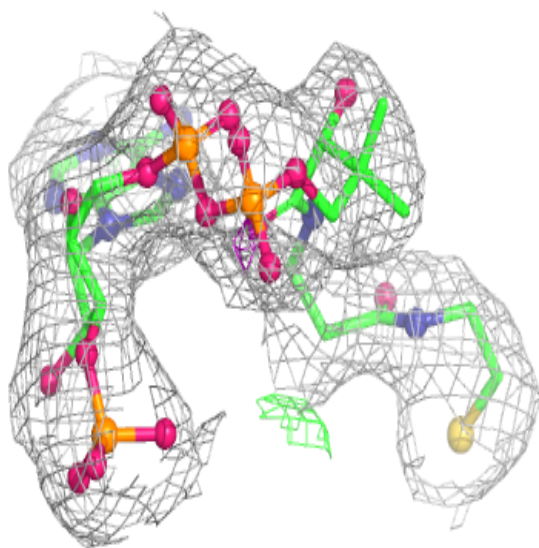
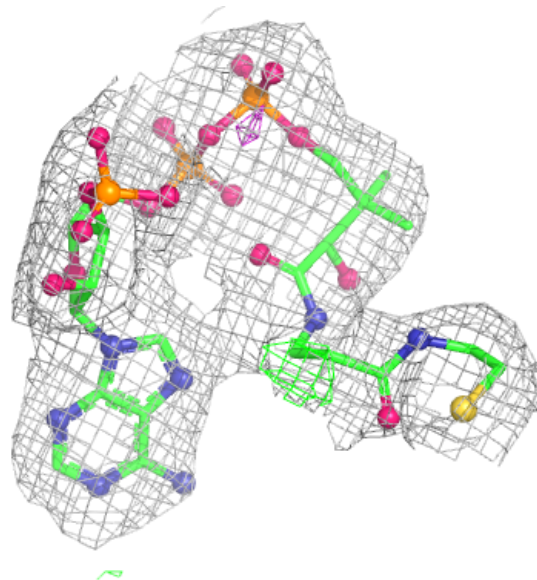
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
3	MN	A	2002	1/1	0.88	0.12	86,86,86,86	0
4	BTI	B	2000	15/15	0.89	0.12	47,53,54,55	0
2	COA	D	2001	48/48	0.92	0.10	45,51,55,56	0
4	BTI	C	2000	15/15	0.93	0.09	36,40,42,43	0
3	MN	B	2002	1/1	0.93	0.09	60,60,60,60	0
2	COA	C	2001	48/48	0.95	0.08	32,36,48,51	0
2	COA	B	2001	48/48	0.95	0.08	37,40,43,45	0
2	COA	A	2001	48/48	0.95	0.08	44,48,57,59	0
3	MN	C	2002	1/1	0.97	0.05	65,65,65,65	0
3	MN	D	2002	1/1	0.98	0.04	65,65,65,65	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.

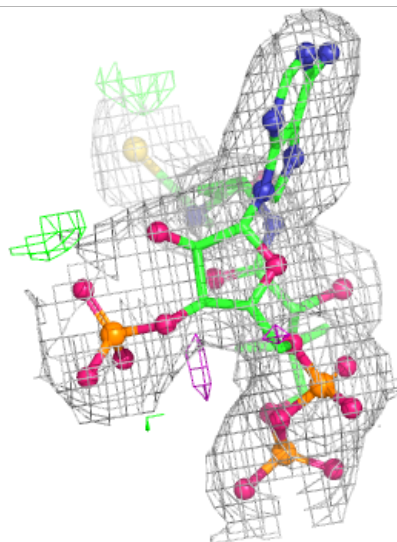
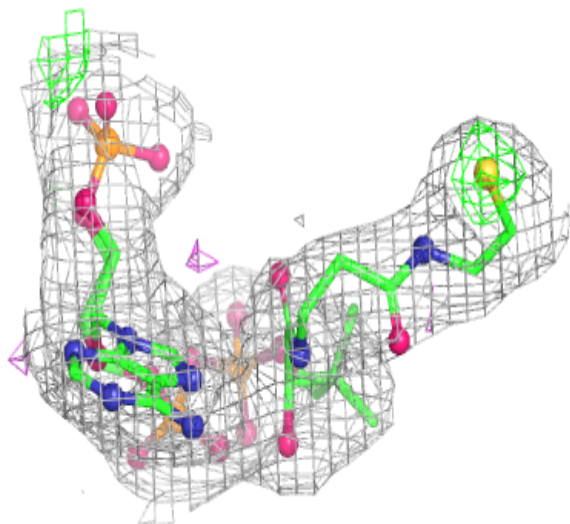
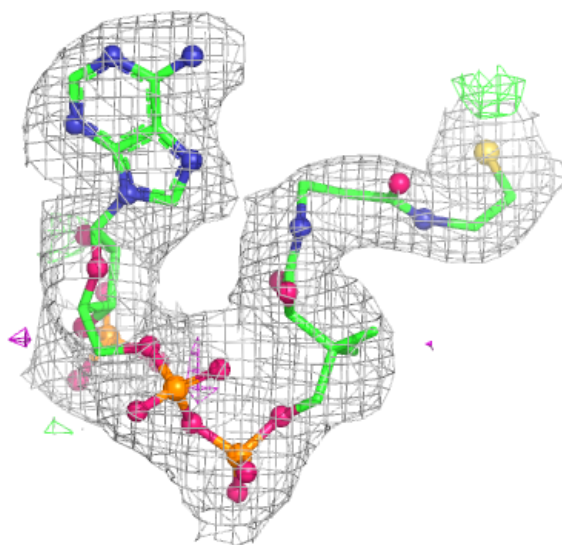
Electron density around COA D 2001:

