W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:40 am BST

PDB ID	:	1CQI
Title	:	Crystal Structure of the Complex of ADP and MG2+ with Dephosphorylated E. Coli Succinyl-CoA Synthetase
Authors	:	Joyce, M.A.; Fraser, M.E.; James, M.N.G.; Bridger, W.A.; Wolodko, W.T.
Deposited on	:	1999-08-06
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

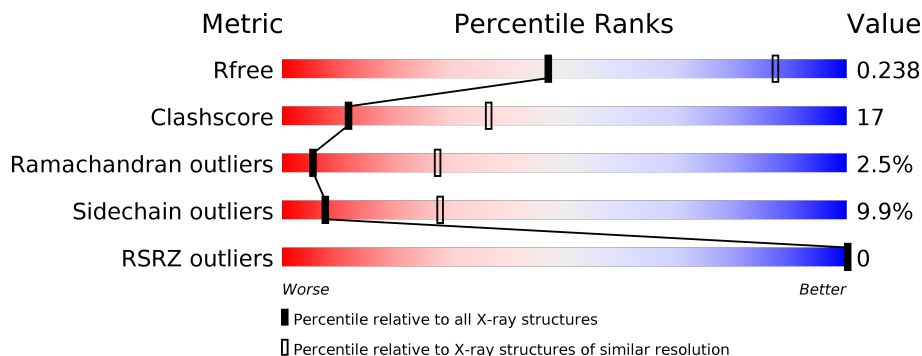|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		17
Ramachandran outliers		2.5%
Sidechain outliers		9.9%
RSRZ outliers		0

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	286	63% 30% 6%
1	D	286	59% 33% 8%
2	B	385	71% 24% •
2	E	385	70% 26% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10054 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.
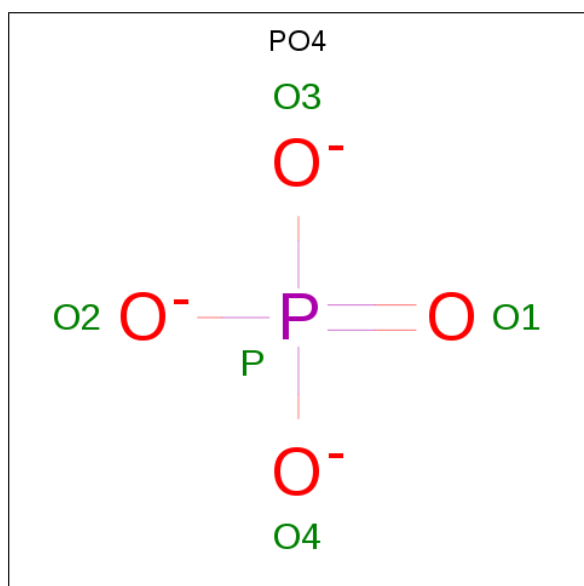
- Molecule 1 is a protein called PROTEIN (SUCCINYL-COA SYNTHETASE ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2061	1307	345	398	11			
1	D	286	Total	C	N	O	S	0	0	0
			2061	1307	345	398	11			

- Molecule 2 is a protein called PROTEIN (SUCCINYL-COA SYNTHETASE BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			
2	E	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	D	1	Total 5	O 4	P 1	0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
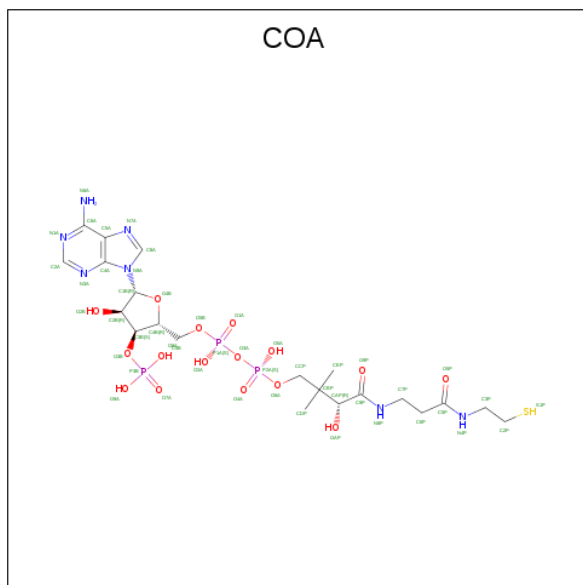
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0

