wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 03:38 PM EDT

PDB ID	:	3TW6
Title	:	Structure of Rhizobium etli pyruvate carboxylase T882A with the allosteric activator, acetyl coenzyme-A
Authors	:	St Maurice, M.; Kumar, S.; Lietzan, A.D.
Deposited on	:	2011-09-21
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

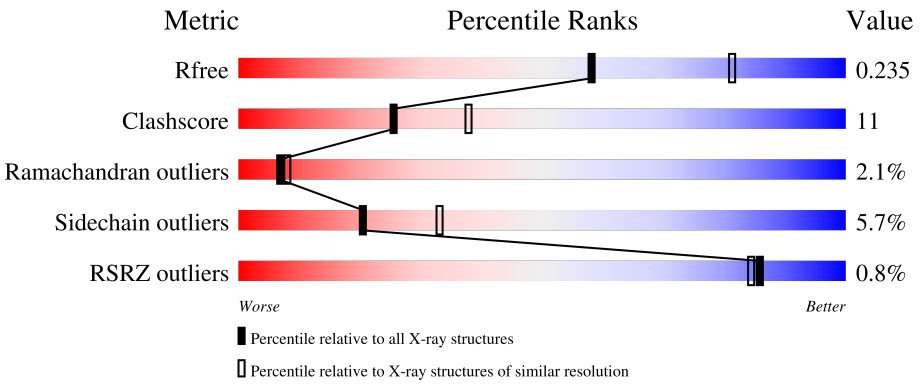
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	1165	% 66% 17% • 14%
1	B	1165	% 77% 17% • • •
1	C	1165	% 72% 16% • 10%
1	D	1165	% 76% 17% • • •

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
2	CL	A	1600	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 32812 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1007	7446	4708	1287	1423	28	10	4	0
1	B	1129	8321	5271	1431	1586	33	0	5	0
1	C	1044	7735	4914	1319	1471	31	0	1	0
1	D	1129	8294	5245	1432	1585	32	0	2	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q2K340
A	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-3	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
A	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
A	0	GLY	-	EXPRESSION TAG	UNP Q2K340
A	1	GLY	-	EXPRESSION TAG	UNP Q2K340
A	882	ALA	THR	ENGINEERED MUTATION	UNP Q2K340
B	-10	MET	-	EXPRESSION TAG	UNP Q2K340
B	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-3	HIS	-	EXPRESSION TAG	UNP Q2K340

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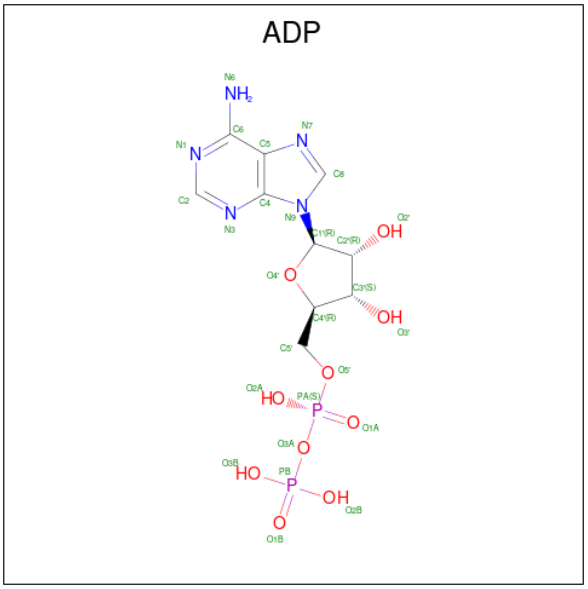
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
B	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
B	0	GLY	-	EXPRESSION TAG	UNP Q2K340
B	1	GLY	-	EXPRESSION TAG	UNP Q2K340
B	882	ALA	THR	ENGINEERED MUTATION	UNP Q2K340
C	-10	MET	-	EXPRESSION TAG	UNP Q2K340
C	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-3	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
C	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
C	0	GLY	-	EXPRESSION TAG	UNP Q2K340
C	1	GLY	-	EXPRESSION TAG	UNP Q2K340
C	882	ALA	THR	ENGINEERED MUTATION	UNP Q2K340
D	-10	MET	-	EXPRESSION TAG	UNP Q2K340
D	-9	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-8	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-7	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-6	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-5	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-4	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-3	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-2	HIS	-	EXPRESSION TAG	UNP Q2K340
D	-1	HIS	-	EXPRESSION TAG	UNP Q2K340
D	0	GLY	-	EXPRESSION TAG	UNP Q2K340
D	1	GLY	-	EXPRESSION TAG	UNP Q2K340
D	882	ALA	THR	ENGINEERED MUTATION	UNP Q2K340

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

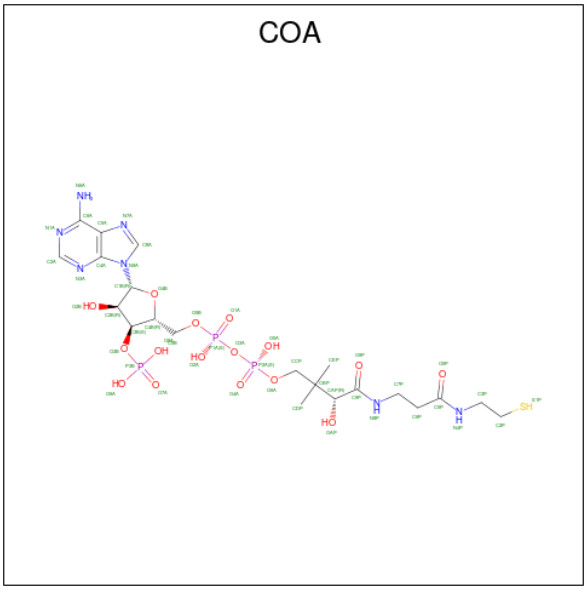
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

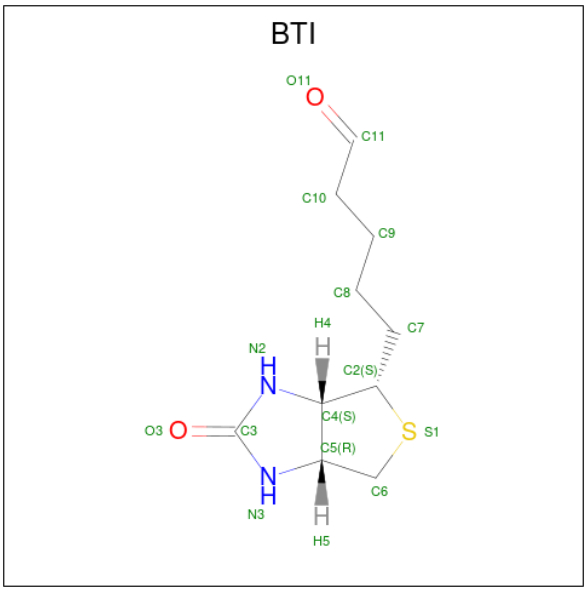
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	2	2	2	0	0
			Total	Mg		
5	B	2	2	2	0	0
			Total	Mg		
5	C	1	1	1	0	0
			Total	Mg		
5	D	2	2	2	0	0

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



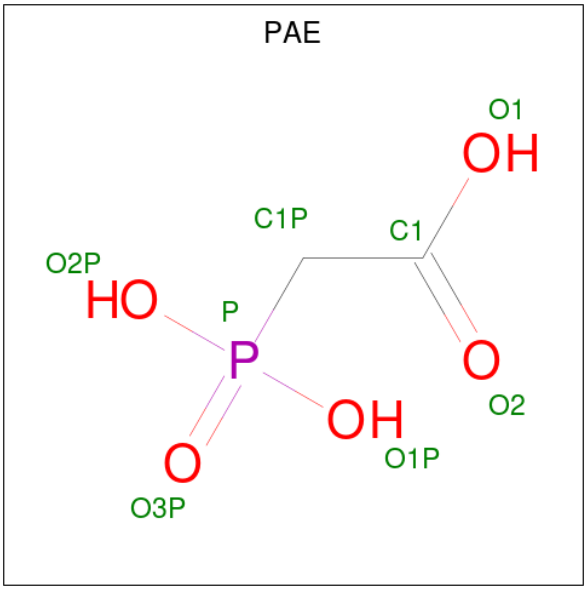
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	32	11	5	13	3	0	0
			Total	C	N	O	P		
6	C	1	33	12	5	13	3	0	0

- Molecule 7 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



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

- Molecule 8 is PHOSPHONOACETIC ACID (three-letter code: PAE) (formula: $C_2H_5O_5P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
8	C	1	16	4	10	2	0	1

- Molecule 9 is water.