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



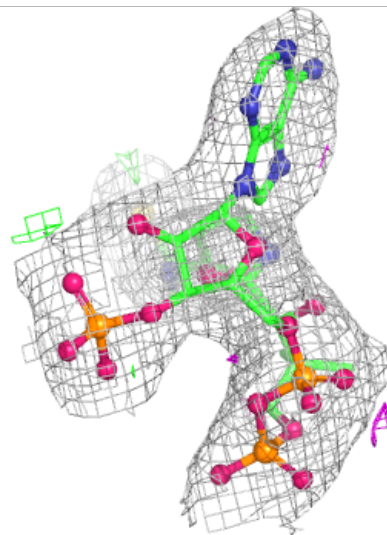
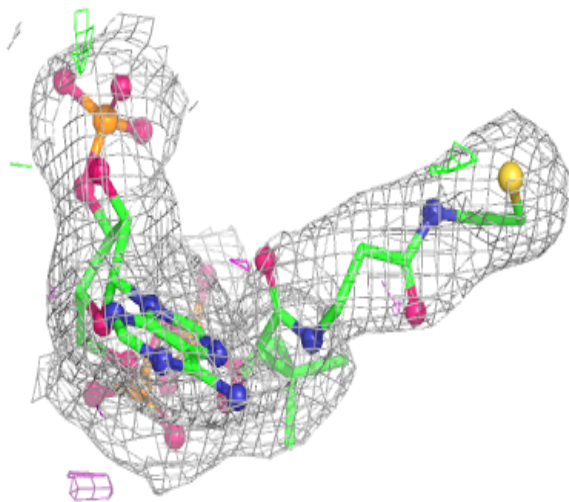
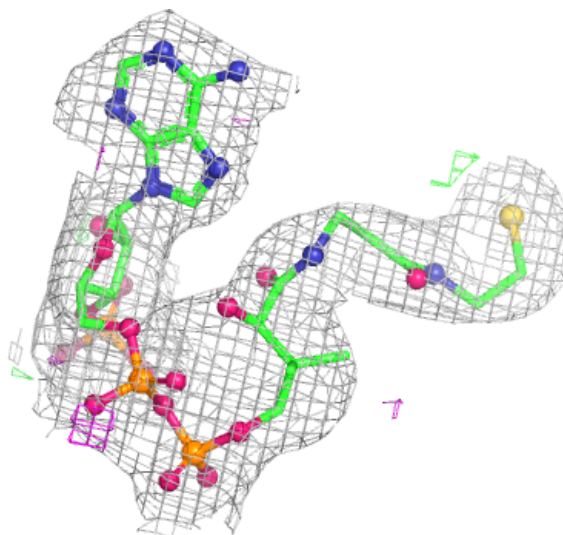
Electron density around COA C 2001:

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



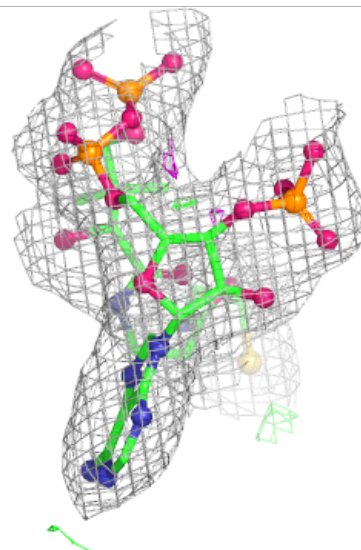
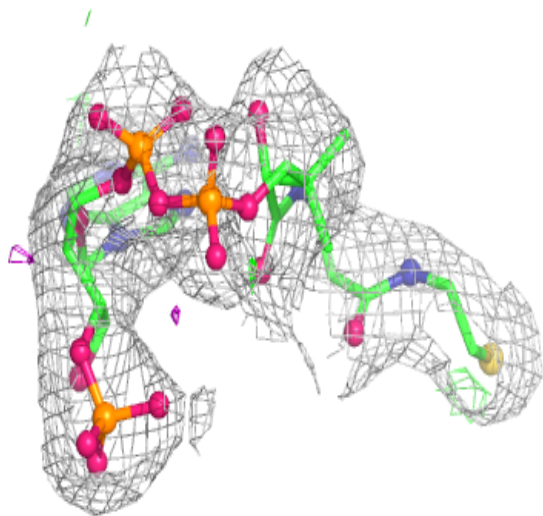
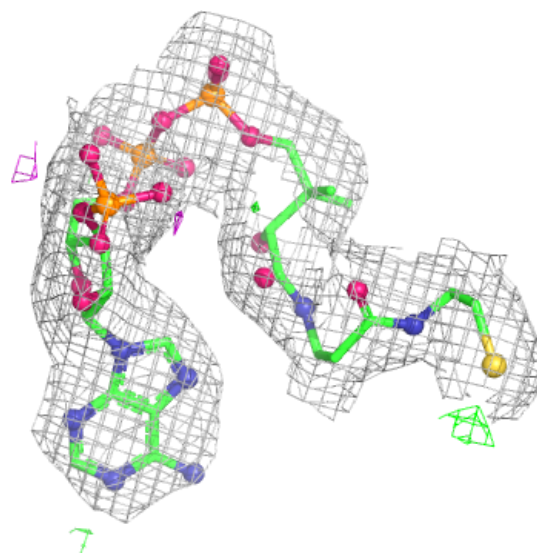
Electron density around COA B 2001:

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



Electron density around COA A 2001:

$2mF_o-DF_c$ (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.