- Molecule 6 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
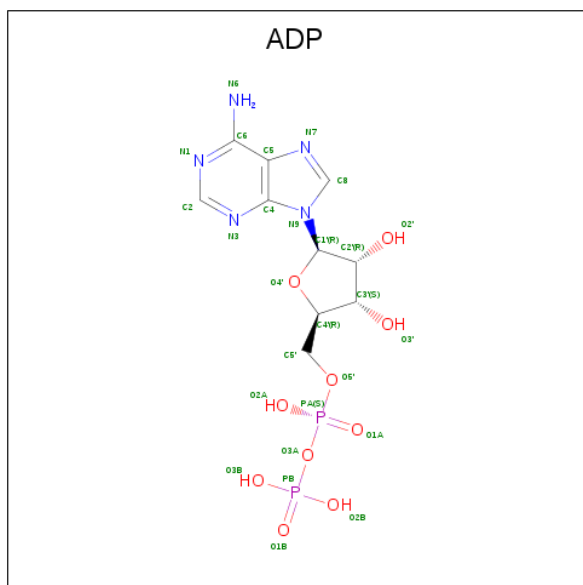
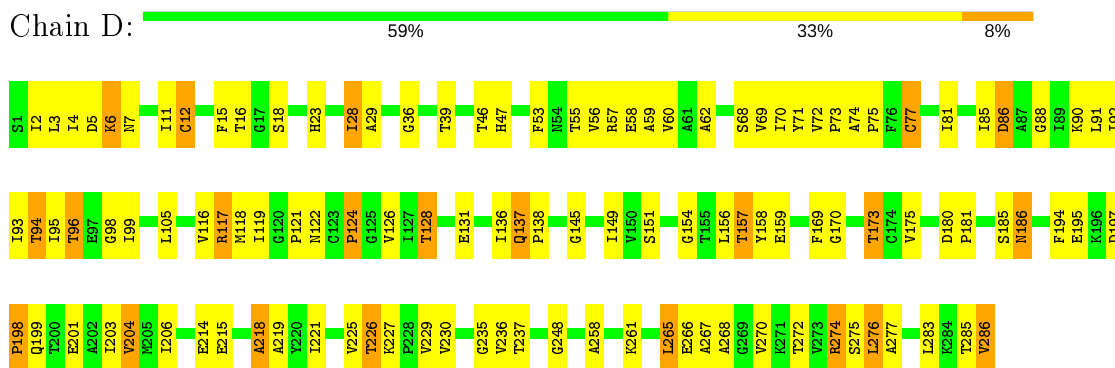| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
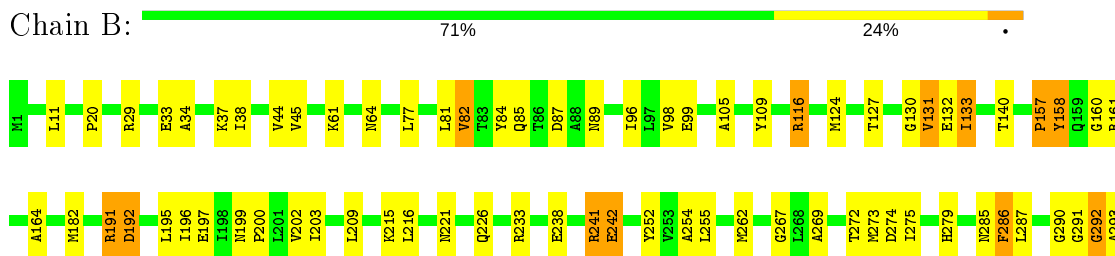
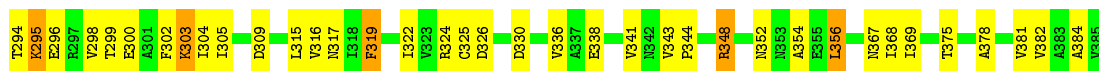- Molecule 1: PROTEIN (SUCCINYL-COA SYNTHETASE ALPHA CHAIN)
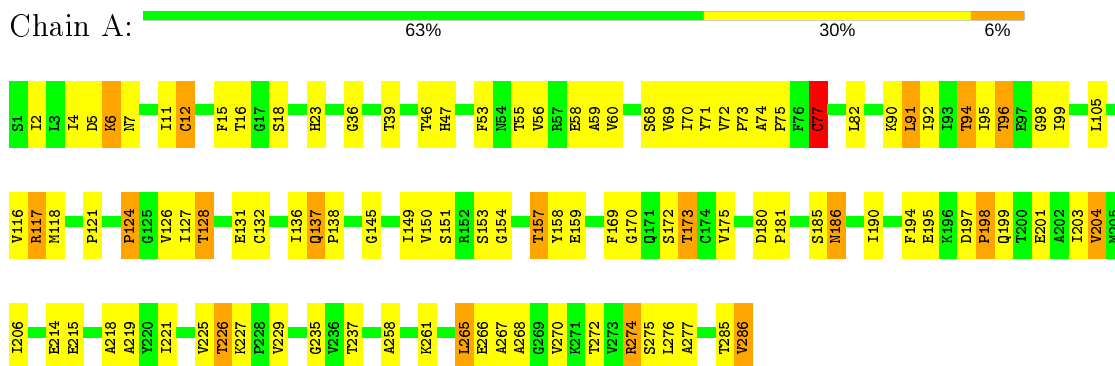
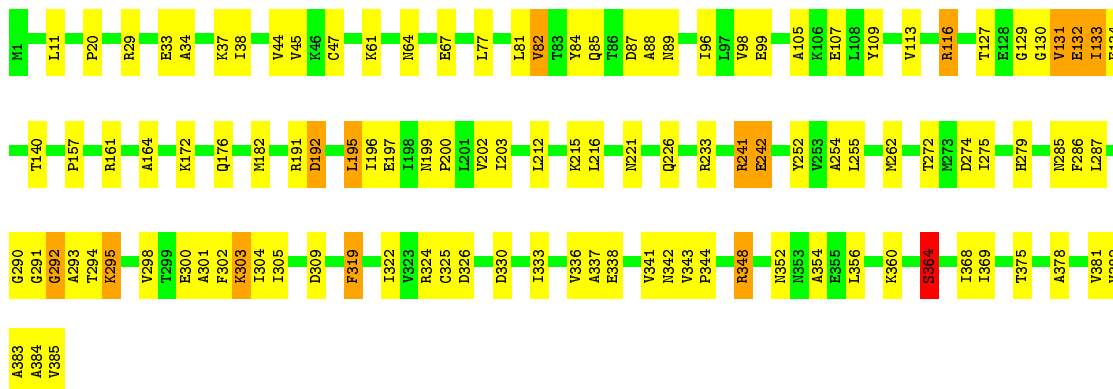- Molecule 1: PROTEIN (SUCCINYL-COA SYNTHETASE ALPHA CHAIN)