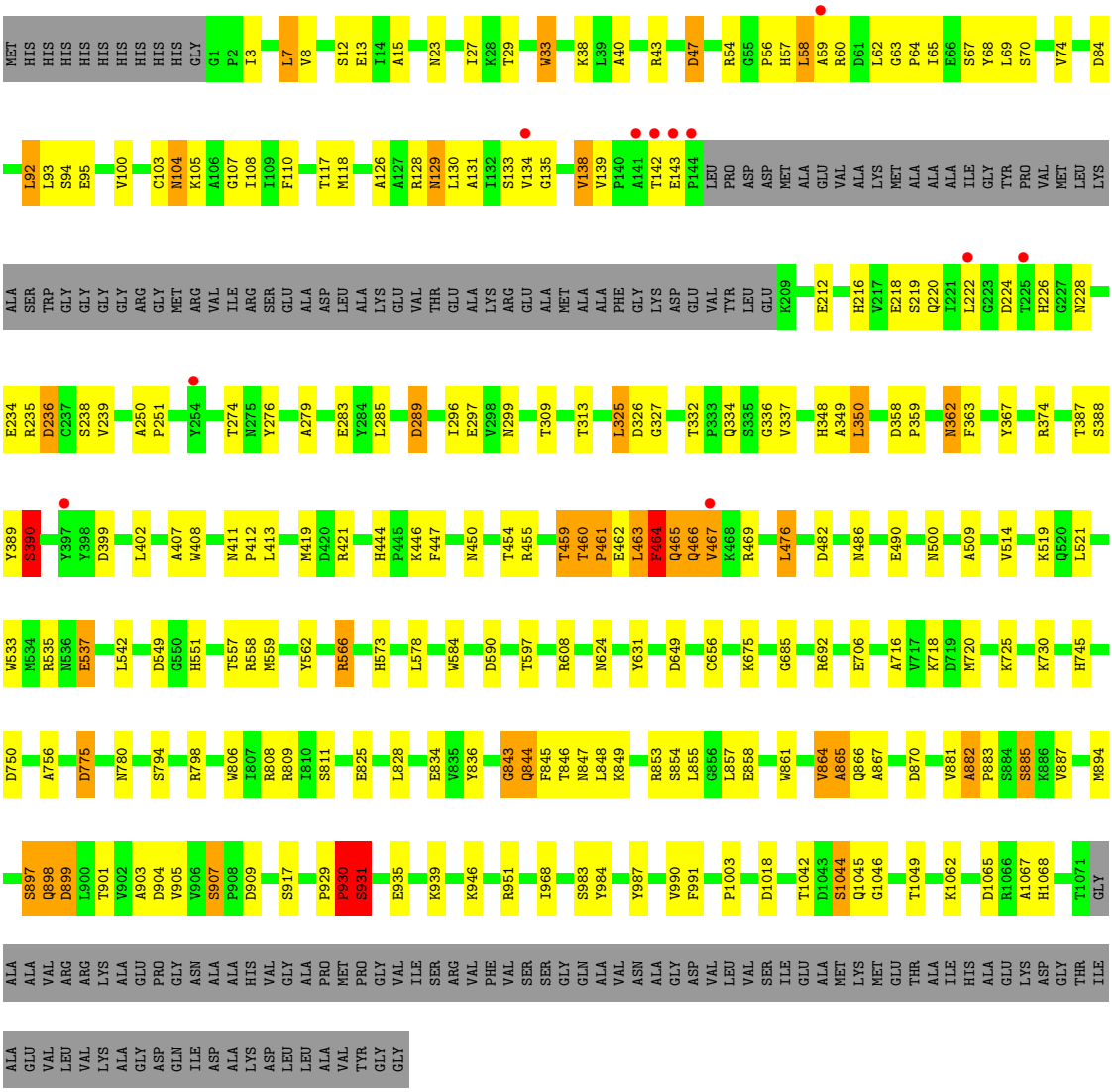
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	193	193	193	0	0
			Total	O		
9	B	244	244	244	0	0
			Total	O		
9	C	157	157	157	0	0
			Total	O		
9	D	199	199	199	0	0

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.

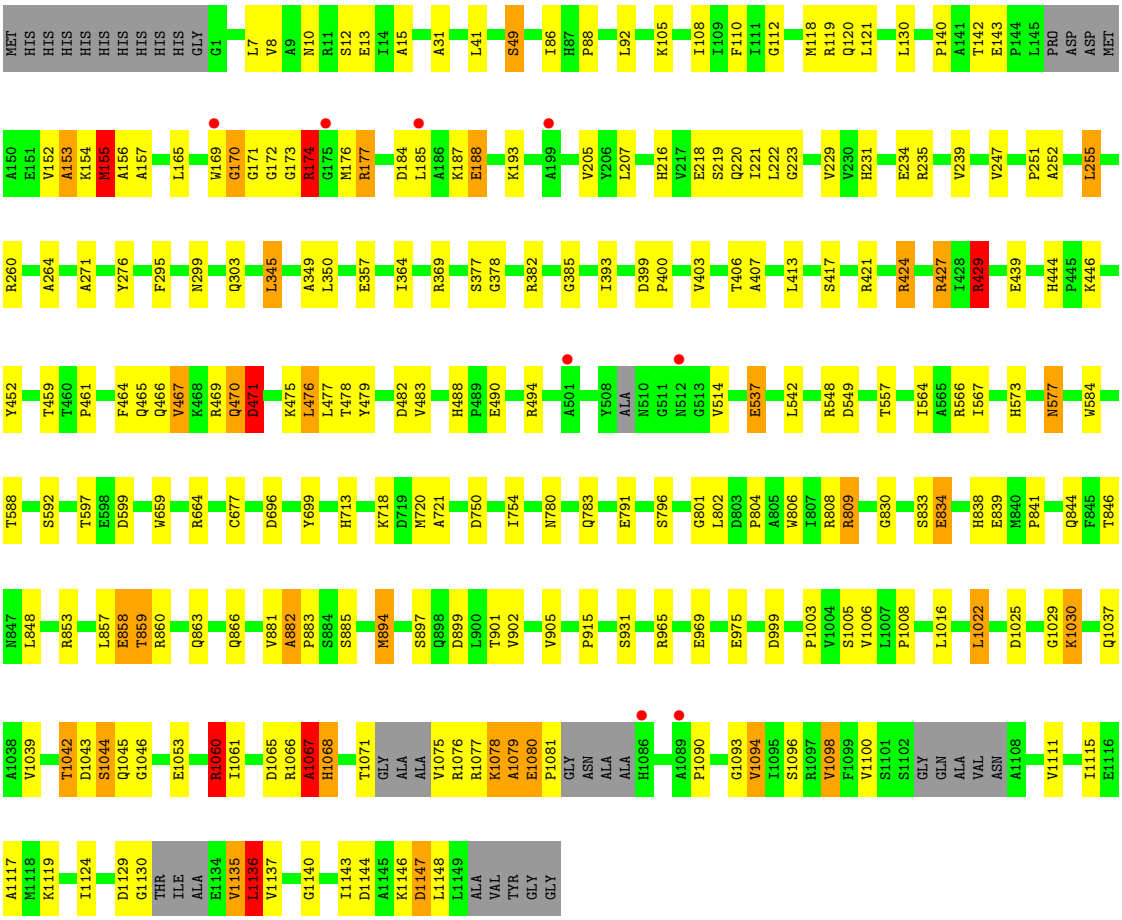
• Molecule 1: Pyruvate carboxylase protein

Chain A:



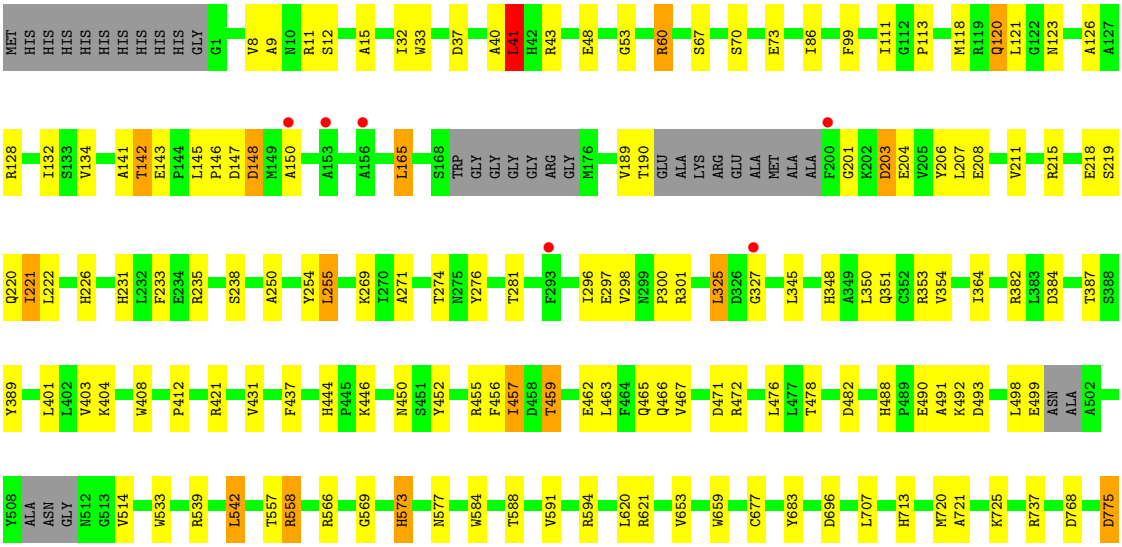
• Molecule 1: Pyruvate carboxylase protein

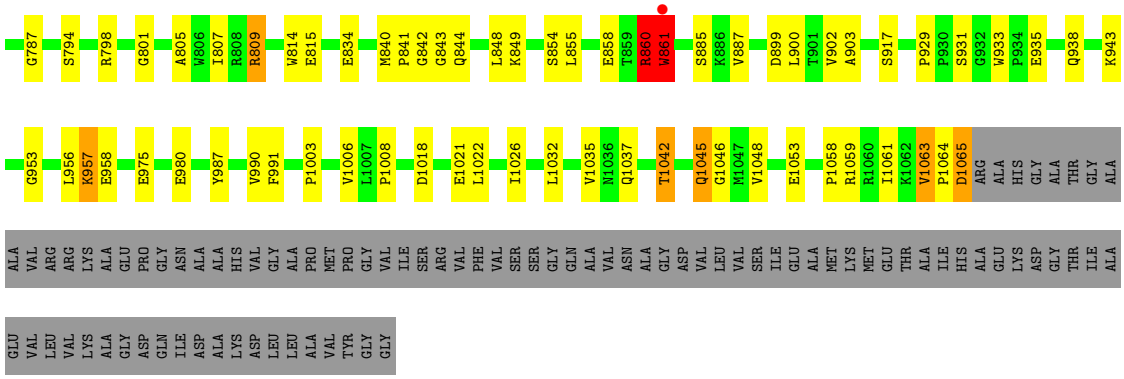
Chain B:



- Molecule 1: Pyruvate carboxylase protein

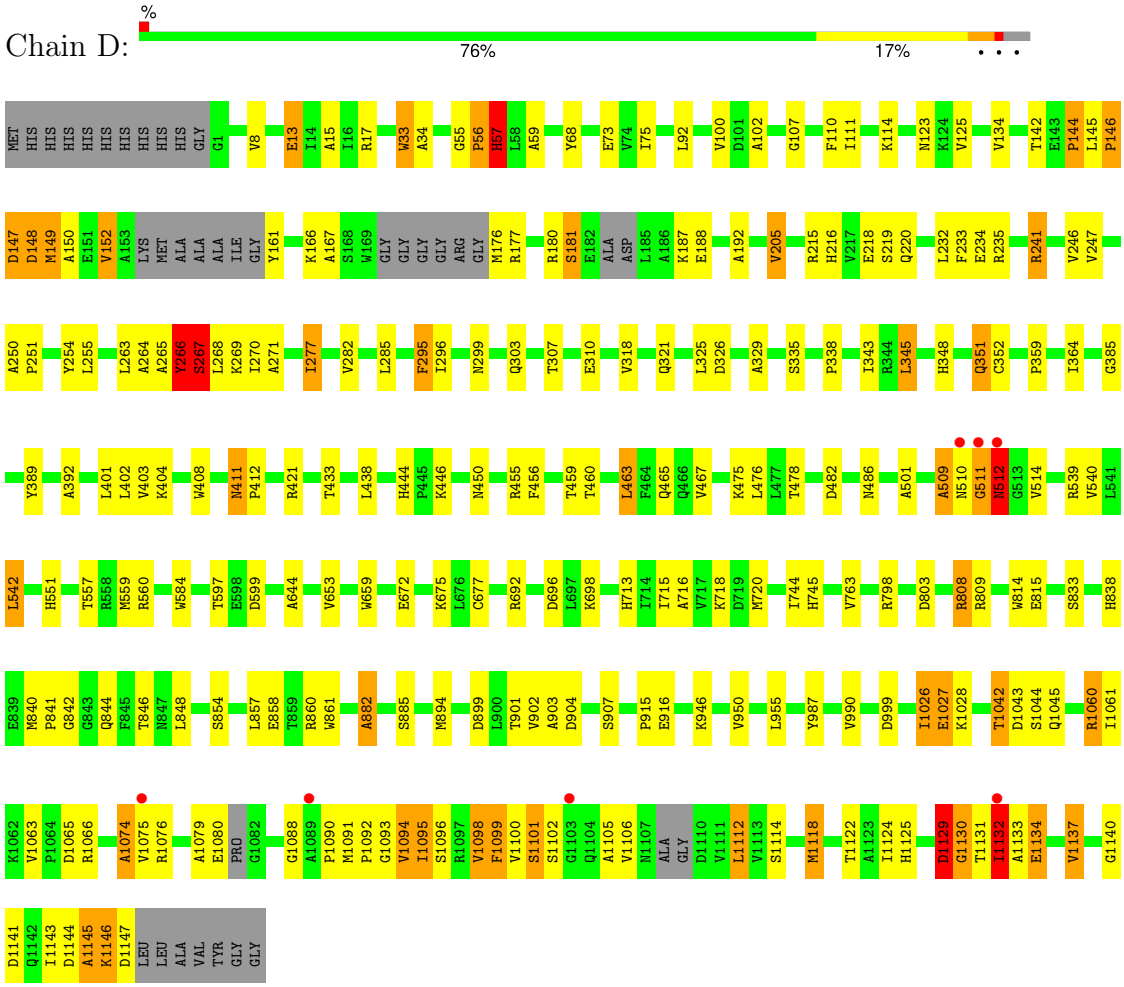
Chain C:





- Molecule 1: Pyruvate carboxylase protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	370.44Å 91.55Å 261.35Å 90.00° 134.71° 90.00°	Depositor
Resolution (Å)	46.43 – 2.40 46.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.43-2.40) 97.1 (46.43-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.189 , 0.235 0.189 , 0.235	Depositor DCC
R_{free} test set	12133 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 21.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.159 for h+2*l,k,-h-l 0.027 for h,-k,-h-l 0.028 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32812	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BTI, KCX, CL, PAE, MG, ADP, COA, ZN

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	0.97	9/7600 (0.1%)	0.98	17/10366 (0.2%)
1	B	0.97	7/8482 (0.1%)	1.01	27/11556 (0.2%)
1	C	0.93	8/7880 (0.1%)	0.96	14/10738 (0.1%)
1	D	1.06	13/8449 (0.2%)	1.00	19/11512 (0.2%)
All	All	0.98	37/32411 (0.1%)	0.99	77/44172 (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	3
1	B	0	4
1	C	0	2
1	D	0	4
All	All	0	13

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1129	ASP	C-O	31.32	1.82	1.23
1	D	1130	GLY	C-O	17.79	1.52	1.23
1	A	105	LYS	CB-CG	-15.45	1.10	1.52
1	B	1130	GLY	C-O	-10.28	1.07	1.23
1	B	1130	GLY	CA-C	8.59	1.65	1.51

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	539	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	B	427	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	B	1022	LEU	CB-CG-CD1	-9.50	94.85	111.00
1	D	696	ASP	CB-CG-OD1	8.91	126.32	118.30
1	C	696	ASP	CB-CG-OD1	8.37	125.83	118.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	GLY	Peptide
1	A	465	GLN	Peptide
1	A	930	PRO	Peptide
1	B	1067	ALA	Peptide
1	B	174	ARG	Peptide

5.2 Too-close contacts (i)

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	7446	0	7019	182	0
1	B	8321	0	7918	169	0
1	C	7735	0	7375	151	0
1	D	8294	0	7872	157	0
2	A	2	0	0	3	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
3	C	27	0	12	1	0
3	D	27	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	A	32	0	11	3	0
6	C	33	0	13	5	0
7	B	15	0	16	3	0
8	C	16	0	4	4	0
9	A	193	0	0	31	0
9	B	244	0	0	9	0
9	C	157	0	0	29	0
9	D	199	0	0	3	0
All	All	32812	0	30276	658	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 11.

The worst 5 of 658 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:591:VAL:HB	9:C:1242:HOH:O	1.34	1.25
1:D:1129:ASP:C	1:D:1129:ASP:O	1.82	1.17
1:B:470:GLN:HA	1:B:471:ASP:CB	1.75	1.14
1:C:621:ARG:NH1	9:C:1265:HOH:O	1.81	1.11
1:D:1075:VAL:H	1:D:1076:ARG:HA	0.99	1.10

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	1005/1165 (86%)	921 (92%)	58 (6%)	26 (3%)	5 5
1	B	1118/1165 (96%)	1042 (93%)	58 (5%)	18 (2%)	9 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1033/1165 (89%)	957 (93%)	61 (6%)	15 (2%)	10	14
1	D	1117/1165 (96%)	1013 (91%)	74 (7%)	30 (3%)	5	5
All	All	4273/4660 (92%)	3933 (92%)	251 (6%)	89 (2%)	7	8

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	SER
1	A	129	ASN
1	A	138	VAL
1	A	461	PRO
1	A	463	LEU

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	717/933 (77%)	669 (93%)	48 (7%)	16	26
1	B	802/933 (86%)	753 (94%)	49 (6%)	18	30
1	C	754/933 (81%)	714 (95%)	40 (5%)	22	37
1	D	798/933 (86%)	756 (95%)	42 (5%)	22	37
All	All	3071/3732 (82%)	2892 (94%)	179 (6%)	20	32

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	431	VAL
1	D	219	SER
1	C	476	LEU
1	C	885	SER
1	D	411	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	231	HIS
1	D	57	HIS
1	C	351	GLN
1	C	536	ASN
1	D	226	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	KCX	D	718[A]	4,1	10,11,12	1.20	1 (10%)	6,12,14	1.45	2 (33%)
1	KCX	C	718[A]	4,1	10,11,12	0.93	0	6,12,14	0.86	0
1	KCX	A	718[A]	4,1	10,11,12	1.02	0	6,12,14	2.59	2 (33%)
1	KCX	B	718[A]	4,1	10,11,12	1.01	1 (10%)	6,12,14	1.05	1 (16%)

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
1	KCX	D	718[A]	4,1	-	2/9/10/12	-
1	KCX	C	718[A]	4,1	-	1/9/10/12	-
1	KCX	A	718[A]	4,1	-	1/9/10/12	-
1	KCX	B	718[A]	4,1	-	1/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	718[A]	KCX	OQ1-CX	2.77	1.26	1.21
1	B	718[A]	KCX	O-C	2.34	1.28	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	718[A]	KCX	CE-NZ-CX	5.41	131.16	121.98
1	D	718[A]	KCX	CD-CE-NZ	-2.54	105.07	112.20
1	B	718[A]	KCX	CE-NZ-CX	2.47	126.17	121.98
1	A	718[A]	KCX	OQ1-CX-NZ	-2.41	121.25	124.92
1	D	718[A]	KCX	CE-NZ-CX	-2.36	117.97	121.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	O-C-CA-CB
1	C	718[A]	KCX	O-C-CA-CB
1	D	718[A]	KCX	O-C-CA-CB
1	D	718[A]	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 19 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	ADP	A	2000	5	24,29,29	1.35	3 (12%)	29,45,45	1.51	5 (17%)
3	ADP	B	2000	5	24,29,29	0.83	0	29,45,45	1.34	4 (13%)
8	PAE	C	2003[A]	-	7,7,7	1.19	0	9,10,10	1.65	1 (11%)
8	PAE	C	2003[B]	5	7,7,7	1.38	0	9,10,10	1.38	2 (22%)
3	ADP	C	2000	5	24,29,29	1.29	3 (12%)	29,45,45	1.35	3 (10%)
3	ADP	D	2000	5	24,29,29	1.10	2 (8%)	29,45,45	1.31	4 (13%)
6	COA	C	4011	-	31,35,50	1.36	6 (19%)	38,54,75	1.54	8 (21%)
6	COA	A	4011	-	30,34,50	1.12	3 (10%)	37,53,75	1.93	9 (24%)
7	BTI	B	2003	-	15,16,16	0.89	1 (6%)	20,21,21	1.67	4 (20%)

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
3	ADP	A	2000	5	-	3/12/32/32	0/3/3/3
3	ADP	B	2000	5	-	1/12/32/32	0/3/3/3
8	PAE	C	2003[A]	-	-	3/5/5/5	-
8	PAE	C	2003[B]	5	-	0/5/5/5	-
3	ADP	C	2000	5	-	4/12/32/32	0/3/3/3
3	ADP	D	2000	5	-	1/12/32/32	0/3/3/3
6	COA	C	4011	-	-	10/21/41/64	0/3/3/3
6	COA	A	4011	-	-	9/20/40/64	0/3/3/3
7	BTI	B	2003	-	-	4/6/27/27	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	ADP	PA-O3A	4.70	1.64	1.59
3	C	2000	ADP	PA-O3A	4.06	1.63	1.59
6	C	4011	COA	O4B-C1B	3.25	1.45	1.40
6	C	4011	COA	C2A-N3A	3.18	1.37	1.32
6	C	4011	COA	P1A-O3A	3.11	1.62	1.59

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4011	COA	O5A-P2A-O3A	-5.95	91.18	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2003	BTI	C2-C4-N2	5.10	118.75	113.34
3	D	2000	ADP	N3-C2-N1	-4.52	122.53	128.67
3	B	2000	ADP	N3-C2-N1	-4.48	122.59	128.67
3	A	2000	ADP	N3-C2-N1	-4.35	122.77	128.67

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	ADP	C5'-O5'-PA-O3A
6	A	4011	COA	C5B-O5B-P1A-O2A
6	A	4011	COA	C5B-O5B-P1A-O3A
6	C	4011	COA	C4B-C5B-O5B-P1A
6	C	4011	COA	CCP-O6A-P2A-O3A

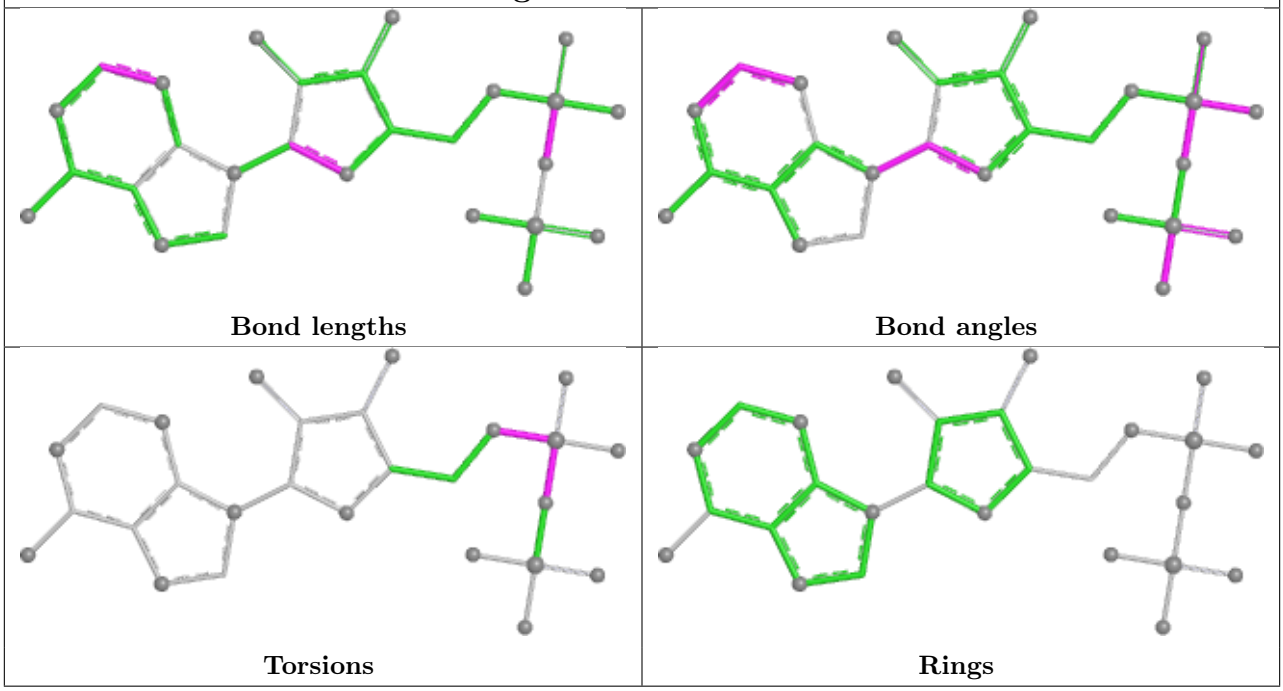
There are no ring outliers.