- Molecule 2: PROTEIN (SUCCINYL-COA SYNTHETASE BETA CHAIN)

T294 K295 E296 R297 V298 T299 E300 A301 F302 K303 I304 I305 D309 L315 V316 N317 I318 F319 I322 V323 R324 C325 D326 D330 V336 E338 V341 N342 V343 P344 R348 N352 N353 A354 E355 L356 N367 I368 I369 T375 A378 V381 V382 A383 A384 V385

• Molecule 2: PROTEIN (SUCCINYL-COA SYNTHETASE BETA CHAIN)

Chain E:

70%   26%   .

M1 L11 P20 R29 E33 A34 K37 I38 V44 V45 K46 C47 K61 N64 E67 L77 L81 V82 T83 Y84 Q85 T86 D87 A88 N89 I96 L97 V98 E99 A105 K106 E107 L108 Y109 V113 R116 T127 E128 G129 G130 V131 E132 I133 E134

T140 P157 R161 A164 K172 Q176 M182 R191 D192 L195 I196 E197 I198 N199 P200 L201 V202 I203 L212 K215 L216 N221 Q226 R233 R241 E242 Y252 V253 A254 L255 M262 T272 M273 D274 I275 H279 N285 F286 L287

G290 G291 G292 A293 T294 K295 V298 T299 E300 A301 F302 K303 I304 I305 D309 F319 I322 V323 R324 C325 D326 D330 I333 V336 A337 E338 V341 N342 V343 P344 R348 N352 N353 A354 E355 L356 K360 S364 I368 I369 T375 A378 V381 V382

A383 A384 V385

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.86Å 99.86Å 407.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.30) 99.1 (19.97-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.50 (at 3.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.247 0.187 , 0.238	Depositor DCC
R_{free} test set	3470 reflections (10.93%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 31.1	EDS
L-test for twinning[2]	$<|L|> = 0.44, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10054	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, PO4, MG, 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	0.80	1/2095 (0.0%)	0.93	2/2838 (0.1%)
1	D	0.77	0/2095	0.92	1/2838 (0.0%)
2	B	0.83	0/2927	0.86	1/3961 (0.0%)
2	E	0.84	1/2927 (0.0%)	0.85	1/3961 (0.0%)
All	All	0.82	2/10044 (0.0%)	0.89	5/13598 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	47	CYS	CB-SG	-8.38	1.68	1.82
1	A	77	CYS	CB-SG	-6.62	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LEU	CA-CB-CG	-6.50	100.35	115.30
2	E	113	VAL	CB-CA-C	-5.56	100.83	111.40
2	B	191	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	91	LEU	CA-CB-CG	-5.08	103.62	115.30
1	A	91	LEU	CA-CB-CG	-5.08	103.62	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	158	TYR	Sidechain

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	2061	0	2117	103	0
1	D	2061	0	2117	106	0
2	B	2885	0	2941	77	0
2	E	2885	0	2941	79	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	48	0	31	2	0
4	D	48	0	31	2	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	27	0	12	1	0
6	E	27	0	12	1	0
All	All	10054	0	10202	353	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 17.

The worst 5 of 353 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)
2:B:124:MET:CE	2:B:124:MET:SD	2.03	1.47
1:A:128:THR:HG23	1:A:173:THR:OG1	1.78	0.84
1:D:2:ILE:HG12	1:D:173:THR:HG21	1.60	0.82
1:A:2:ILE:HG12	1:A:173:THR:HG21	1.59	0.82
1:D:128:THR:HG23	1:D:173:THR:OG1	1.79	0.81

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	284/286 (99%)	242 (85%)	34 (12%)	8 (3%)	5	25
1	D	284/286 (99%)	236 (83%)	37 (13%)	11 (4%)	3	18
2	B	383/385 (100%)	342 (89%)	36 (9%)	5 (1%)	12	40
2	E	383/385 (100%)	349 (91%)	24 (6%)	10 (3%)	5	27
All	All	1334/1342 (99%)	1169 (88%)	131 (10%)	34 (2%)	5	27

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	292	GLY
1	D	96	THR
2	E	292	GLY
2	E	325	CYS
1	A	6	LYS