9 monomers are involved in 24 short contacts:

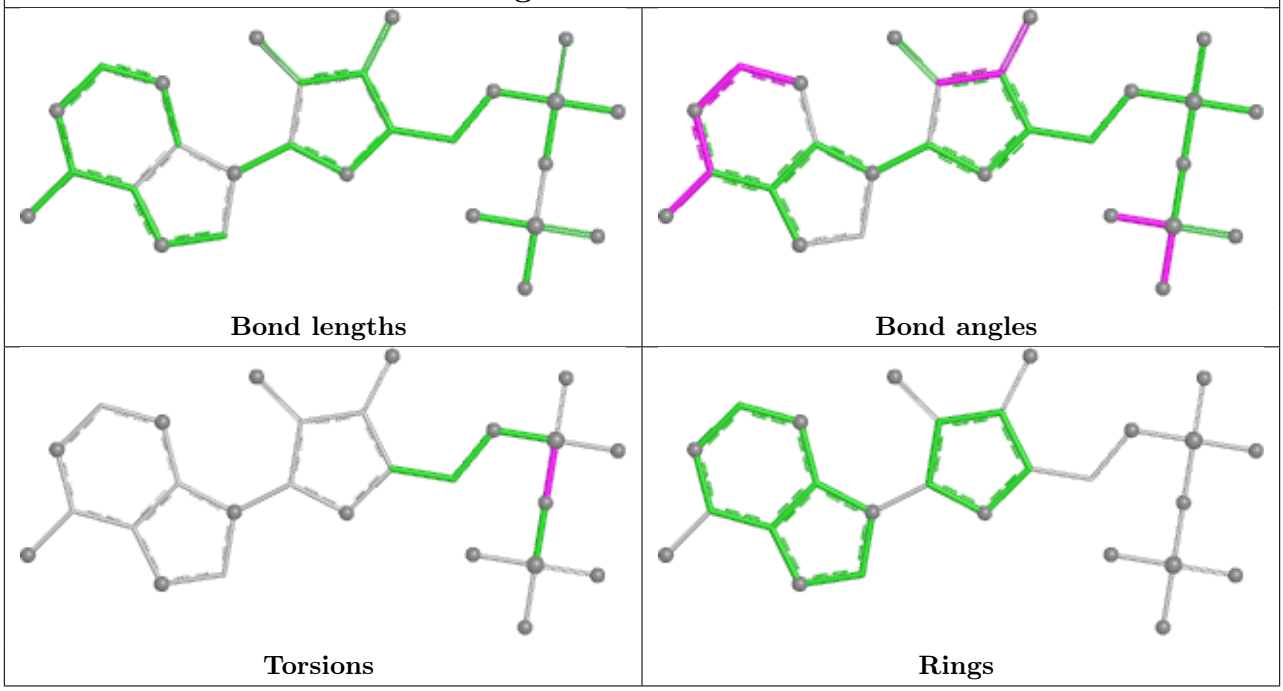
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	ADP	3	0
3	B	2000	ADP	3	0
8	C	2003[A]	PAE	1	0
8	C	2003[B]	PAE	3	0
3	C	2000	ADP	1	0
3	D	2000	ADP	3	0
6	C	4011	COA	5	0
6	A	4011	COA	3	0
7	B	2003	BTI	3	0

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 then 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.