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	216/216 (100%)	196 (91%)	20 (9%)	9	30
1	D	216/216 (100%)	194 (90%)	22 (10%)	7	27
2	B	296/296 (100%)	266 (90%)	30 (10%)	7	27
2	E	296/296 (100%)	267 (90%)	29 (10%)	8	29
All	All	1024/1024 (100%)	923 (90%)	101 (10%)	8	28

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	338	GLU
1	D	90	LYS
2	E	309	ASP
2	B	356	LEU
1	D	16	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	342	ASN
2	B	353	ASN
2	E	221	ASN
2	B	226	GLN
2	E	94	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 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	COA	D	702	1	41,50,50	1.02	4 (9%)	52,75,75	1.87	8 (15%)
6	ADP	E	802	5	24,29,29	0.97	3 (12%)	29,45,45	1.04	3 (10%)
6	ADP	B	801	5	24,29,29	1.02	1 (4%)	29,45,45	1.06	3 (10%)
3	PO4	A	601	-	4,4,4	1.89	2 (50%)	6,6,6	0.77	0
4	COA	A	701	1	41,50,50	1.05	3 (7%)	52,75,75	1.89	10 (19%)
3	PO4	D	602	-	4,4,4	1.83	2 (50%)	6,6,6	0.62	0

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	COA	A	701	1	-	11/44/64/64	0/3/3/3
4	COA	D	702	1	-	10/44/64/64	0/3/3/3
6	ADP	E	802	5	-	2/12/32/32	0/3/3/3
6	ADP	B	801	5	-	3/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	COA	C6P-C5P	2.71	1.56	1.51
3	A	601	PO4	P-O2	-2.65	1.46	1.54
4	A	701	COA	OAP-CAP	2.54	1.47	1.42
3	D	602	PO4	P-O2	-2.53	1.47	1.54
4	A	701	COA	C6P-C5P	2.44	1.56	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	COA	O6A-CCP-CBP	7.55	122.69	110.55
4	D	702	COA	O6A-CCP-CBP	7.31	122.29	110.55
4	D	702	COA	C6P-C5P-N4P	-6.44	105.58	116.42
4	A	701	COA	C6P-C5P-N4P	-5.94	106.42	116.42
4	D	702	COA	O5P-C5P-N4P	3.89	130.35	123.01

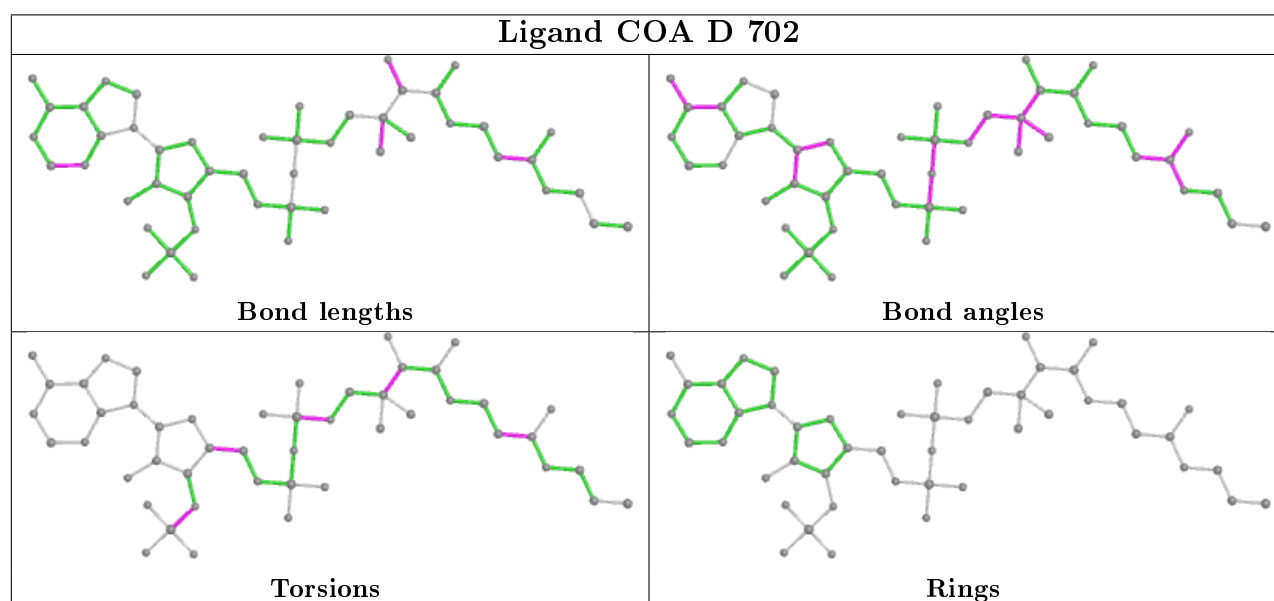There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	702	COA	C3B-O3B-P3B-O7A
4	D	702	COA	C3B-O3B-P3B-O8A
4	D	702	COA	OAP-CAP-CBP-CEP
4	D	702	COA	C9P-CAP-CBP-CEP
4	A	701	COA	C3B-O3B-P3B-O7A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	COA	2	0
6	E	802	ADP	1	0
6	B	801	ADP	1	0
4	A	701	COA	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 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 COA D 702

Bond lengths | Bond angles

Torsions | Rings

Ligand ADP E 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand COA A 701

Bond lengths

Bond angles

Torsions

Rings
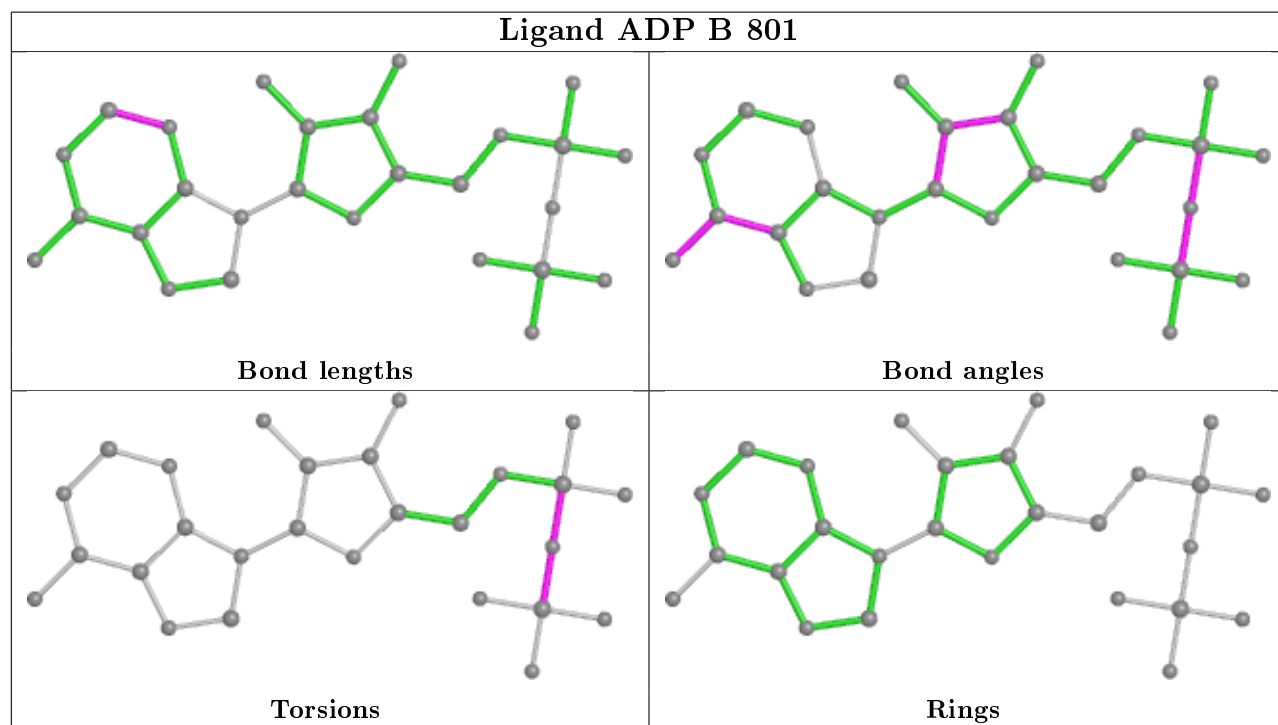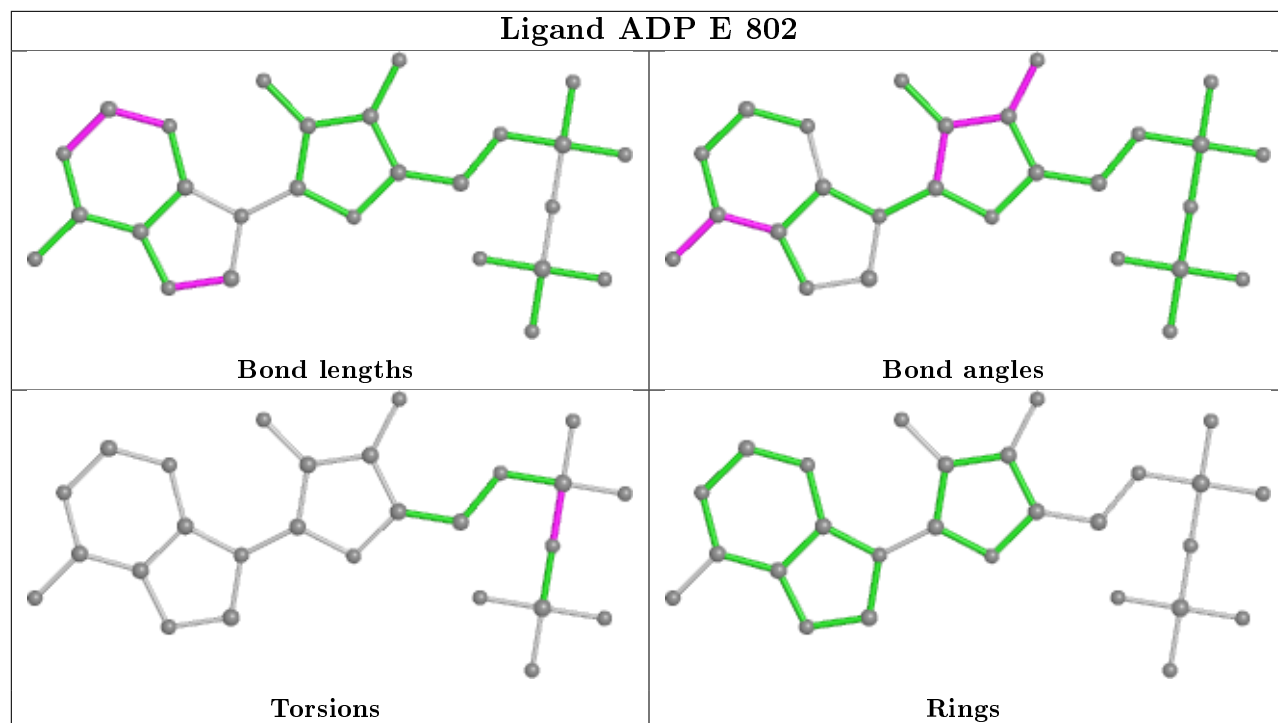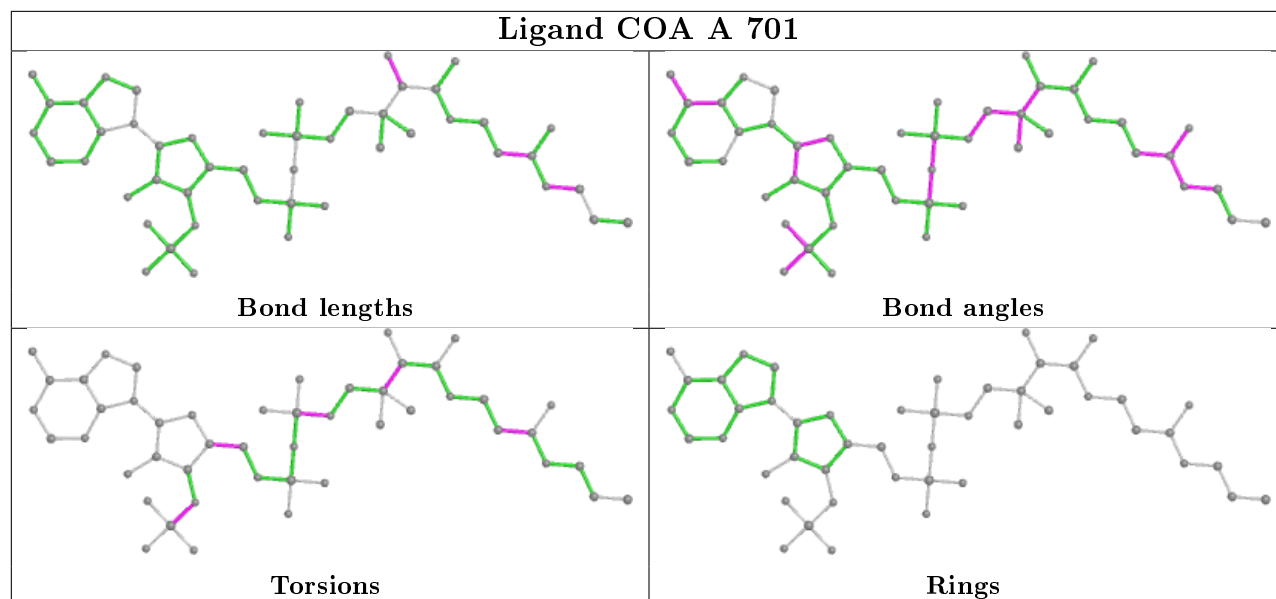
5.7 Other polymers (i)