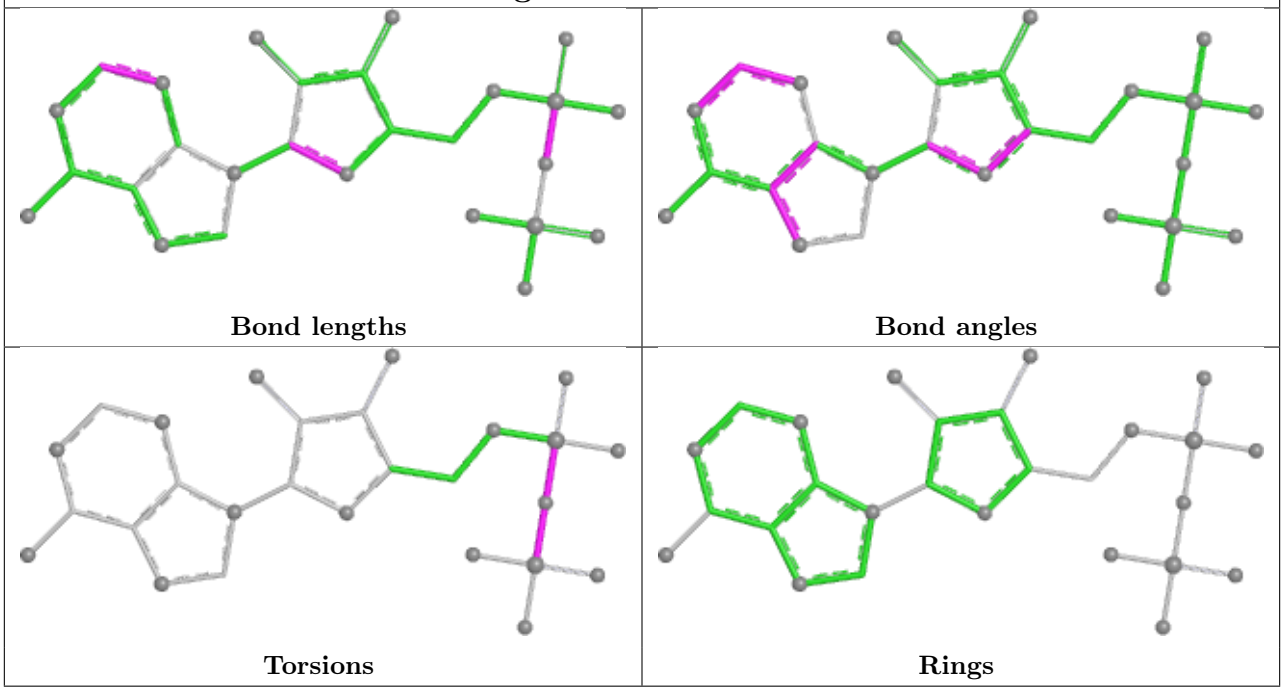
Ligand ADP A 2000



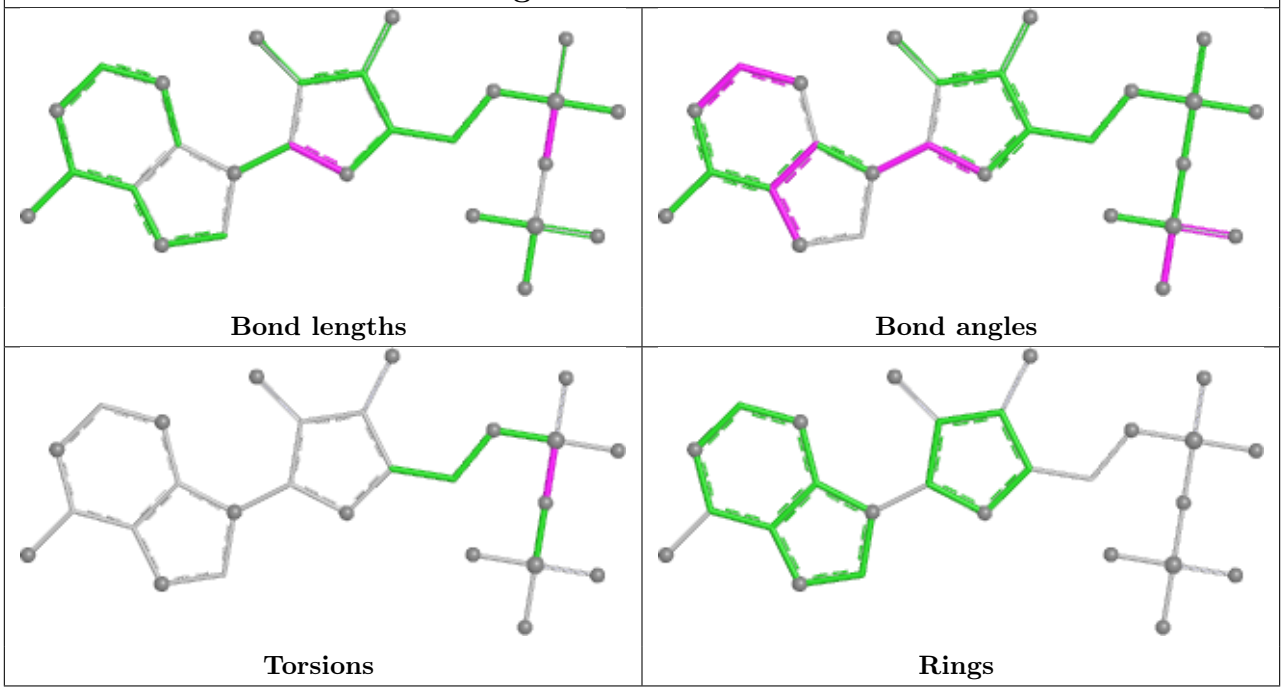
Ligand ADP B 2000



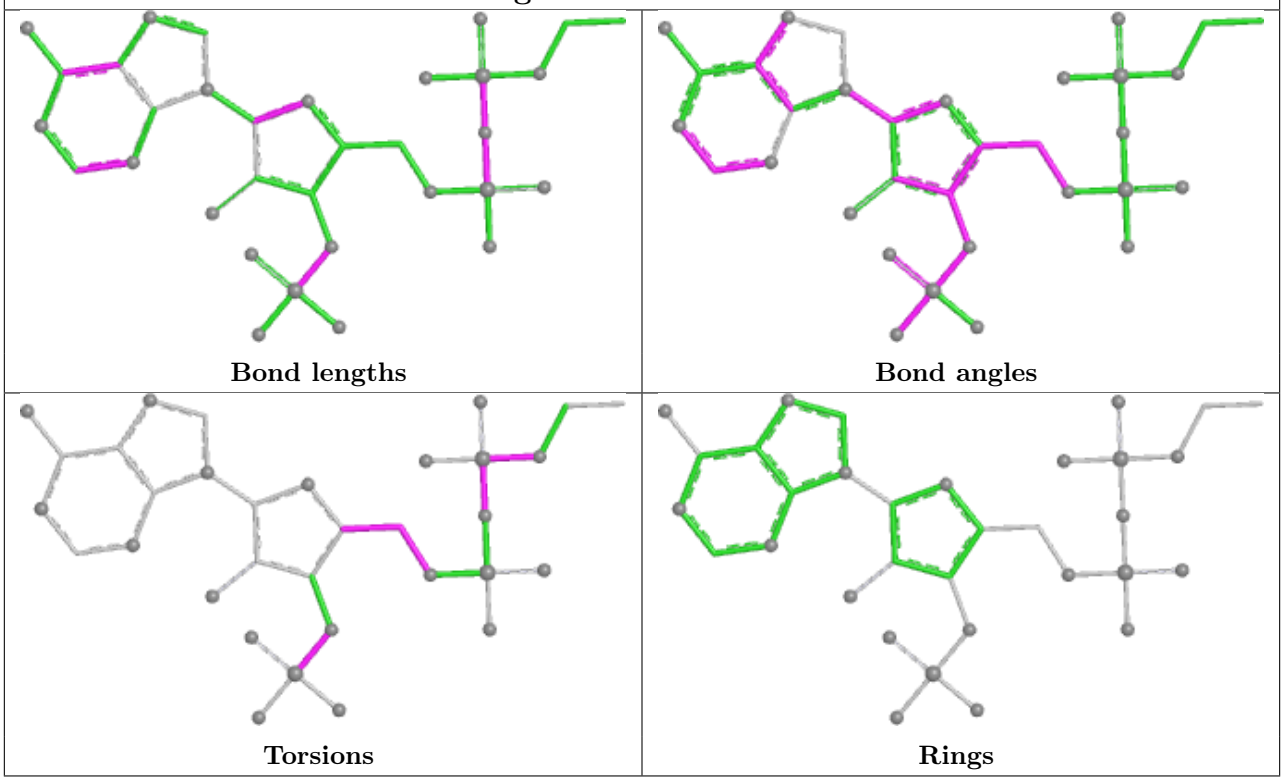
Ligand ADP C 2000



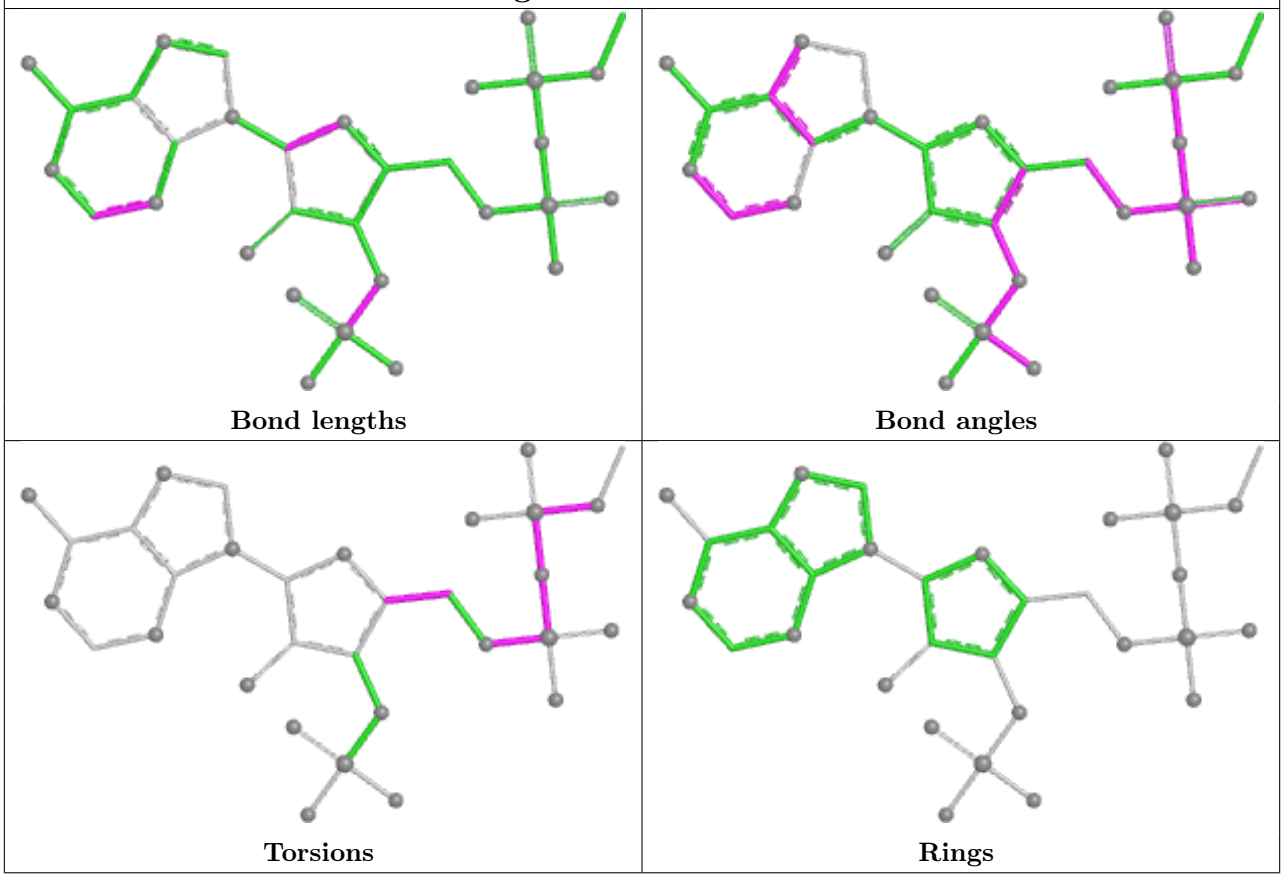
Ligand ADP D 2000



Ligand COA C 4011



Ligand COA A 4011



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	1006/1165 (86%)	-0.32	11 (1%)	80	79	17, 47, 90, 142	3 (0%)
1	B	1128/1165 (96%)	-0.41	8 (0%)	87	86	16, 43, 77, 114	3 (0%)
1	C	1043/1165 (89%)	-0.38	7 (0%)	87	86	18, 47, 82, 111	2 (0%)
1	D	1128/1165 (96%)	-0.37	7 (0%)	89	88	17, 43, 93, 135	3 (0%)
All	All	4305/4660 (92%)	-0.37	33 (0%)	86	84	16, 44, 86, 142	11 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	ALA	4.1
1	A	467	VAL	3.8
1	D	1075	VAL	3.7
1	A	144	PRO	3.4
1	A	141	ALA	3.3