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	286/286 (100%)	-0.87	0	100	100	2, 27, 66, 86	0
1	D	286/286 (100%)	-0.64	0	100	100	2, 40, 80, 100	0
2	B	385/385 (100%)	-0.84	0	100	100	2, 29, 70, 97	0
2	E	385/385 (100%)	-0.83	0	100	100	2, 28, 75, 100	0
All	All	1342/1342 (100%)	-0.80	0	100	100	2, 30, 74, 100	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.
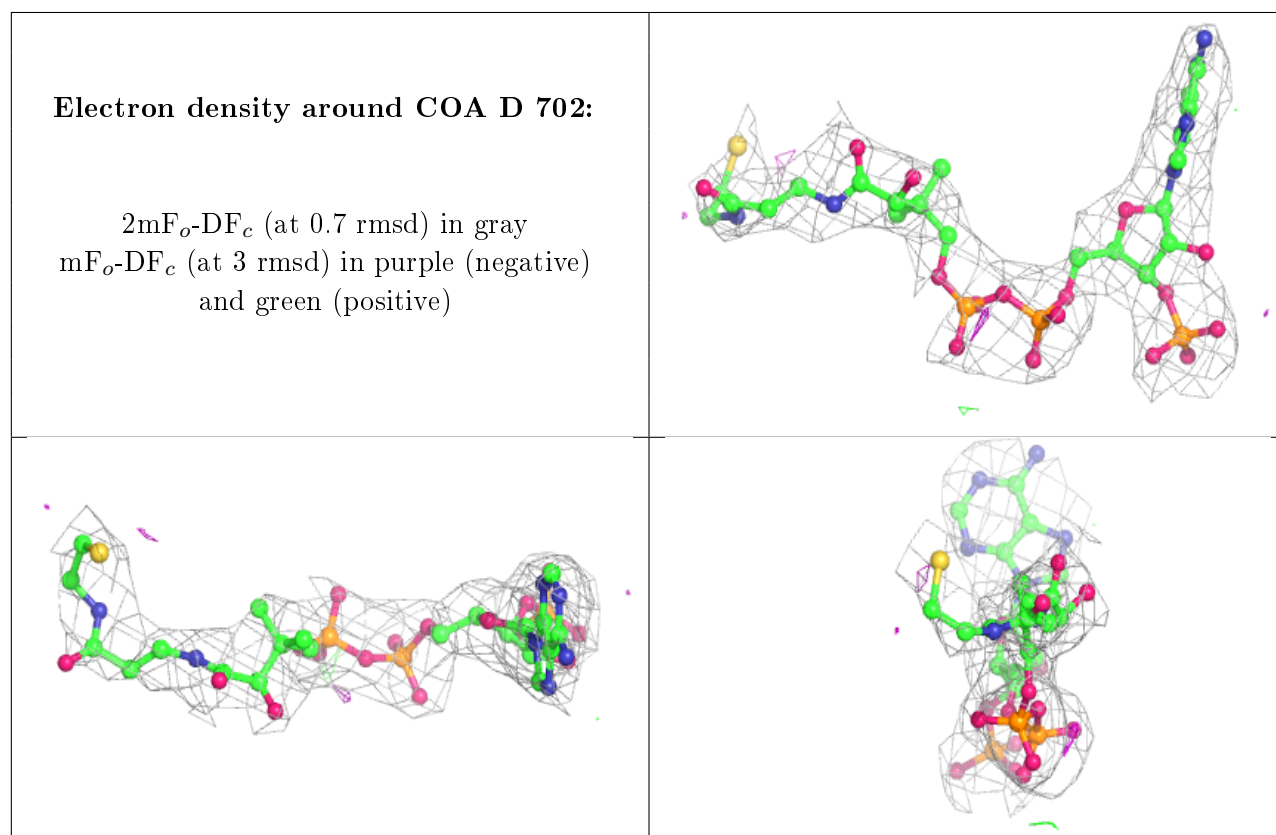
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	E	502	1/1	0.93	0.11	17,17,17,17	0
4	COA	D	702	48/48	0.96	0.14	25,29,70,75	0