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	KCX	B	718[A]	12/13	0.98	0.11	19,21,25,26	0
1	KCX	C	718[A]	12/13	0.98	0.09	20,21,23,24	0
1	KCX	D	718[A]	12/13	0.98	0.13	18,19,22,22	0
1	KCX	A	718[A]	12/13	0.99	0.11	19,20,22,24	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

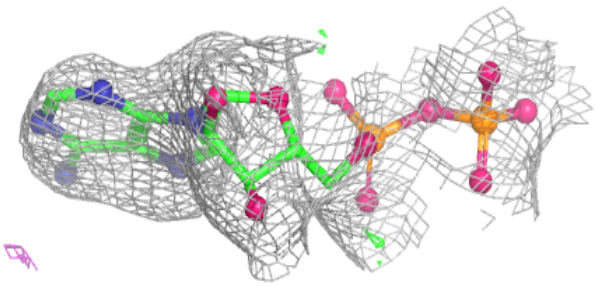
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	2002	1/1	0.79	0.10	78,78,78,78	0
3	ADP	A	2000	27/27	0.81	0.15	80,102,116,122	0
7	BTI	B	2003	15/15	0.83	0.16	49,71,85,87	0
8	PAE	C	2003[A]	8/8	0.84	0.23	55,70,76,76	8
8	PAE	C	2003[B]	8/8	0.84	0.23	82,90,96,99	8
6	COA	C	4011	33/48	0.88	0.17	58,82,116,116	0
6	COA	A	4011	32/48	0.89	0.13	63,78,99,120	0
5	MG	D	2002	1/1	0.93	0.17	60,60,60,60	0
5	MG	B	2002	1/1	0.94	0.18	50,50,50,50	0
2	CL	A	1600	1/1	0.95	0.07	55,55,55,55	0
5	MG	C	2002	1/1	0.95	0.06	55,55,55,55	0
3	ADP	D	2000	27/27	0.96	0.15	53,59,82,91	0
3	ADP	C	2000	27/27	0.96	0.15	52,60,79,80	0
3	ADP	B	2000	27/27	0.97	0.13	41,52,55,58	0
2	CL	C	1600	1/1	0.97	0.14	49,49,49,49	0
4	ZN	D	2001	1/1	0.98	0.06	43,43,43,43	0
2	CL	A	1601	1/1	0.99	0.17	23,23,23,23	0
2	CL	D	1600	1/1	0.99	0.21	39,39,39,39	0
5	MG	D	2005	1/1	0.99	0.10	16,16,16,16	0
2	CL	D	1601	1/1	0.99	0.22	25,25,25,25	0
2	CL	B	1600	1/1	0.99	0.17	35,35,35,35	0
5	MG	A	2005	1/1	0.99	0.08	18,18,18,18	0
2	CL	B	1601	1/1	0.99	0.23	22,22,22,22	0
5	MG	B	2005	1/1	0.99	0.08	17,17,17,17	0
4	ZN	A	2001	1/1	1.00	0.07	38,38,38,38	0
4	ZN	B	2001	1/1	1.00	0.08	40,40,40,40	0
4	ZN	C	2001	1/1	1.00	0.07	41,41,41,41	0
2	CL	C	1601	1/1	1.00	0.24	24,24,24,24	0

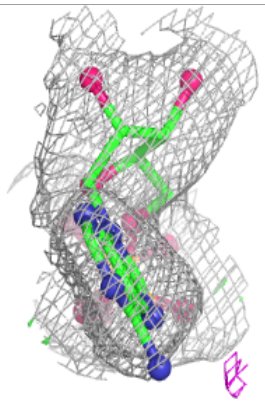
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around ADP A 2000:

$2mF_o$-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 4011:

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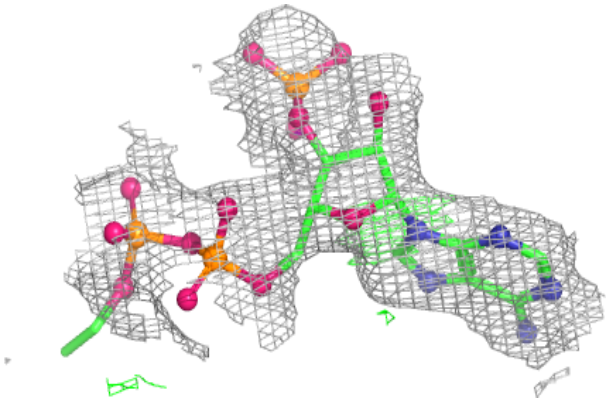
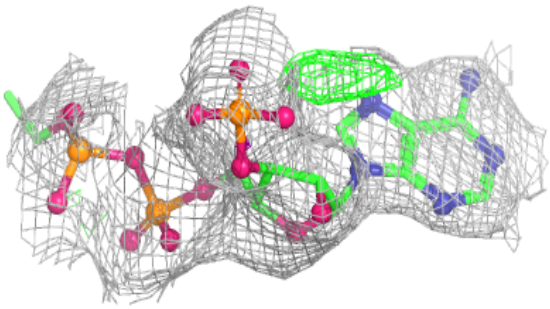
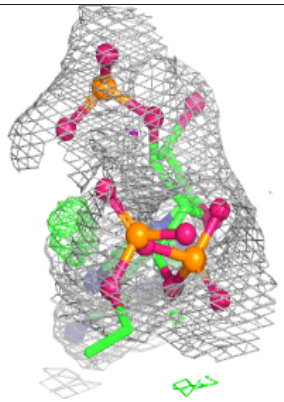
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around COA A 4011:

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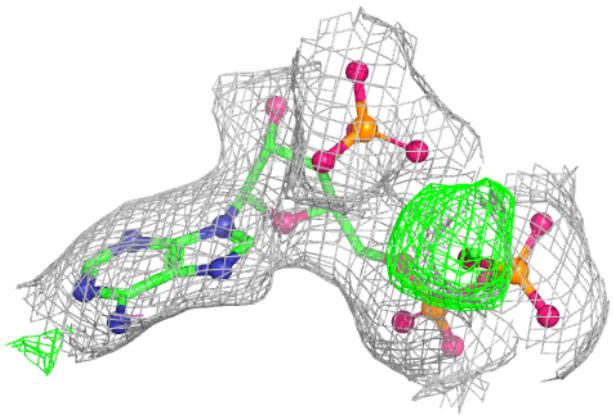
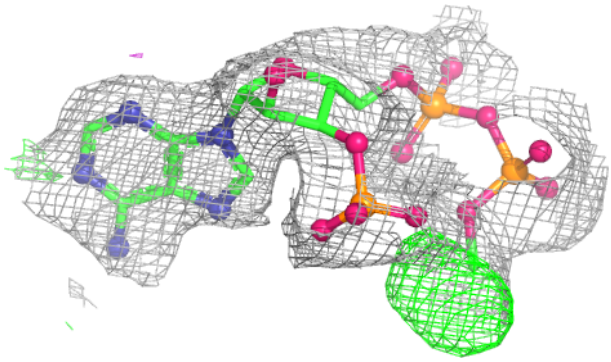
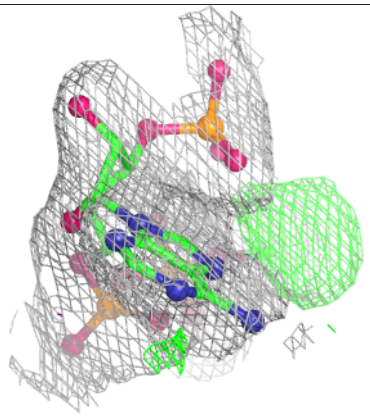
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ADP D 2000:

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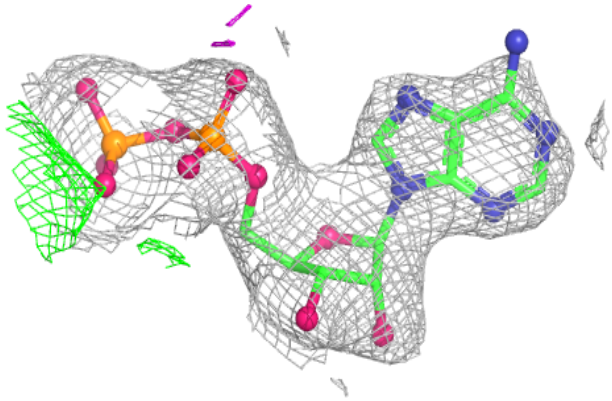
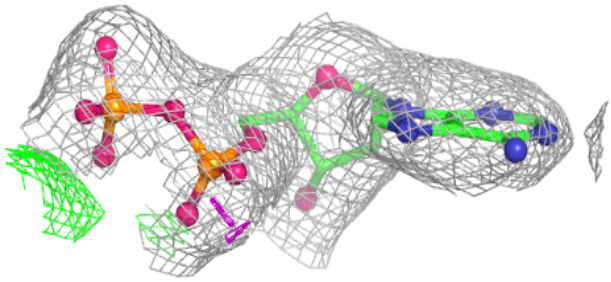
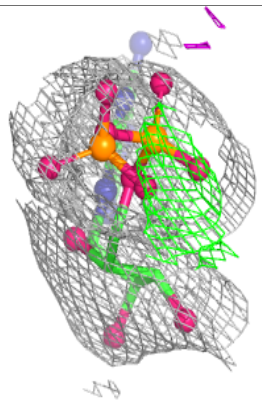
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

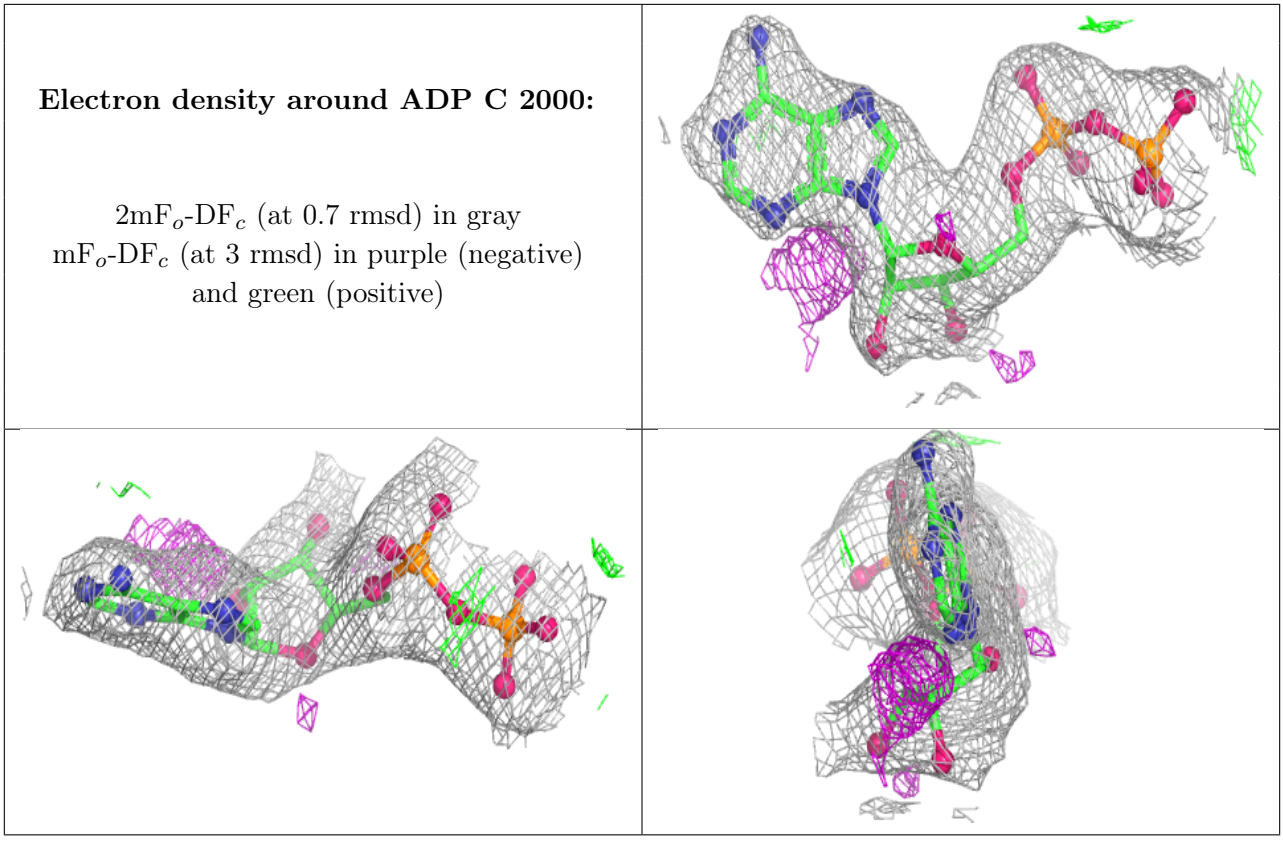






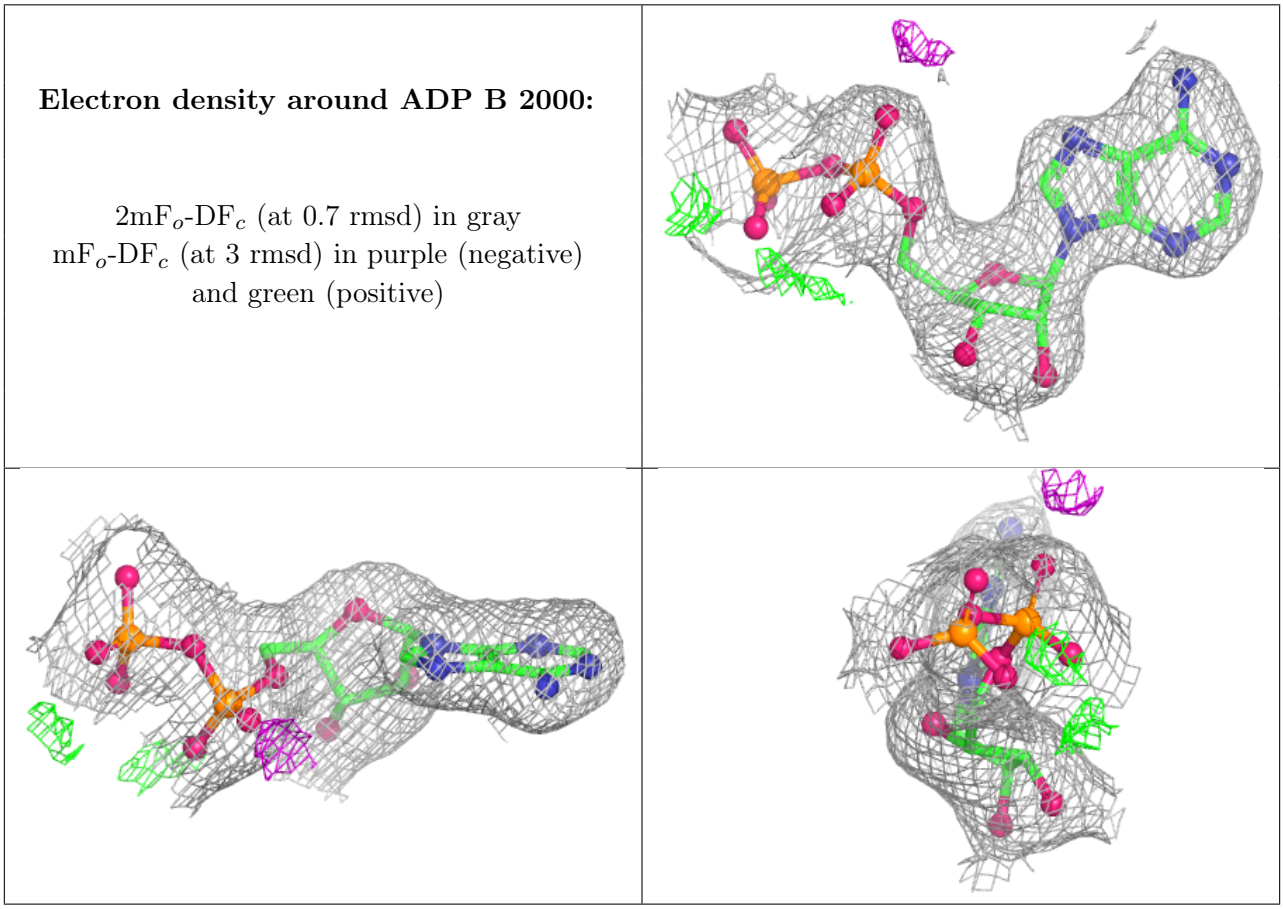
Electron density around ADP C 2000:

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



Electron density around ADP B 2000:

$2mF_o$-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.