6	ADP	E	802	27/27	0.96	0.13	32,34,38,39	0
5	MG	B	501	1/1	0.96	0.07	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COA	A	701	48/48	0.96	0.15	39,47,73,77	0
3	PO4	D	602	5/5	0.96	0.13	27,30,31,33	0
6	ADP	B	801	27/27	0.97	0.11	28,29,33,34	0
3	PO4	A	601	5/5	0.99	0.09	16,18,19,19	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.
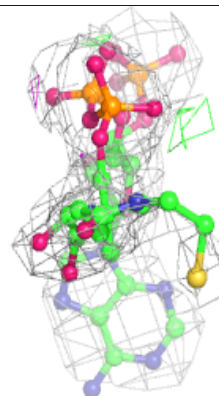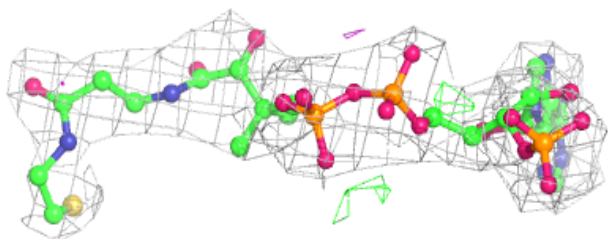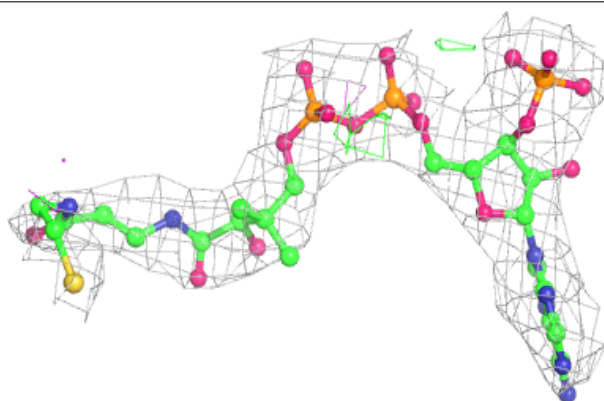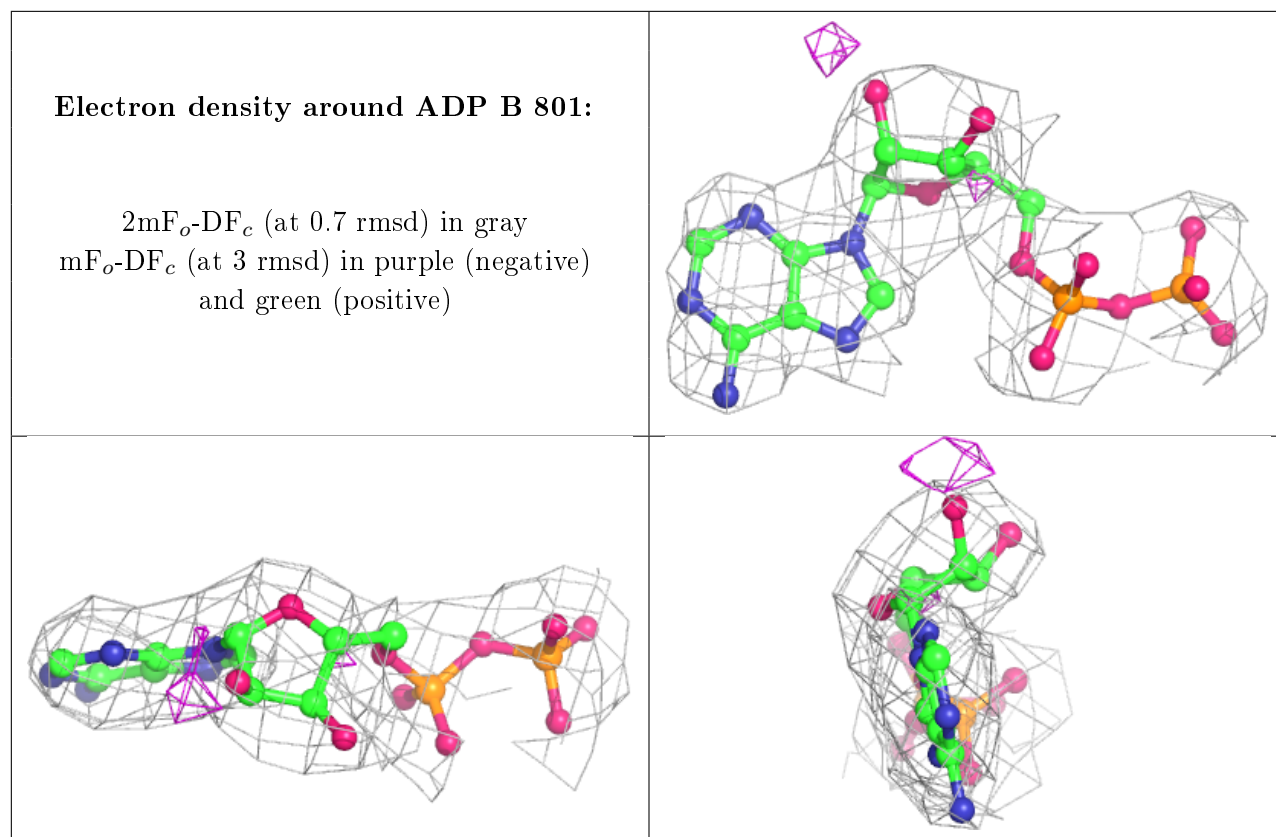
Electron density around COA D 702:

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 E 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
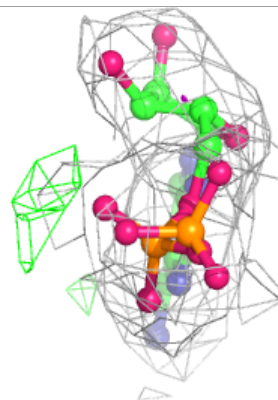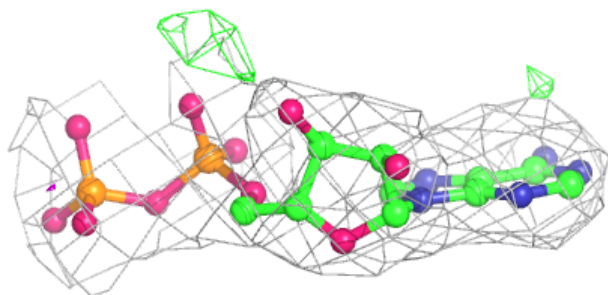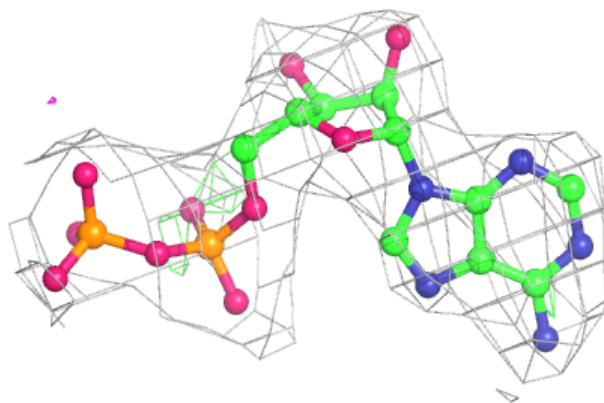
Electron density around COA A 701:

$2mF_o$-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 801:

$2mF_o$-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 ⓘ

There are no such residues in this entry.